UNIVERSITI
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Dynamic Modelling of Carbon Dioxide Absorber for Different Solvents

by

Pravin Chandra Segaran
13906

A project dissertation submitted in partial fulfilment of
the requirements for the
Bachelor of Engineering (Hons)
(Chemical)

January 2014

University Technology of PETRONAS
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CERTIFICATION OF APPROVAL

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Approved by,

(Dr. Haslinda Binti Zabiri)
Supervisor

UNIVERSITI TEKNOLOGI PETRONAS
TRONOH, PERAK
January 2014

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.

PRAVIN CHANDRA SEGARAN

ABSTRACT

In the recent era, the green house alleviation technologies have been fully emphasized and implemented due to the rapid climate change. Fossil fuelled power plants contribute to the globally carbon dioxide (CO_2) emission. Post combustion CO_2 capture (PCC) and natural gas processing plant CO_2 capture processes have attained a high consideration and interest which led to significant progress in CO_2 capture. Chemical absorption is the well-established and commercialized technology compare to other technologies in CO_2 capture. Choice of solvent is very important to optimize the performance of absorber.

The aim of this project is to simulate the rate based CO_2 absorber model using two different types of solvent to check the CO_2 removal efficiency considering the same operational conditions of the absorption column. This project emphasis only on the solvent parameters since the manipulate variable of this project is solvent, while the inlet gas stream is considered constant parameters. For this project, the CO_2 absorption process modelling was done using air as the gas inlet stream. The developed models for each solvent were implemented in Matlab.

The developed models are comprised of mass balance, energy balance, rate transfer, interface and hydraulic model. The scope of this project involved the evaluation of three different solvents which are monoethanolamine (MEA) and sodium hydroxide (NaOH).

The results of developed models are validated with the literature. The analysis of simulation results highlights that the CO_2 absorption process more likely happens at the lower segment of the absorber. As the gas flow from bottom to top of the absorber, the gas phase CO_2 concentration and the gas temperature decrease. The solvent concentration declines from upper to lower segment of the absorber while the solvent temperature rises from upper to lower segment of the absorber. Both MEA and NaOH solvents results are agreed to the pilot scale experimental results.

The developed model can be used to evaluate the efficacy and capability of ANY novel solvent in a simulated environment before it is being tested on actual experimental set-up. Therefore the best solvent can be determined. The objective of the project is accomplished.

ACKNOWLEDGEMENTS

First and foremost, I would like to express my deepest appreciation and gratitude to all those who provided me the possibility to complete this report. My warmest thank upon the God for providing me time and knowledge to establish this report while doing my practical at the same time. However, all of these could not be achieved if I was not able to take final year project course. It was a great honour for me to be working with my supervisor in order to succeed this project.

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Furthermore, I would also like to acknowledge with much appreciation the crucial role of the Final Year Project Coordinator, Dr. Abrar Inayat who furnishes training and talks for producing a better final year project report. Besides that, Dr. Abrar has given support and advice when I have problems regarding the report.

With love and thanks to my both parents for giving a fully support to me until I finished my final year project. Lastly, I would like to thank everyone who involved during this project and the co-operation and advises that they gave to me.

Thank you.

NOMENCLATURE

a	interfacial area packing (m2/m3)
C_{CO_2G}	gas phase CO_2 concentration (kmol/m3)
C_{pG}	heat capacity of gas (kJ/kmol K)
C_{pL}	heat capacity of solution (kJ/m3 K)
D_j	diffusivity of component j (m2/s)
E	enhancement factor
G_{air}	molar flow rate of air (m^3/m^2h)
H_{CO_2}	henry's law constant of CO_2 (kmol/m^3 kPa)
h_G	heat transfer coefficient (kJ/s m^2 K)
H_R	heat of absorption and reaction (kJ/kmol)
H_S	heat of vaporization of solvent (kJ/kmol)
k_2	reaction rate constant (m^3/kmol s)
k_L^o	physical liquid mass transfer coefficient (m/s)
k_G	physical gas mass transfer coefficient (kmol/m^2 s kPa)
L	liquid flow rate, m^3/m^2 s
N_{CO_2G}	molar flux of CO_2 (kmol/m^2s)
P	total pressure, kPa
p_{CO_2}	partial pressure of CO_2 (kPa)
S_{CO_2}	source term representing the rate of chemical absorption of CO_2
T_i	temperature of gas or liquid (K)
u	gas velocity in the z direction along the column height (m/s)
w	percentage of mass of solvent present in the solution
X	Concentration of solvent (kmol/m^3)
Y_{CO_2}	mole ratio of CO_2 in the gas phase
z	distance from bottom of packing to top (m)
α	CO_2 loading
B (subscript)	Reagent in the liquid

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CHAPTER 1:
INTRODUCTION

1.1. Background

The world population is increasing yearly, thus the demand for the energy worldwide is increasing too. The source of current energy generations is fossil fuels combustion power plant. These power plants which produce the energy are the main source of CO_2 emissions. Emissions of greenhouse gases cause the catastrophic climate change in the world that must be reduced. Due to the concerns on the climate changes, initiatives to reduce CO_2 emissions are taken. Four main available technical routes to capture CO_2 from fossil fuel power plants are pre-combustion, post-combustion, chemical looping combustion and oxy-fuel. Kohl and Nielsen (1997) have mentioned that post combustion CO_2 capture is the most well establish technology (as cited in Notza, Mangalapallyb, and Hasse, 2012).

Natural gas is the foremost alternate source of energy with lower environmental effect. Natural gas have some pollutants such as CO_2 and H_2S, which can causes excessive environmental threats when diffuse into the atmosphere and slowed down natural gas processes. Hence the need of capturing CO_2 content in natural gas is much important than compare to the combustion of fossil fuel power plant CO_2 capture. Thus this ensures that natural gas is a less environmental impact energy source. Delivering natural gas to the client is expensive. The most common method to transport natural gas to client is through pipelines. When the pipeline length increases, the natural gas has to be liquefied.

At very low temperature and as low as atmospheric pressure operation, natural gas will be undergoes transformation into liquid form, this is known as liquefaction process. Ebenezer (2005) has mentioned that CO_2 can cause process bottle necks in the pipeline and thereby reduce the plant efficiency at a low temperature and pressure. Due to these factors, the CO_2 from natural gas has to be removed before liquefaction process. Removal of CO_2 from natural gas will ensure good environmental performance, to achieve the Liquefied Natural Gas (LNG) product conditions and prevent corrosion.

Based on Kohl and Nielsen (1997), numerous gas treating processes are available for removal of CO_2 such as absorption process and membrane separation (as cited in Ebenezer, 2005). David, Kellogg and Pankaj (2003) have indicated that the chemical absorption process is been used widely in existing base load LNG facilities (as cited in Ebenezer, 2005). Based on Rufford, Smart, Watson, Graham, Boxall, Diniz da Costa and May (2012), in the natural gas industry, the most established technology for CO_2 removal is absorption process using amine.

There are many available solvents used in chemical absorption process such MEA, methyl-diethanolamine (MDEA), 2-amino-2-methyl-1-propanol (AMP) and ammonia. Each solvent will have different absorption performance depends to the operating conditions. Many studies are conducted to invent new efficient solvents to have higher the absorption efficiency.

Modelling CO_2 removal process is a hot topic since past years, this is due to the demand of green technology and concern of climate changes. Modelling of CO_2 removal process is more effective because the whole CO_2 removal process plant can be replicated in the computer. This enables to study the whole process by altering the parameters without spending time in the real plant and carry out the test run. This method can optimize the process of the plant effectively. Modelling needs a simulation and modelling tools.

Computer-aided process simulation and modelling tools are very essential and helpful tools in the process industries and they are globally recognized. Simulation and modelling tools are used to investigate and optimize the operational procedure. There are many advance simulation and modelling tools nowadays such as MATLAB, gPROMS, Modelica and Aspen Plus.

There are lack of research on dynamic modelling of CO_2 absorption process for natural gas processing plant and research on modelling different solvents CO_2 absorption process. This project therefore summarizes the modelling of different solvents CO_2 absorber for natural gas processing plant.

1.2. Problem Statement

Huge amount of natural gas reserves in Malaysia are undeveloped due to high CO_2 content. The technology for CO_2 removal process for high CO_2 content natural gas is still not well-established. Building and operating infrastructure to evaluate the process performance is a costly scheme and time consuming proposition. Simulation and modelling software provides a low cost and time saving to evaluate the CO_2 capture performance. However there is lack in the literature on the model development of CO_2 absorber for natural gas. There are many uncertainties in the existing literature regarding on the CO_2 absorber modelling. Valid dynamic models of CO_2 absorber needed to simulate the performance of absorber by varying the parameters without disturbing the operating absorber in the plant.

Many solvents are introduced for the CO_2 absorption process. Different solvents provide different absorber performance. The energy requirement and capital costs of an absorption plant are be influenced by the type of solvent. There is lack of research in developing models for different type of solvents for the CO_2 absorber for natural gas. With exists of models for different types of solvent, the performance of the absorption can be evaluated and thereby the best solvent determined.

1.3. Objectives

The aim of this research is very straightforward to prevent the project diverge from the scope. The objectives of this project are:

- To develop the dynamic models of CO_2 absorber for different type of solvents.

- To simulate the CO_2 absorber model using two different types of solvent to check the CO_2 removal efficiency considering the same operational conditions of the absorption column.

Developing models for each solvent enable the absorption efficiency for each solvent compared and thereby can indicate the better solvent. This proposed analysis is crucial for future analysis to evaluate the efficacy and capability of ANY novel solvent in a simulated environment before it is being tested on actual experimental set-up.

It provides a low cost approach to assess ANY novel solvent performance and to provide certain insights in terms of its scale-up feasibility and preliminary economics.

1.4. Scope of Study, Relevancy and Feasibility

The scope of this project is modelling and simulation. This project is not involved in experimental work. The area of study of this project is removal of CO_2 from air through absorption process using different solvents. The purpose of developing dynamic models is to study the performance of the absorber with different solvents. The models developed in this project are mass balance, energy balance, rate transfer, interface and hydraulic model.

Matlab is the simulation and modelling tool that used in this project. This advance tool is easily available in the market, very well known for its capacity for modelling a process. This tool is feasible for developing, validating, executing and deploying dynamic process models. In this tool the models of the process can be adjusted or can be defined by the user itself under the user define function. The defined model will be simulated in the way the user wants. This tool is very flexible and useful.

The models for different solvents CO_2 absorber are developed in the Matlab via multiple shooting and expeuler method. The scope of this project involved the evaluation of two different solvents which are MEA and NaOH.

The overall result of this project is validated with the literature since there is limitation for the validation of other solvents with the pilot plant data in University Technology of PETRONAS. The results of simulation from the developed MEA-CO_2 absorber models are validated by comparing to results obtained by Mac Dowell, Samsatli, and Shah (2013) and Faisal M. K. and Tariq M. (n.d.). Both Mac Dowell et al. (2013) and Faisal et al. (n.d.) have validated the models and results using available pilot plant data Tontiwachwuthikul et al. (1992). Therefore the developed models in this project are indirectly validated with the pilot plant data. Once the models are validated, the models are modified for different solvents (NaOH) to study the performance of the absorber.

This project is feasible and can be accomplished within the allocated time line. This is because the scope of this project just focuses on absorber only. On top of that, the solvent studied in this project is only three which is feasible for the given time frame. Besides that, the simulation tool used in this project is very effective and flexible as per explained earlier. The literatures studied for this project were taken from various resources that are relevant to this project and are not more than about 9 years gap from the current date. Most of the literatures reviewed are from year 2012 and 2013. This shows that all the literatures used in this project are the recent in order to ensure the accurate and more precise information are used.

CHAPTER 2:
LITERATURE REVIEW

2.1. CO_2 Capture

Greenhouse gas such as CO_2 mitigation technology became an important technology since past few years due to the fears of rapid climate change. Jayarathna, Lie and Melaaen (2013) mentioned that the fossil fuel-fired power plants are recognised to be the key CO_2 emission source. Therefore many researches have done on the CO_2 capture for the fossil fuel-fired power plant in order to achieve the goals in CO_2 emission reduction.

Table 1: CO_2 emission express in thousand tonnes of carbon (US Department of Energy, 2013)

CO_2 Emission (express in thousand tonnes of C)			
Country	2010	2011	2012
India	547811	567319	611226.3
Malaysia	59122	58294.98	58952.86
China	9896	10712.82	10483.04
Japan	319257	320144.8	342270
US	1481609	1450140	1396791
UK	134580	124692.9	128494
Total World	9167000	9459937	9666501

Based on Table 1, U.S. Department of Energy (2013) reported that the overall emission of CO_2 of the world increased from 2010 to 2012. However in some country like US (United State), the emission is reduced from year 2010 to 2012. This shows that the efforts are taken to reduce the CO_2 emission.

According to Adams and Davison (2007) (as cited in Cousinsa, Wardhaughb and Feronb, 2011) the most common technologies used for the removal of CO_2 from fossil-fuel fired power plant are:

- Oxyfuel combustion
- Pre-combustion capture
- Post combustion capture (PCC).

Cousinsa et al. (2011), Sonderbya, Carlsena, Fosbola, Kiorboeb Lars and Solms (2012) and Jayarathnaa, Liea, and Melaaen (2013) agreed to Kohl and Nielsen (1997) that PCC is considered to be the well-established technology for CO_2 removal in fossil fuel power plant. Among the available literatures, the most of them are related to modelling of PCC technology.

While for natural gas processing plant, natural gas contains high volume of CO_2 and H_2S compounds which is corrosive and cannot be burned efficiently and safely. Therefore the PCC technology is not suitable for natural gas processing plant. Hubbard (2010) stated that natural gas supplied to customers by pipeline has the maximum level of CO_2 that permitted which is usually less than 3% (as cited in Rufford et al., 2012).

Both process conditions available in the natural gas processing facility and post-combustion flue gas treatment may be not same. According to Rufford et al. (2012), the important differences between these applications are the CO_2 partial pressure and the quantity of CO_2 to be removed. Usually the natural gases feed are at high pressures (greater than 3000 kPa) while flue gases are normally at near atmospheric pressure. Amount of CO_2 that needed to be removed from natural gas is greater than the amount for flue gas.

2.2. Chemical CO_2 Absorption Process

Based on David, Kellogg and Pankaj (2003) (as cited in Ebenezer, 2005) and Rufford et al. (2012), chemical CO_2 absorption process is well known in the natural gas industry. Jayarathnaa, Liea and Melaaen (2013) and Sonderbya, Carlsena, Fosbola, Kiorboeb and Solms (2012) mention that chemical solvent absorption process is the most mature technology used in PCC. This shows the chemical absorption process is well established in both natural gas processing plant and PCC.

In chemical absorption process, CO_2 is captured from the inlet gas by solvent in a packed absorber column. Then 'CO_2 rich' solvent flow into desorber column and release the CO_2 due to the high temperature. Regenerated 'CO_2 lean' solvent will be cooled down and recycled to the absorber (Sonderbya et al., 2012).

The absorption process for natural gas processing and PCC are using the same concept but differ in the operating condition since natural gas contains higher CO_2 partial pressure than the flue gas. Figure 1 shows the process flow of an absorption process for natural gas processing plant.

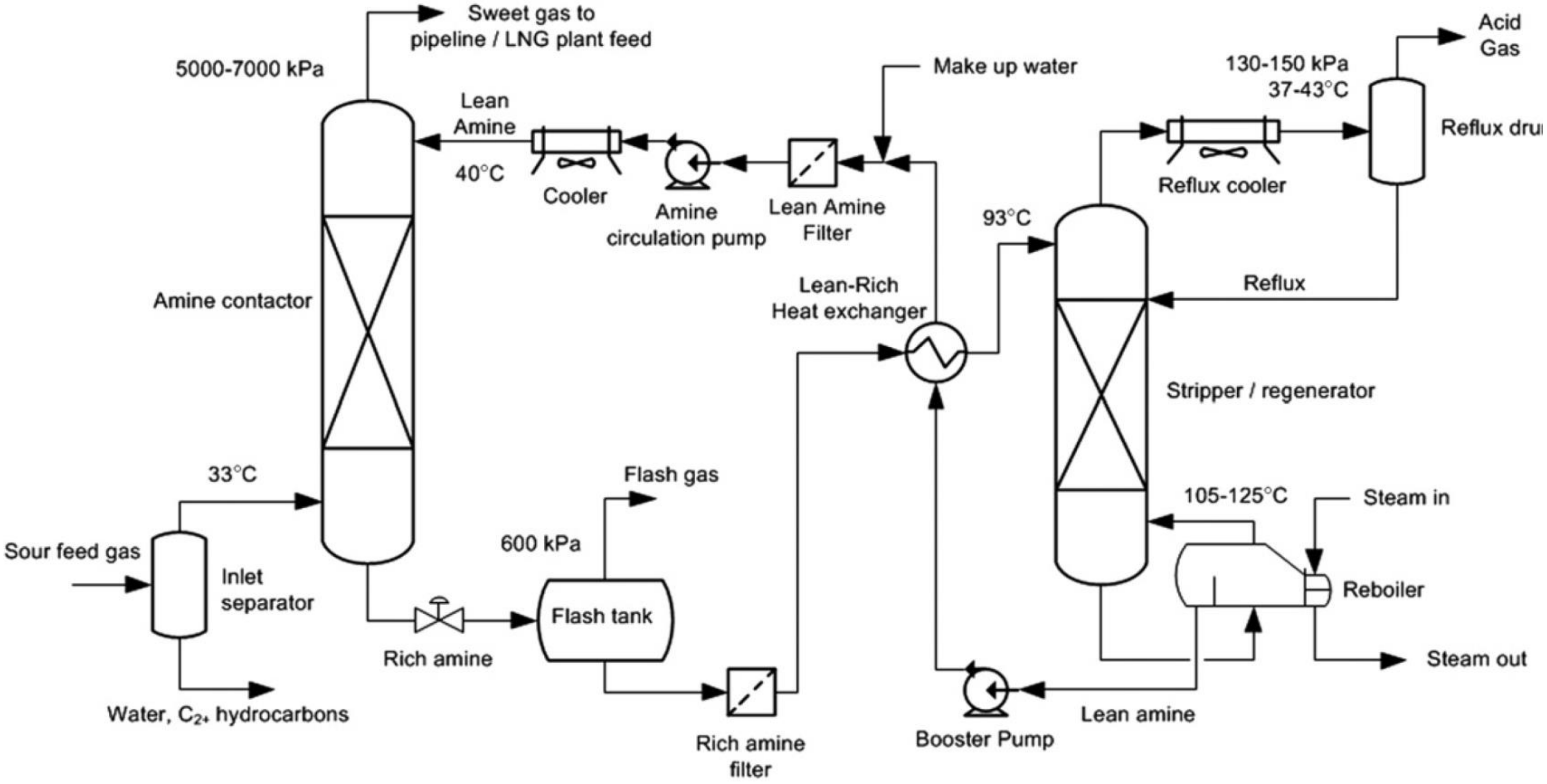


Figure 1: Typical chemical CO_2 adsorption system for natural gas processing plant (Hubbard, 2010) (as cited in Rufford et al., 2012).

2.3. Study of Parameters and Models for CO_2 Absorption Process

There are many parameters that can be manipulated for the performance study of CO_2 absorption process. Zhang and Guo (2013) mentioned that rise of the CO_2 loading of the lean solvent will lead to the reduction of CO_2 removal efficiency. The CO_2 removal efficiency increases at the low temperature of the lean solvent and decreases at the high temperature.

Ebenezer (2005) and Mac Dowell, Samsatli, and Shah (2013) justified that when amine concentration rises, the sweet gas CO_2 concentration declines. The mass transfer zone and position of the maximum temperature in column are detected to travel up the column when decrease in solvent flow rate (Mac Dowell et al., 2013). Sonderbya et al. (2012) described that when flow rate of absorbent and absorption height increases, the CO_2 recovery rises. The CO_2 recovery decreases as the lean CO_2-loading of the absorbent rises.

From the preliminary research, it is learnt that there are a few software feasible for developing the model of this project such as gPROMS, MATLAB and Aspen Plus. Gaspar and Cormos (2012) used MATLAB to develop rate based models for absorption capacity assessment of CO_2 capture process. The developed models are generic model, mass transfer models and hydraulic models. Besides that, Mac Dowell et al. (2013) have developed thermodynamic model and packed column models in gPROMS for analysis of an amine-based PCC absorption column.

There are two approaches for modelling the CO_2 capture, equilibrium-based and rate-based. The equilibrium-based modelling assumes that liquid and vapour phases reach equilibrium at theoretical stages and perfect mixing occurs at each stage (Lawal et al., 2009b). The rates of absorption and desorption in reactive distillation are determined by two main mechanisms, mass transfer and chemical reaction. In rate-based modelling, the vapour–liquid equilibrium occurs at the phase interface. The mass transfer between the vapour and liquid phases is modelled based on the two-film theory and the Maxwell-Stefan formulation (Lawal et al., 2010b). The rate-based approach is more rigorous, but the accuracy of the calculation is higher than equilibrium rate (Bui, Gunawan, Verheyen, Feron, Meuleman and Adeloju, 2014).

2.4. Study of Solvent for CO_2 Absorption Process

There are many types of solvent being used to perform CO_2 absorption process study. Ebenezer (2005) used many types of solvents for different types of CO_2 removal processes which are chilled methanol, propylene carbonate and dimethylether of polyethylene glycol. While Australian National Low Emissions Coal Research and Development (2012) used MEA, MDEA, AMP and piperazine (PZ) to study the environmental impact. Sipocza and Tobiesen (2012) considered ammonia, potassium carbonate and ionic liquids as solvent for economic evaluation. Kothandaraman (2010) has performed a solvent comparison study using chilled ammonia, potassium carbonate and MEA. According to Zhang and Guo (2013), MEA solvent not suitable to use above 122°C because MEA will face degradation and corrosion.

Zhang and Guo (2013) used aqueous ammonia solution for the CO_2 absorption and regeneration processes of a research scale pilot plant. Zhang and Guo (2013) have mentioned that using aqueous ammonia solvent has benefits such as less corrosion and no degradation. However aqueous ammonia solution has restrictions such as NH_3 slip problem, require huge amount of additional energy for regeneration process and crystallization of NH_4HCO_3.

Guo, Feng, Song, Xiao and Shen (2012) have conducted a simulation of CO_2 removal for crude synthetic natural gas (SNG) upgrade by the Selexol process concerning power requirement and separation performance. The solvent used in the process is Selexol, a mixture of dimethylethers and polyethylene glycol with the formulation of $CH_3(CH_2CH_2O)nCH_3$.

Rufford et al. (2012) have done research on few solvent types and concluded that:

- Amine based

  Primary and secondary amine (MEA and DEA) react fast than tertiary amine (MDEA). MDEA has loading capacity than MEA. Moderately hindered amines are considered have high rates of CO_2 absorption and high capabilities for CO_2 absorption.

- Aqueous ammonia

Lower energy necessities however high costs for the complexity of the ammonia process (Kohl and Nielsen, 1997). The sweetened gas has to be recompress in aqueous ammonia processes.

- Physical solvent and hybrid solvent processes

Lower heat requirement for regeneration compare to amine or potassium carbonate sorbents. Most physical solvents absorb water unlike the aqueous amine, aqueous ammonia and potassium carbonate which saturate the inlet gas with water. Circulation rates of physical solvent are high. Hybrid solvent need lower heat requirement for regeneration, has high acid gas loading capacities, low foaming tendency, and low corrosion capacity.

- Switchable solvents and ionic liquid

Ionic liquid added amine mixtures have advantages such as lower solvent circulation rates, higher amine loadings and lower energy requirements but they are insoluble in water.

MEA has the fastest rate of reaction compared to the DEA followed by AMP and then MDEA. MEA has highest CO_2 absorption performance compare to AMP, DEA and MDEA but MEA is the most corrosive and high rate of degradation compare to others (Gaspar & Cormos, 2012). These discussions were coherent with the research done by Peeters, Faaij, & Turkenburg (2007). Peeters et al. (2007) have mentioned that solvents with higher absorption rates will decrease the absorber size.

All the literature stated that MEA is the best choice for the chemical absorption process. This is because MEA has highest rate of reaction and the energy penalty for CO_2 absorption is lower than the other solvent which claim by Kothandaraman (2010). However there are still many research are being carrying out to produce a better solvent than MEA in term of the high corrosiveness and high degradation disadvantages as discovered by Gaspar & Cormos (2012).

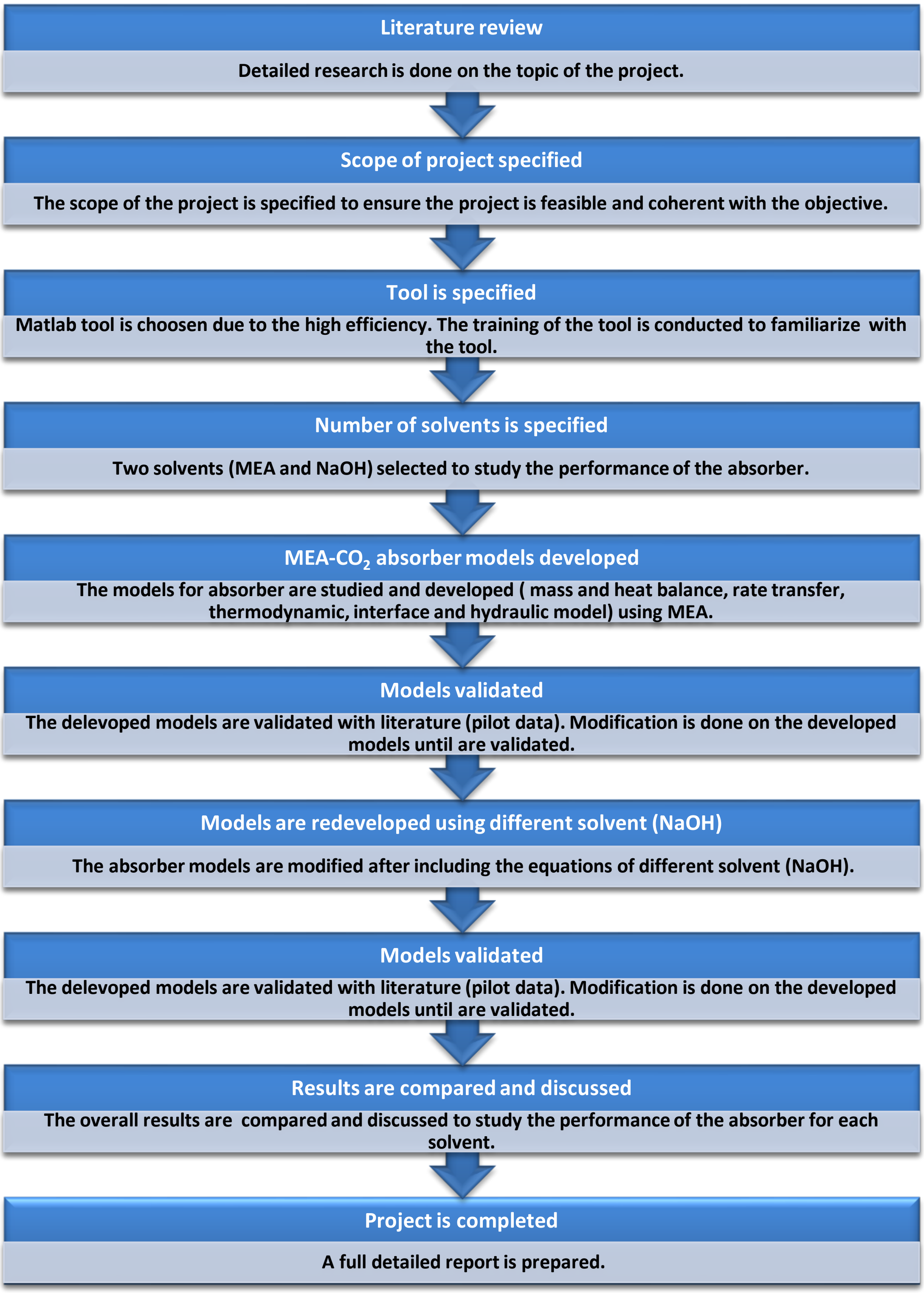
A detailed study of the available literatures is done and tabulated in APPENDICES.

CHAPTER 3:

PROJECT METHODOLOGY

3.1 Project Overall Methodology

The overall methodology of this project is shown in the Figure 2.



Literature review

Detailed research is done on the topic of the project.

Scope of project specified

The scope of the project is specified to ensure the project is feasible and coherent with the objective.

Tool is specified

Matlab tool is choosen due to the high efficiency. The training of the tool is conducted to familiarize with the tool.

Number of solvents is specified

Two solvents (MEA and NaOH) selected to study the performance of the absorber.

MEA-CO_2 absorber models developed

The models for absorber are studied and developed (mass and heat balance, rate transfer, thermodynamic, interface and hydraulic model) using MEA.

Models validated

The delevoped models are validated with literature (pilot data). Modification is done on the developed models until are validated.

Models are redeveloped using different solvent (NaOH)

The absorber models are modified after including the equations of different solvent (NaOH).

Models validated

The delevoped models are validated with literature (pilot data). Modification is done on the developed models until are validated.

Results are compared and discussed

The overall results are compared and discussed to study the performance of the absorber for each solvent.

Project is completed

A full detailed report is prepared.

Figure 2: Methodology of the project

3.2 Model Development Methodology

Mechanisms of the chemical absorption process have to be clearly studied and defined for developing a complete mathematical model. Treybal (1969) and Panday (1983) were the one worked earlier on developing the model for the CO_2 absorption and were used as reference to developed model in this project. Figure 3 shows the two-film theory that used to develop the mass and energy transfer model.

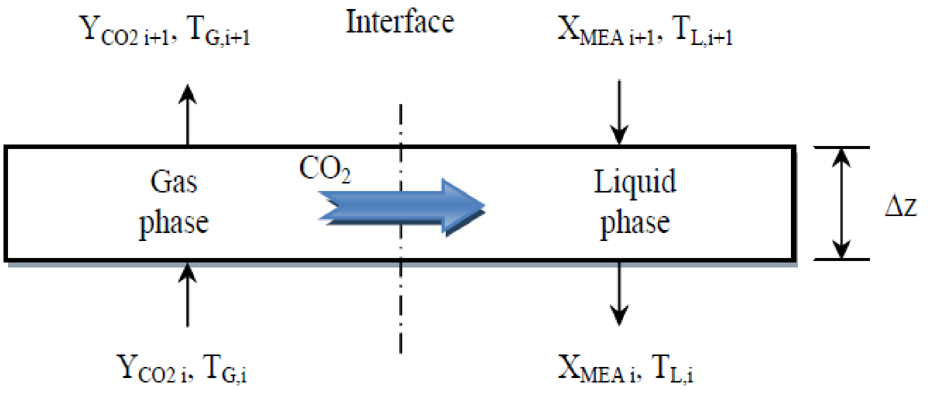


Figure 3: Schematic two film theory

Reaction Kinetics

This is the most important and challenging part of the model development. This is because the model development for kinetics reaction will be different and vary for each solvent. Without a good understanding and detail parameters, an accurate model could not be obtained. The enhancement factor, E is one of the difficult characteristics of modeling gas absorption with chemical reaction.

$$E = 1 + \frac{1}{\left[\left[\frac{1}{E_i - 1}\right]^{1.35} + \left[\frac{1}{E_1 - 1}\right]^{1.35}\right]^{1/1.35}}$$

Where:

$$E_i = 1 + \left[\frac{C_{B,L}C_D}{bD_{A,L}C_{A,i}}\right],\ E_1 = \left[\frac{\sqrt{M}}{\tan\sqrt{M}}\right] \text{ and } M = \left[\frac{D_{A,L}k_2\, C_{B,L}}{(k_L^o)^2}\right]$$

$$D_{CO_2,L} = D_{CO_2,water}\left[\frac{\mu_{water}}{\mu_L}\right]^{0.8}$$

$$D_{CO_2,water} = 2.35\ \times 10^{-6}\left[\frac{-2119}{T_L}\right]^{0.8}$$

$$\frac{\mu_{water}}{\mu_L} = \exp\left[\frac{(21.18w + 2373)[\alpha(0.01015w + 0.0093T - 2.2589) + 1]w}{{T_L}^2}\right]^{0.8}$$

$$H_{CO_2} = 10^{\left(5.3 - 0.035 C_{solvent} - \frac{1140}{T}\right)}$$

Rate constant, k_2 depends on the solvent's reaction properties. For MEA, the rate constant is second order and can be determine as shown below:

$$\log k_2 = 10.99 - 2152/T_L$$

For NaOH, the rate constant is shown below:

$$\log k_2 = 11.895 - \frac{2382}{T_L} + 0.221 I_c - 0.016 I_c^2$$

Material and Energy Balances

Mass transfer rates

$$\frac{dN_{CO_2 G}}{dz} = S_{CO_2}$$

$$N_{CO_2 G_{i+1}} = N_{CO_2 G_i} - S_{CO_2} \Delta z$$

$N_{CO_2 G} = uC_{CO_2 G} = G_{air} Y_{CO_2}$

Gas phase CO_2 concentration:

$$\frac{dC_{CO_2 G}}{dz} = \frac{S_{CO_2}}{u}$$

$$S_{CO_2} = \frac{p_{CO_2}}{\frac{1}{k_{CO_2 G} a} + \frac{H_{CO_2}}{k_{CO_2 L} a\, E}}$$

Solvent concentration in the solution can be determined by:

$$X_{solvent_i} = X_{solvent_{i+1}} + \frac{(Y_{CO_2 i} + Y_{CO_2 i+1}) b G_{air}}{L_{water}}$$

Gas phase energy balance:

$$G_{air}Y_{CO_2}C_{pG}\frac{dT_G}{dz} = h_G\mathrm{a}(T_G + T_L)$$

Liquid phase energy balance:

$$\mathrm{LC_{pL}}\frac{\mathrm{dT_L}}{\mathrm{dz}} = \mathrm{G_{air}Y_{CO_2}C_{pG}}\frac{\mathrm{dT_G}}{\mathrm{dz}} + \mathrm{G_{air}(H_R + H_S)}\frac{\mathrm{dY_{CO_2}}}{\mathrm{dz}}$$

Parameters

There are many parameters used in the models that the values are taken from the literatures. The correlations are referred from the available literatures. For example the a, k_{CO_2L} and k_{CO_2L} were taken from the correlations used by Onda et al. (1968). All the literatures used in this project are listed in the REFERENCES.

3.3 Proposed Simulation Methodology

There are plenty of methods available to run simulation in Matlab, however the best and most efficient method has to be selected in order to give a smooth and accurate results. "Shooting method" has been used in this project because it is a best method for the iteration procedure. In this method, the four intervals were used to obtain the result. This method is used to solve two-point boundary value problems and with optimisation steps. Where the total length of the absorber column is 6.55 m, so it is divided into 4 differential elements and the discretised mass and energy balance equations were assigned for each element to solve the equations.

Direct multiple "shooting method":

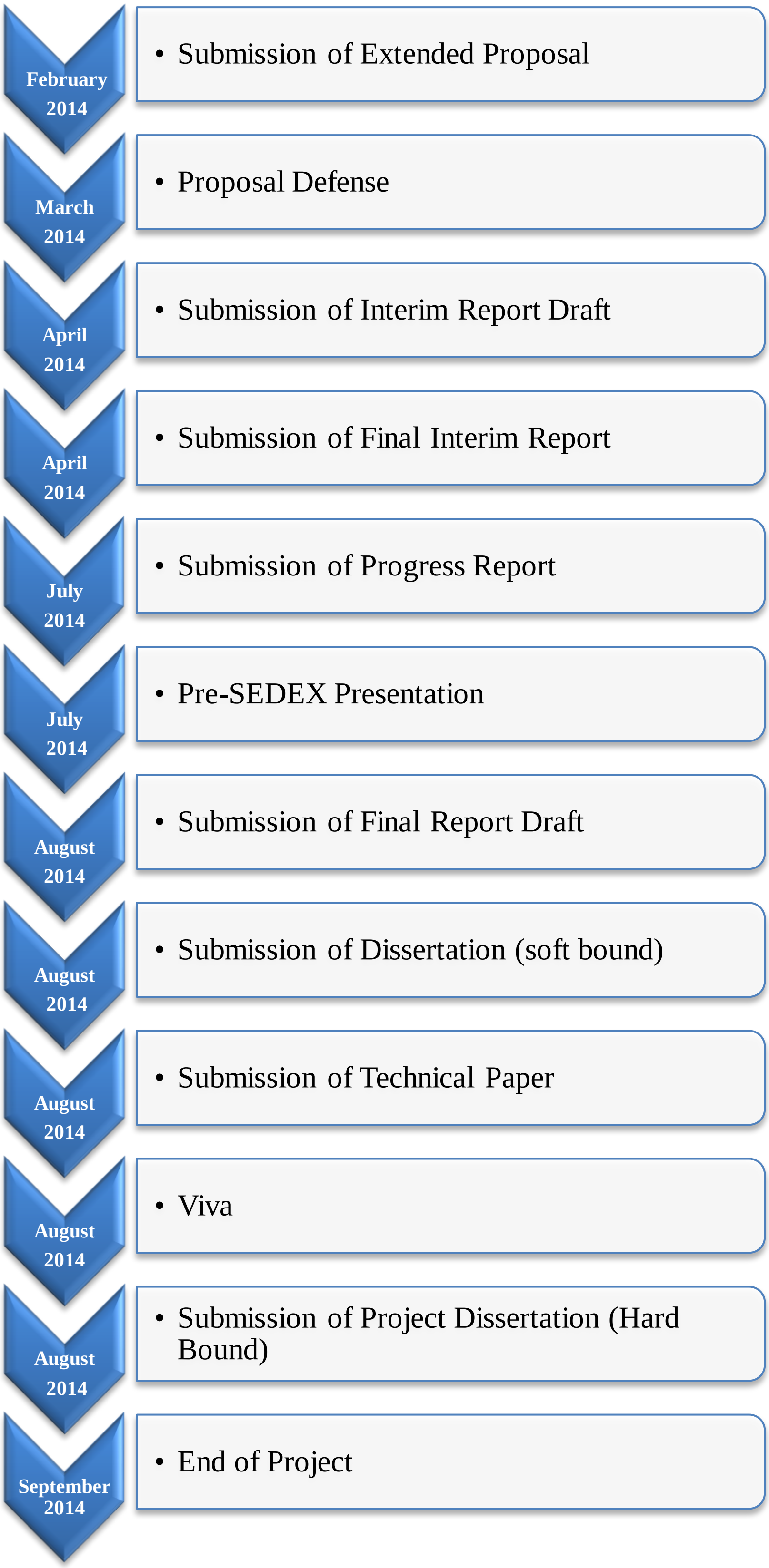
- a numerical method for the solution of boundary value problems
- divides the interval over which a solution is sought into several smaller intervals
- solves an initial value problem in each of the smaller intervals
- imposes additional matching conditions to form a continuous solution on the whole intervals.

The general description of the direct multiple “shooting method” that used in this project is shown below.

1. Partitions the interval $[z_a, z_b]$ by introducing additional intervals:
   $z_a = z_0 < z_1 < \ldots < z_N = z_b$.
2. Starts by guessing the values of yk at all interval points zk with $0 \leq k \leq N - 1$.
3. Let y(z; zk, yk) denote the solution emanating from the kth interval, that is, the solution of the initial value problem:
   $y'(t) = f(z, y(z)), \; y(z_k) = y_k$.
4. All these solutions can be pieced together to form a continuous trajectory if the values y match at the intervals. Thus, solutions of the boundary value problem correspond to solutions of the following system of N equations:
   $y(z_1 ; z_0, y_0) = y_1$
   $\vdots$
   $y(z_{N-1} ; z_{N-2}, z_{N-2}) = y_{N-1}$
   $y(z_N ; z_{N-1}, y_{N-1}) = y_b$.
5. The central N−2 equations are the matching conditions, and the first and last equations are the conditions $y(z_a) = y_a$ and $y(z_b) = y_b$ from the boundary value problem.
6. The multiple shooting method solves the boundary value problem by solving this system of equations. In this project, the equations are solved using MATLAB nonlinear optimization routine.

3.4 Project Key Milestones

The key milestones of this project are shown in Figure 4.



February 2014	Submission of Extended Proposal
March 2014	Proposal Defense
April 2014	Submission of Interim Report Draft
April 2014	Submission of Final Interim Report
July 2014	Submission of Progress Report
July 2014	Pre-SEDEX Presentation
August 2014	Submission of Final Report Draft
August 2014	Submission of Dissertation (soft bound)
August 2014	Submission of Technical Paper
August 2014	Viva
August 2014	Submission of Project Dissertation (Hard Bound)
September 2014	End of Project

Figure 4: Project key milestones

3.5 Project Gantt Chart

The Gantt chart of this project is shown as below.

ACTIVITIES	WEEKS																													
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
Title selection and allocation (Meeting with coordinator for briefing).	■	■																												
Announcement of supervisor and project title.		■																												
First meeting with supervisor.		■																												
Preparation of paper work and presentation.		■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	
Study of literature on the CO_2 removal from natural gas.		▨	▨	▨																										
IRC training – E Resources and introduction to EndNote.				▨																										
Tabulating the data from the literature as the reference.			▨	▨																										
Conformation of scope of study of the project.					▨																									
Selection of tool and training on the tool.						▨	▨	▨																						
Solvent study and selection								▨	▨																					

ACTIVITIES	WEEKS																													
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
Research methodology lecture.							🟦																							
IRC training: EndNote hands-on										🟦	🟦																			
Simulation tool familiarization and training							🟦	🟦	🟦	🟦	🟦																			
CO_2 absorber models development											🟦	🟦	🟦	🟦	🟦															
Study and development of the solvents equation.															🟦															
CO_2 absorber models re-development																🟦	🟦	🟦												
Simulation of CO_2 absorption process and data comparison and recoding																			🟦	🟦	🟦	🟦								
Validation of results and models																						🟦	🟦	🟦						
Submission of Extended Proposal							■																							
Proposal Defence								■																						
Submission of Interim Report Draft													■																	
Submission of Final Interim Report														■																
Submission of marks by supervisor for FYP 1															■															
Submission of Progress Report																						■								

ACTIVITIES	WEEKS																													
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
Pre-SEDEX Presentation																									■					
Submission Final Report Draft																										■				
Submission of Dissertation (soft bound)																											■			
Submission of Technical Paper																											■			
Viva																												■		
Submission of Project Dissertation (Hard Bound)																														■

CHAPTER 4:
RESULT AND DISCUSSION

The results that have been obtained until the date of this report are discussed below.

4.1. Model Validation

The developed model in this project is validated with the experimental data obtained by Tontinwachwuthikul et al. (1992), as mention earlier. The experiments were done in a pilot size packed absorber. Most of the simulation and modeling projects are validated with these results. In the experiments, a 6.55 m height packed absorption column with 0.1 m internal diameter was used. 12.7 mm ceramic Berl saddles were packed in the column. The operating pressure of the column is 103.15 kPa.

Figure 5 shows the flow of the gas stream inlet and solvent stream inlet conditions used for the validation purpose. The gas enters the absorber at bottom and flow to top while the solvent is counter flow in the direction of the gas. In Figure 5, the solvent stream inlet conditions are for MEA solvent. Whereas for NaOH solvent conditions are listed in the table

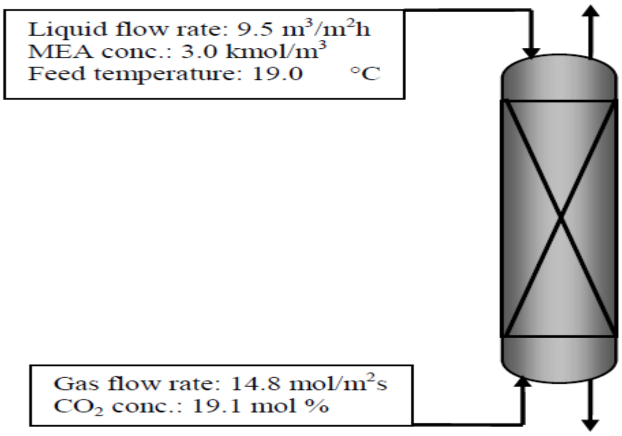


Figure 5: Schematic of the CO_2 absorber process conditions

Table 2 : NaOH solvent conditions

NaOH Inlet Stream	
NaOH feed (kmol/m3)	2
Liquid flow rate (m3/m2 h)	13.5
Feed temperature (°C)	15

4.2. CO_2 Mole Fraction Profile

Figure 6 shows the profile of gas phase CO_2 mole fraction along the column height using MEA solvent. From the result obtained, the agreement between the simulation result and the experimental result are very good. The mole fraction of CO_2 is slightly over-predicted around 2 to 5 meters from to bottom of column. This may be due to the minor deviations in the empirical correlations used in this project.

Figure 7 shows the profile of gas phase CO_2 mole fraction along the column height using NaOH solvent. From the result obtained, the agreement between the simulation result and the experimental result are not so good. This is because the some parameters of the NaOH were not able to obtain such as heat capacity and physical liquid mass transfer coefficient of NaOH. Therefore rough estimated values are used and caused the inaccuracy in the results.

The CO_2 concentration of in gas phase reduces along the distance from the bottom of column to top as the CO_2 is being continuously absorbed by the solvent. From the results, it can be conclude that the CO_2 absorption process more likely happens at the bottom of the absorber. Amount of the CO_2 being absorbed is depend on the pressure of gas stream and solvent concentration and temperature. Due to the space and time limitation, the results for dynamic change of the parameters are not included.

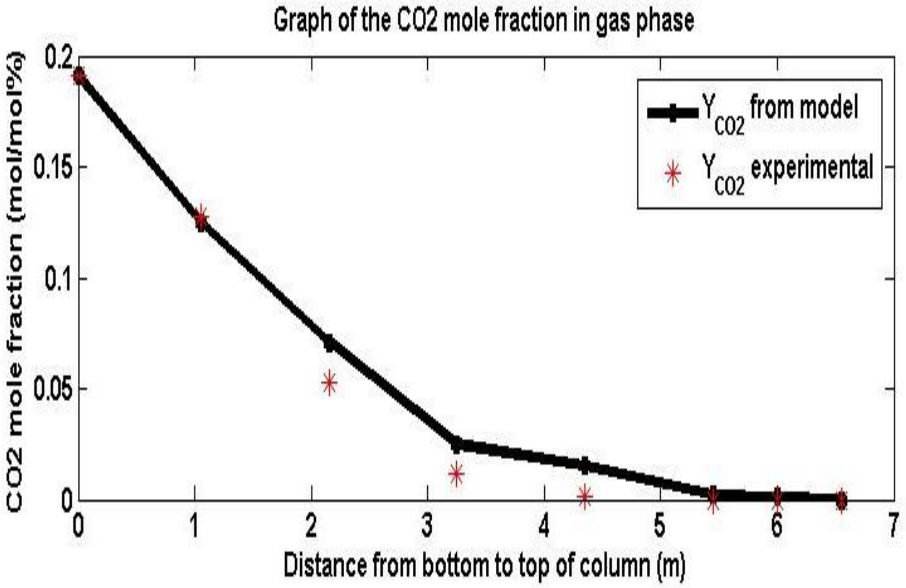


Figure 6: Relationship between CO_2 mole fraction in gas and distance from lower segment to upper segment of column (MEA Solvent)

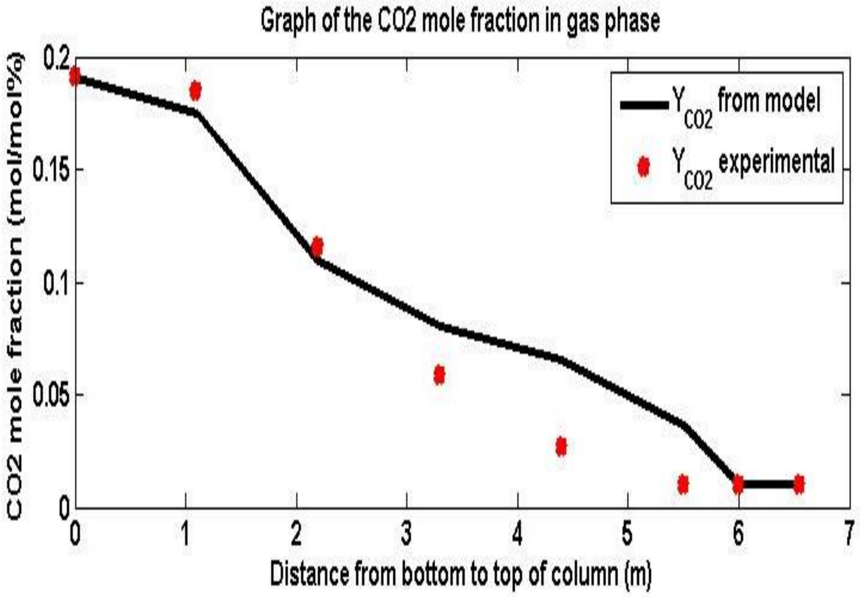


Figure 7: Relationship between CO_2 mole fraction in gas and distance from lower segment to upper segment of column (NaOH Solvent)

4.3. Gas Temperature Profile

Figure 8 shows the profile of gas phase temperature across the column height using MEA solvent. Based on the graph, the agreement between the simulation results and experimental results are good. Minor variation can be obtained from the experimental and simulation results. This variation is due to the usage of only four intervals in shooting method to discretize the model. Small interval will cause roughness in the curve.

Figure 9 shows the profile of gas phase temperature throughout the length of the column height using NaOH solvent. The graph shows that there are discrepancies in the middle of the column. This is due to the parameter of absorption heat or reaction of NaOH-CO_2 and the heat transfer coefficient of NaOH were unable to determine. Estimated values are used in this project. These parameters play significant role in the gas temperature profile.

Based on the graphs, the temperature of inlet gas reduces along the flow from the bottom to top of absorber. This is because the heat of reaction is absorbed by the solvent solution. Thus the gas temperature profile is related and contributed to the solvent temperature profile. The results show that the enhancement factors differ significantly along the absorber. Largest changes in enhancement factors occurred at the bottom of the absorber where the chemical reaction happened mostly.

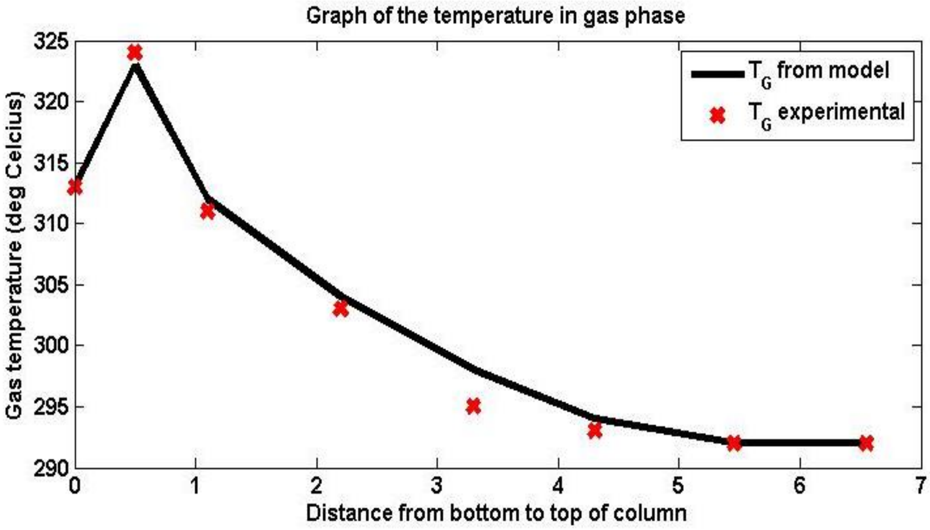


Figure 8: Relationship between gas temperature and distance from lower segment to upper segment of column (MEA Solvent)

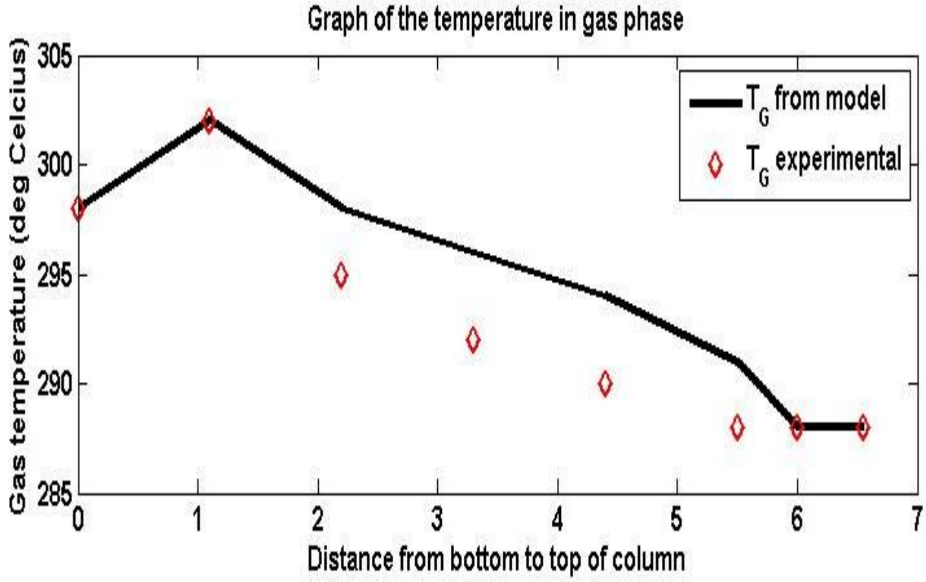


Figure 9: Relationship between gas temperature and distance from lower segment to upper segment of column (NaOH Solvent)

4.4. Solvent Temperature Profile

Figure 10 shows the profile of solvent temperature throughout the length of the column height for MEA solvent. The agreement between the experimental results and simulation results are good however there are some minor variations. These variations can be reduced and eliminated by increasing the intervals in shooting method to discretize the model.

Figure 11 shows the profile of solvent temperature throughout the length of the column height for NaOH solvent. The agreement between the simulation results and experimental results are good, however there is discrepancy in the middle of the column. This is because the parameter of heat of vaporization and heat capacity of NaOH were not accurate.

The solvent temperature profile shows the temperature of solvent increases along the flow of the solvent from top of column to bottom. The heat produced due to absorption and reaction between CO_2 and solvent is the root of the high temperature of the solvent close to the lower segment of the absorber. The reaction is fairly less at top of the absorber thus the solvent temperature is almost constant or varies little. The solvent temperature profile also depend on the solubility of inlet gas

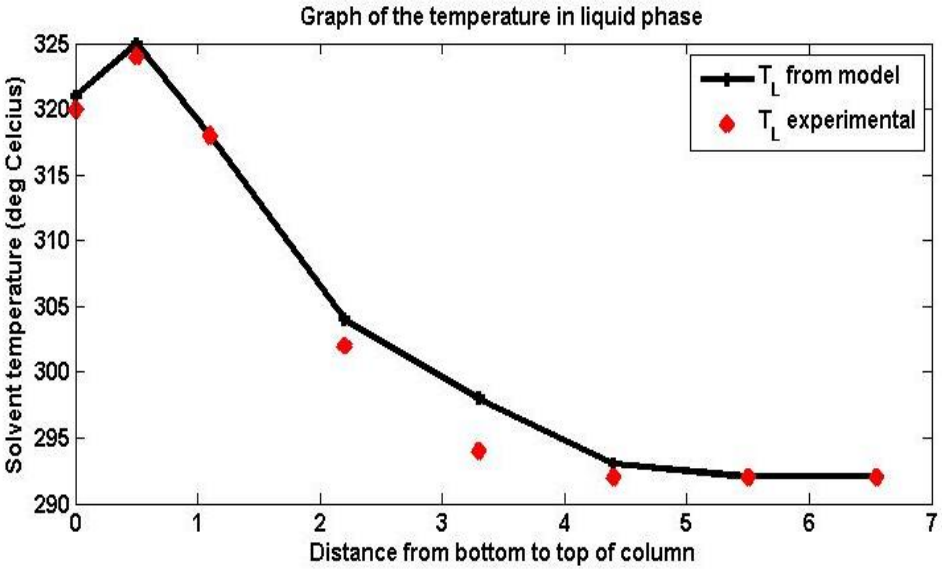


Figure 10: Relationship between solvent temperature and distance from lower segment to upper segment of column (MEA Solvent)

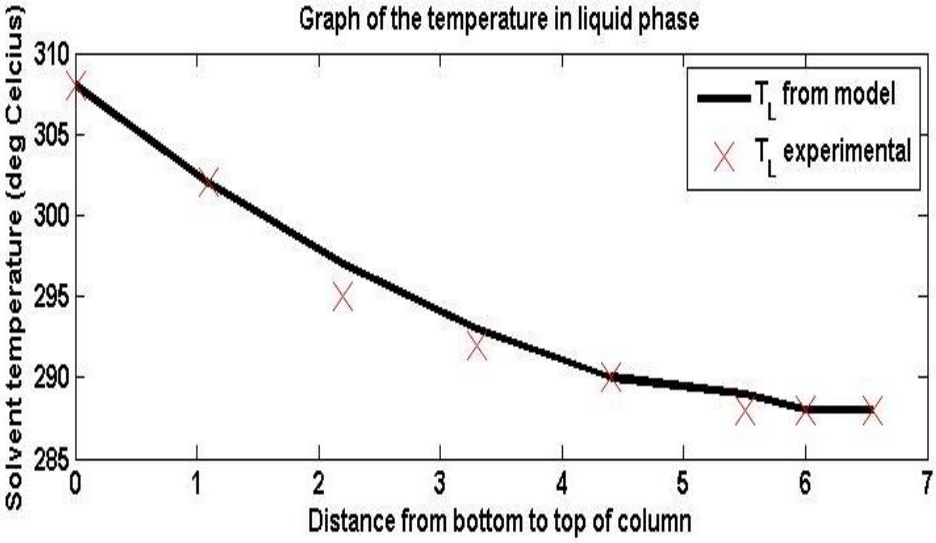


Figure 11: Relationship between solvent temperature and distance from lower segment to upper segment of column (NaOH Solvent)

4.5. Summary

The overall agreement between the simulation and experimental results are good. Therefore the developed CO_2 absorber model for different solvent can be confirmed to be valid. The developed model can be used to study the performance of different types of solvent and thereby can determine the best solvent.

In this project, the comparisons of the solvents are not in the scope of this project. The purpose of this research is just to design the model for different solvents. Two different solvents used in this project to validated the model with the existing result in the literature.

CHAPTER 5:
CONCLUSION AND RECOMMENDATION

Good agreements were found between the results of this project with the validated literature results. The literature results are from pilot scale experimental data obtained from Tontiwachwuthikul et al. (1992). However the models can be modified to produce better and accurate results by further research on the chemical properties of the solvent and CO_2 reaction.

From the results obtained, it could be summarized that the CO_2 absorption process more likely happens at the lower segment of the absorber. As the inlet gas flow from lower to upper segment of the column, the gas phase CO_2 concentration and the gas temperature decrease. MEA concentration decreases from upper to lower segment of the absorber because of the CO_2 absorption. The solvent temperature increases from top to bottom of the absorber due to the reaction heat of CO_2 with solvent.

This project has managed to determine the absorption performance for two different solvents. Thus through this project, ANY new solvent can be evaluated by comparing the performance of the CO_2 absorber. Therefore best solvent can be determined by comparing the performance of the CO_2 absorber.

The models developed in this project could be used to simulate CO_2 absorber under any conditions after some modification applied to the model. Thus is project is consider an important source for future research on CO_2 absorption for natural gas processing plant. Besides that the effect of the CO_2 absorption performance due to the dynamic changes in temperature, flow rate and concentration parameters can be study through these developed models.

In conclusion, the objective of this project is achieved. This project has successfully completed as per scheduled.

The results obtained in this project have good agreement with the pilot scale experimental data. However the accuracy of the results can improved by the following recommendation:

- The number of intervals used in the “shooting method” of this project can increased to improve the accuracy and smoothness in the results.
- This project can be further modified by conducting detailed research on the chemical reaction parameters including the solvent parameters.

The recommendations for future work are as the following

- This project can be further modified for the natural gas plant CO_2 absorption process simulation.
- For the future work, this project can extend the scope of study by including stripper column.

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APPENDICES

Authors & Title	Description	Result	Parameters	Software	Solvent	Reference
Zhang M., Guo Y. Rate based modelling of absorption and regeneration for CO2 capture by aqueous ammonia solution	A rate-based model Simulate the CO_2 absorption and regeneration processes of a research scale pilot plant. Flue gas Absorber and stripper	Under the optimal operation conditions, the regeneration energy is 3.63 MJ/kg CO_2, lower than that reported for the research scale pilot plant (4–4.2 MJ/kg CO_2).	1. CO_2 absorption process • Effects of the flow rate of the lean solvent Increase of the flow rate will increase the heat requirement for the reboiler. Lower flow rate cannot achieve the target of the amount of CO_2 captured. • Effects of the NH3 concentration of the lean solvent Increase of concentration is favourable for the absorption of the CO_2, but will increase the extra energy requirement of the NH3 abatement system due to more severe NH3 slip. • Effects of the CO_2 loading of the lean solvent Increase of the CO_2 loading will lead to the decrease of CO_2 removal efficiency, but it will reduce the NH3 slip and regeneration energy. • Effects of the temperature of the lean solvent	Aspen Plus	Aqueous ammonia (the regeneration temperature should not exceed 122 °C, value above which degradation of MEA and corrosion will become intolerable.) CO2 capture process using aqueous ammonia has advantages such as no degradation and less corrosion. But it still suffers several critical limitations such as NH3 slip problem, crystallization of NH4HCO3 in the condenser, and a great amount of supplementary energy for regeneration process, CO2 compression, and cooling necessities.	http://dx.doi.org/10.1016/j.apenergy.2013.04.074 2013

Authors & Title	Description	Result	Parameters	Software	Solvent	Reference
			When temperature increases, the CO_2 removal efficiency increases at the low temperature but decreases at the high temperature. The NH3 concentration in the exit gas increases rapidly with the temperature of the lean solvent increasing. 2. CO_2 regeneration process • Effects of the condenser temperature The increase in temperature will cause the regeneration energy decreases with the CO_2 output increasing and the reboiler heat duty decreasing. • Effects of the boilup ratio With the boilup ratio increasing, the CO_2 and the NH3 flow rates increase more rapidly, the reboiler heat duty increases, the regeneration energy also increases. CO_2 escapes from the solvent more easily than the NH3 and H2O • Effects of the diameter and packed height of the stripper Effects of the increase of inner diameter on the CO_2 output and the NH3 concentration in the CO_2 product stream are more significant than that of the			

Authors & Title	Description	Result	Parameters	Software	Solvent	Reference
			packed height. Size of the stripper increasing, the CO_2 output and the NH3 concentration in the CO_2 product stream both increase as the residual time of the rich solvent in the stripper becomes longer. The regeneration energy decreases slightly with the size of the stripper increasing. • Temperature distributions along the packed height absorber The temperature of the liquid phase increases along its flow direction due to the heat of absorption and the heat transfer between the liquid phase and the gas phase. The temperature of the gas phase decreases along its flow direction In the stripper, the temperatures of both the liquid phase and the gas phase increase at the bottom of the stripper due to the heat supply from the reboiler, and decrease at the top the stripper due to the condenser			
Gáspár J., Cormos A. Dynamic modelling	Modelling and simulation, carbon dioxide capture in packed absorption	Developed model for: • Mass and heat balances • Gas–liquid mass transfer model	• Changing the power plant load (increasing the volumetric ratio between gas flow rate and liquid flow rate and decreasing the volumetric ratio between gas flow rate and liquid	MATLAB/Simulink	(MEA)	http://dx.doi:10.1016/j.compchemeng.2010.10.001

Authors & Title	Description	Result	Parameters	Software	Solvent	Reference
and validation of absorber and desorber columns for post-combustion CO_2 capture	columns to be used in power sector. Dynamic mathematical model Absorber and stripper	- Hydraulic and physico-chemical properties - Thermodynamic model - Reboiler model (The temperature of the liquid phase in the reboiler must be lower than the boiling point of the solution, because the alkanolamines degenerate at higher temperatures).	flow rate) The power plant performance is reduced significantly with excessive increase of the absorber load and a decreasing of the gas flow rate to liquid flow rate ratio (FG/FL) allowed an increasing of CO_2 capture rate. Amine solution temperature influences the stripper performance and the steam requirement - Decreasing the temperature of the input rich amine stream By reducing the temperature of the desorber feed stream, causes the decreasing of the amine regeneration process yield. The desorber feed stream temperature is more sensitive than to the flue gas to liquid solvent ratio			2010
Jayarathna S., Lie B., Melaaen M. Dynamic modelling of the absorber	A model for the absorption column of a post-combustion CO_2 capture plant is developed following the	Model developed for - Main model equations - Interfacial mass transfer - Reaction kinetics and phase equilibrium - Physical properties and other parameters	- Start-up simulation Almost all the CO_2 could be absorbed at smaller gas rates, and as the gas rate increases, the percentage removal decreases depending on the absorption rate, contact time and phase equilibrium. - Simulation of varying load conditions	Matlab	MEA	http://dx.doi.org/10.1016/j.compchemeng.2013.03.002 2013

Authors & Title	Description	Result	Parameters	Software	Solvent	Reference
of a post-combustion CO_2 capture plant: Modelling and simulations	rate based approach to represent heat and mass transfer. The Kent–Eisenberg model is used to compute the transfer and generation rates of the species. Absorber only	The gas side mass transfer coefficient has a direct effect on the overall heat transfer coefficient according to the Chilton–Colburn analogy. The specific heat capacity of the MEA solution decreases as CO_2 loading increases. MEA - low volatility.	The temperature bulge appears to be increasing as the gas rate increases. This can be due to the increased amount of CO_2 absorbed into a specific amount of MEA solution, which has increased the amount of heat released per specific amount of the solution. If the gas rate to the absorber increases, the removal efficiency faces a drop due to the decreased contact time. • Influence from the stripper The reduced initial CO_2 content in the solvent stream will increased absorption capacity The temperature of liquid in the bottom half of the column is reduce to lower due to the increased specific heat capacity of the solution as a result of the reduced CO_2 loading.			
Guo W., Feng F., Song G., Xiao J., Shen L. Simulation and energy performan	A simplified process simulation of CO_2 removal for crude synthetic natural gas (SNG) upgrade by the Selexol process	Less pressure difference between crude SNG and absorption pressure favours the energy performance of CO_2 removal process. Sensitivity analysis indicates that the CO_2 removal efficiency	Process modelling: • Selexol solvent flow rate • Separation ratios • Power consumptions of pump and refrigeration system	Aspen Plus	Selexol (mixture of dimethyl ethers polyethylene glycol with the formulation of CH3(CH2CH2O)nCH3). There is no heat duty for the Selexol process. MEA and DEA washing techniques required less	http://dx.doi:10.1016/S1003-9953(11)60412-X 2012

Authors & Title	Description	Result	Parameters	Software	Solvent	Reference
ce assessment of CO_2 removal from crude synthetic natural gas via physical absorption process	concerning power requirement and separation performance SNG is produced from biomass Only absorber	significantly influences the total power CO_2 consumption excluding crude SNG and SNG compressions of the CO_2 removal process, as well as HHV of SNG			power consumption rather than membrane and PSA techniques.	
Cousinsa A., Wardhaughb L.T., Feronb P.H.M. A survey of process flow sheet modifications for energy efficient CO_2 capture from flue gases	Fifteen process flow sheet modifications for chemical based CO_2 absorption processes are reviewed to reduce the energy penalty and improve absorption performance. Flue gas	Past review: • For post combustion capture, Eide et al. (2005) suggest using membrane contactors in the absorber to increase the specific contact area for mass transfer and reducing the size of the absorber column • A 30% reduction in energy requirements over conventional MEA processes is claimed if there is pre-contactor prior to the	Potential flow sheet modifications: • Multi-component columns • Inter-stage temperature control • Heat-integrated stripping column (reduce the energy penalty) • Split flow process (applied to the NG process) • Vapour recompression • Matrix stripping • Heat integration	Aspen Plus custom modeller ®.	MEA Type of solvent can influence the energy consumption	http://dx.doi:10.1016/j.ijggc.2011.01.002 2011

Authors & Title	Description	Result	Parameters	Software	Solvent	Reference
using chemical absorption		absorber and live steam addition in the stripping column (Chakma, 1997) Energy saving increase with increasing plant complexity				
Sipöcza N., Tobiesen F. A. *Natural gas combined cycle power plants with* CO_2 *capture: Opportunities to reduce cost*	A detailed analysis covering a thermodynamic and economic evaluation of a 440MWe natural gas combined cycle power plant with an integrated CO_2 removal plant.	Absorber intercooling, the solvent temperature is reduced, facilitating a higher rich loading and thus increasing the solvent absorption capacity. Way to reduce the energy consumption of the CO_2 capture process: • split flows • double matrix stripper and an internal heat exchange stripper • Lean vapour recompression(LVR), vacuum-and multi-pressure stripping Power plant with EGR	System design (3 different configuration of integrated plant) (this paper focus on cost and economical study)	IPSEpro CO_2SIM (rate-based approach)	MEA Solvent study: • new amines and blends of amines • ammonia • potassium carbonate • ionic liquids	http://dx.doi:10.1016/j.ijggc.2012.01.003 2012

Authors & Title	Description	Result	Parameters	Software	Solvent	Reference
		and extended MEA absorption plant is the most efficient with respect to OPEX and has slightly higher CAPEX than EGR.				
Jayarathna S. A., Liea B., Melaaen M. C. Amine based CO_2 capture plant: Dynamic modelling and simulations	A dynamic model for simulating an amine based CO_2 absorption plant is developed to predict the effect on the plant operation caused by the disturbances from the up-stream power plant and the operating conditions of the plant itself. Non-equilibrium rate approach. Absorber and	Models: • Column models • Condenser and re-boiler models • Heat exchanger model • Buffer tank model • Mass transfer and specie generation modelling	When flow rate of inlet gas increases, • Removal efficiency has faced a reduction • Effect the temperatures When volume flow rate of the lean amine has increased, • Reduction of the absorbed CO_2 per mole of MEA • Reduction in the amount of heat released per mole of MEA. • reduction in the liquid phase temperature • lean loading value dropped corresponding to the decreased rich loading value • re-boiler duty has increased due to the increased re-boiler feed rate When V/F fraction of the re-boiler has been increases, • The re-boiler duty has increased • Amount of CO_2 released has increased	MATLAB	MEA	http://dx.doi.org/10.1016/j.ijggc.2013.01.028 2013

Authors & Title	Description	Result	Parameters	Software	Solvent	Reference
	stripper.					
Rufford T.E, Smart S., Watson G.C.Y., Graham B.F., Boxall J., Diniz da Costa J.C., May E.F.. The removal of CO 2 and N2 from natural gas: A review of conventional and emerging process technologies	Overview of conventional and developing gas processing technologies for CO2 and N2 removal from natural gas. 5 different process technologies Designed to produce pipeline quality gas (typically 2% CO2, < 3% N2) and gas to feed a cryogenic gas plant.	Differences in the NG and post combustion flue gas CO2 capture: • CO2 partial pressure • Level of CO2 removal required Focuses primarily on CO2 absorption processes, but also introduces technologies for N2 rejection by the selective absorption of CH4 in hydrocarbon solvents Chemical absorption processes with amine solutions are the most commonly used acid gas removal technologies in the natural gas industry (GPSA Engineering Data Book, 2004). CO2 absorb by sorbent and regenerated by heating.	Two major cost factors: • The required sorbent circulation rate, which is determined by the amount of CO_2 that must be removed from the feed gas and the CO_2 loading capacity of the sorbent • The energy required to regenerate the sorbent		Physical solvents, such as the mixture of polyethylene glycol–dimethyl ethers • Amine based Primary and secondary amine (MEA and DEA) react fast than tertiary amine (MDEA). MDEA has loading capacity than MEA. Moderately hindered amines, such as 2-amino, 2-methyl, 1-propanol (AMP), are characterized by high rates of CO_2 absorption and high capacities for CO_2 • Potassium carbonate The absorber and stripping columns operate in a temperature range of 100–116 °C • Aqueous ammonia Potentially lower energy requirements than amine, but the energy savings are not	http://dx.doi.org/10.1016/j.petrol.2012.06.016 2012

Authors & Title	Description	Result	Parameters	Software	Solvent	Reference
		Chemical absorption processes for acid gas treating is likely to remain in the near future for the largest scale gas processing applications because these processes have high separation powers for CO2 The acid gas loading capacity of physical solvents at low to moderate CO2 partial pressures is generally lower than that of chemical absorbents. However, physical solvent processes have lower energy requirements for regeneration because heat absorption for physical solvents is much lower than the heat of absorption for chemical solvents The process disadvantages with conventional amine treating processes include:			sufficiently large to offset the additional costs associated with complexity of the ammonia process (Kohl and Nielsen, 1997) and the need to recompress the sweetened gas in AAPs. • Physical solvent and hybrid solvent processes Heat inputs required for regeneration of a physical solvent are generally much lower than the heat required for the regeneration of amine or potassium carbonate sorbents. Many physical solvents also absorb water, in contrast to the aqueous amine, AAP and potassium carbonate technologies which saturate the sweet gas with water Weakness: physical solvent circulation rates are high. Advantages of the hybrid solvent technologies over conventional amine	

Authors & Title	Description	Result	Parameters	Software	Solvent	Reference
		• the large amounts of energy required for regeneration of the amine, • the relatively low CO2 loading capacity of amines requires high solvent circulation rates and large diameter, high-pressure absorber columns, • the corrosive amine solutions induce high equipment corrosion rates • degradation of amines to organic acids • co-absorption of hydrocarbon compounds such as benzene, toluene, ethyl benzene and xylene (BTEX) which subsequently are emitted with the acid gas stream (Collie et al., 1998; Morrow and Lunsford, 1997)			absorption technologies include low energy consumption for regeneration of the solvent, high acid gas loading capacities, low foaming tendency, and reduced corrosion. Drawback of the mixed-solvent processes is that hydrocarbon losses (to the solvent) are slightly higher than the typical losses in conventional amine processes. • ionic liquids and switchable solvents I L + amine mixtures, reduced energy requirements relative to conventional aqueous amine solvent, higher amine loadings and lower solvent circulation rates but they are insoluble in water.	

Authors & Title	Description	Result	Parameters	Software	Solvent	Reference
Kothandaraman A. Carbon Dioxide Capture by Chemical Absorption: A Solvent Comparison Study	Evaluate the performance of three different solvents. Each solvent system, many parametric simulations were performed to identify the effect on energy consumption in the system Different flow sheet configurations were explored to optimize the energy recuperation for each system. Coal flue gas and NGCC flue gas;	From the standpoint of energy consumption, for existing power plants the use of MEA is found to be the best choice while for future design of power plants, potassium carbonate appears to be an attractive alternative. Monoethanolamine, • Process flexibility in the MEA system was limited by degradation reactions. • Energy penalty for CO_2 capture lower Potassium carbonate • Energy penalty for CO_2 capture higher Chilled ammonia • High partial pressure of CO_2 in the flue gas is require	MEA • Effect of capture percentage • Effect of packing • Effect of absorber height • Effect of solvent temperature • Effect of desorber height • Effect of desorber pressure • Breakdown of energy requirement in the reboiler • Effect of cross-heat exchanger • Other methods of energy recuperation Potassium carbonate • Effect of packing • Effect of desorber height • Effect of desorber pressure Chilled ammonia • Analysis of the absorber • Analysis of the desorber	ASPEN Plus	Monoethanolamine, potassium carbonate and chilled ammonia	A thesis 2010
Peeters A.N.M.,	Detailed analysis of the	In general lower value for the chemical binding	Chemical absorption unit: • Regeneration energy	Excel Aspen	Amines aqueous solution (MEA)	http://dx.doi:10.101

Authors & Title	Description	Result	Parameters	Software	Solvent	Reference
Faaij A.P.C., Turkenburg W.C. *Techno-economic analysis of natural gas combined cycles with post-combustion CO_2 absorption, including a detailed evaluation of the development potential*	potential future costs and performance of post combustion CO_2 absorption in combination with a natural gas combined cycle (NGCC). The energy consumption and capital costs of an absorption plant largely depend on solvent and absorber characteristics.	energy will result in a lower absorption rate. High effective solvent loading will cause a smaller solvent flow in the amine plant Increase in specific surface area will result in a lower pressure drop in the absorber results in lower energy consumption The energy consumption for regeneration can be split into three parts: • CO_2 binding energy. • Energy required for heating the solution. • Water evaporation A lower regeneration energy requirement will reduce the size of the reboiler needed; and higher solvent loadings will reduce the size of the	• Heat integration • CO_2 loading • Absorption rate • Pressure drop in the absorber • Flue gas recycle (Many factors/parameters that might reduce the cost and energy consumption are discussed in result and discussion part)	Plus	Absorption characteristics of the solvent: • chemical binding energy • absorption rate • effective solvent loading • absorption temperature • desorption temperature • sorbent concentration • Solvent stability Solvents with higher absorption rates will decrease absorber size Higher solvent concentrations will result in a smaller stripper size. Corrosive effect – type of solvent (MEA most corrosive).	6/S1750-5836(07)00068-0 2007

Authors & Title	Description	Result	Parameters	Software	Solvent	Reference
		amine pumps.				
Notza R., Mangalapallyb H. P., Hasse H. Post combustion CO_2 capture by reactive absorption: Pilot plant description and results of systematic studies with MEA	Reports on results of systematic studies of the CO_2 capture with MEA that were carried out in the pilot plant. Flue gas Main task in optimizing the process for CO_2 removal from power plant flue gases by reactive absorption is the reduction of the energy requirement	Two reference experiments, • Low CO_2 partial pressure in the flue gas • High CO_2 partial pressure Study on absorber, desorber and evaluation of the energy requirement. Regeneration energy consists of four different contributions, • desorption of CO_2 (desorption enthalpy), • generating stripping stream, • heating up of the solvent, • heating up of the condensate reflux.	Parameter studies: • Variation of the solvent flow rate (important parameter because most influence the process) • Variation of the desorber pressure • Variation of the solvent composition • Variation of the lean solvent temperature • Variation of the CO_2 partial pressure • Variation of the fluid dynamic load in the absorber • Variation of the CO_2 removal rate • Variation of the flue gas temperature		MEA (Determination of the amine content by gas chromatography is included in this paper)	http://dx.doi:10.1016/j.ijggc.2011.11.004 2012
Amrollahi Z., Ystad P. A. M., Ertesvåg I.	Discusses the selection of most important parameters	The power output reduction due to CO_2 capture and compression was decreased from 48	Case of study: • Base case model • Absorber inter-cooling model (Case 1)	UniSim Design	MEA	http://dx.doi:10.1016/j.ijggc.2012.01.00

Authors & Title	Description	Result	Parameters	Software	Solvent	Reference
S., Bolland O. Optimized process configurations of post-combustion CO_2 capture for natural-gas-fired power plant – Power plant efficiency analysis	necessary to obtain 90% capture ratio and the lowest energy consumption for the CO_2 capture and compression plants. Six different CO_2 capture process configurations were simulated. The increased operating pressure of the stripper led to a reduction in the thermal energy requirement of the stripping process but higher degradation rates and corrosion	MW for the base case chemical absorption process to 42.5 MW for the case with absorber inter-cooling and lean vapour recompression The major reduction of energy requirement of the reboiler, led to overall work demand reduction for Cases 4 and 5. The best optimized process with lowest work demand was the fifth case. 1.86 bar – Stripping column operating pressure.	• Split-flow model • Absorber inter-cooling combined with split-flow model • Lean vapour recompression (LVR) model • LVR combined with absorber inter-cooling model (Case 5)			5 2012

Authors & Title	Description	Result	Parameters	Software	Solvent	Reference
	problem should be expected (Abu-Zahra et al., 2007).					
Gaspar J., Cormos A. Dynamic modelling and absorption capacity assessment of CO_2 capture process	Aim: check the mass transfer and hydraulic correlation models predictive capacity and to investigate the dynamic behaviour and absorption performance of four different type alkanolamine.	Reaction rate, which decreases in order: MEA>DEA >AMP >MDEA. High viscosity and high CO_2 solution loading - MEA, AMP and MDEA High viscosity and small CO_2 solution loading - DEA CO_2 absorption performance: MEA>AMP>DEA>MDEA. The disadvantage of the use of MEA compared to DEA is that corrosive and presents a medium biodegrability and relatively high toxicity. MDEA and AMP show high toxicity and lowest	Rate based modelling: • Generic model. Assumptions. • Mass transfer models • Chemical reaction • Hydraulic models • Physical and chemical properties • Influence of the phase ratio on absorption efficiency The solvents are evaluated based on: • Dynamic behaviour • absorption performance • Rate-based	Matlab/Simulink 2008	MEA, DEA, AMP and MDEA	http://dx.doi:10.1016/j.ijggc.2012.01.016 2012

Authors & Title	Description	Result	Parameters	Software	Solvent	Reference
		biodegrability, so they are the most dangerous on an environmental viewpoint. 1st choice = MEA.2nd choice = MDEA				
Sønderbya T. M., Carlsena K. M., Fosbøla P. L., Kiørboeb Lars G., Solms N. A new pilot absorber for CO_2 capture from flue gases: Measuring and modelling capture with MEA solution	A pilot absorber column for CO_2 recovery from flue gases was constructed and tested with aqueous 30wt% MEA and pilot plant data were compared with a mathematical rate based packed-column model. Flue gas Absorber only	CO_2 recovery increases with an increase in flow rate of absorbent and absorption height, it decreases as the lean CO_2-loading of the absorbent increases. The liquid flow has greatest influence on the absorption efficiency when the absorption height is low. Absorber = (40-60 °C) Striper = (100-140 °C) CO_2 concentration of inlet flue gas = 4–20vol%.	(Analysis method for CO_2 content is given in this paper)	UNIQUAC	30wt % MEA.	http://dx.doi.org/10.1016/j.ijggc.2012.10.010 2012
Mac	A dynamic,	Model development:	Parameter studied:	gPROM	Monoethanolamine	http://dx.d

Authors & Title	Description	Result	Parameters	Software	Solvent	Reference
Dowell N., Samsatli N.J., Shah N. Dynamic modelling and analysis of an amine-based post-combustion CO_2 capture absorption column	non-equilibrium model of a packed column for the chemisorption of CO_2 from dilute gas streams has been proposed. Uses the SAFT-VR equation of state to describe the thermo physical properties and fluid-phase behaviour.	• Thermodynamic model • Proposed model (A packed column as represented as a cascade of dynamic, non-equilibrium, non-adiabatic) • Packed column model equations (6 model developed under this) The mass transfer zone and position of the temperature maximum are observed to move up the column when decrease in solvent flow rate.	• Variation in the inlet loading of the lean solvent stream • Variation in the inlet temperature of the lean solvent stream (running the absorption column at higher temperatures may result in systems which have lower CAPEX) • Variation in the amine content of the lean solvent stream (increase in amine concentration, increases the absorption capacity) • Variation in the flow rate of the lean solvent stream (reducing the solvent flow rate reduced the extent of CO_2 capture) • Modification of the inlet gas stream • Dynamic modelling studies	S		oi.org/10.1016/j.ijggc.2012.10.013 2013
Hoffa K. A. and Svendsenb H. F. CO_2 absorption with membrane contactors	Presents a case study where membrane contactors are compared with absorption towers for post combustion CO_2 capture and for natural	Absorber size may potentially be reduced by 75%, given that liquid is flowing on the shell side of the membrane units. Membrane contactors may provide significant improvements in offshore CO_2 capture, both from		CO_2 SIM	MDEA, MEA and Piperazine	http://dx.doi:10.1016/j.egypro.2013.05.190 2013

Authors & Title	Description	Result	Parameters	Software	Solvent	Reference
vs. packed absorbers- Challenges and opportunities in post combustion capture and natural gas sweetening	gas sweetening The current work is based upon three different gas treatment options: • Post combustion CO_2 capture from offshore gas turbines • Sweetening of natural gas with 10% CO_2 to pipeline specification of 2.5% • Same as above with LNG specification of 50 ppm	gas turbine flue gas and in sweetening of natural gas. Models: • Mass transfer flux • VLE model				

Authors & Title	Description	Result	Parameters	Software	Solvent	Reference
Åkessona J., Faberb R., Laird C. D., et al Models of a post-combustion absorption unit for simulation, optimization and non-linear model predictive control schemes	A dynamic model of a chemical absorption process is developed, and used for solving optimal control problems. The goal of the project is to apply nonlinear model predictive control on the separation plant to minimize its energy usage.		The input variables of the test case are: • Flue gas inlet flow and properties • Clean gas pressure • Liquid recirculation rate • Reboiler duty • Product stream outlet pressure	Modelica Dymola	Aqueous monoethanolamine (MEA)	2011
Australian National Low Emissions Coal Research and Development	Choosing an amine solvent for amine-based post combustion capture with minimal environmental adverse impact.	Rank the solvents from greatest to lowest risk as: PZ > MDEA > AMP = MEA Degradation rates: MEA > MDEA > PZ=AMP		Aspen-Plus	Monoethanolamine (MEA), methyl-diethanolamine (MDEA), 2-amino-2-methyl-1-propanol (AMP) piperazine (PZ) and their blends	Project report 2012

Authors & Title	Description	Result	Parameters	Software	Solvent	Reference
Environmental Impacts of Amine-based CO_2 Post Combustion Capture (PCC) Process	(Aqueous amino solvents may undergo oxidative and thermal degradation during the post combustion capture) Black coal-fired power plant flue gas	Risk of nitrosamine formation: PZ > MDEA > MEA > AMP Most volatile amine will have maximum emissions in quantity for a worst case of industrial accident: PZ > AMP > MEA > MDEA Conclusion: ranked in order of their likely maximum adverse impact to minimal adverse impact as: PZ > AMP > MEA > MDEA Oxidation Degradation occurs in absorber and cross exchanger (a chemical reaction of amine with oxygen and other impurities). Thermal Degradation occurs in stripper and				

Authors & Title	Description	Result	Parameters	Software	Solvent	Reference
		reboiler (involves degradation of its carbamate form which occurs due to exposure to 100 C or higher temperatures during CO_2 stripping).				
Kunal M., Jain P. K., Pathak S.K. and Panwar M.L Impact of changing MDEA parameters on Absorption of H_2S and CO_2	MDEA is used in sweetening of natural gas for removal of H_2S via absorption accompanied by CO_2 absorption. The impact of changing the parameter of MDEA on the absorption performance is studied.	Increase in concentration, increases the H_2S content in outlet stream very marginally Increase in temperature, increases the H_2S content in outlet stream invariably CO_2 in MDEA solution increases when the concentration and temperature increases. Recommendations: Concentration = 450-500 g/L Temperature = 35-45 C	Temperature and concentration of MDEA	Experimentation	MDEA	2010
Ebenezer S. A. Removal of carbon	A comprehensive review of different processes	Physical absorption processes (Higher CO_2 partial pressure and lower temperature favours the solubility of CO_2 in the	Discussion of results: • As the concentration of amine increases, the % mole concentration of CO_2 in the sweet gas decreases.	HYSYS	• Selexol process (Carbide selexol, physical solvent made of dimethyl ether of	http://www.ipt.ntnu.no/~jsg/student

Authors & Title	Description	Result	Parameters	Software	Solvent	Reference
dioxide from natural gas for LNG production	available and suitable for removal of CO_2 from natural gas to meet LNG production specifications.	solvents) - Selexol process - Rectisol process - Fluor process Chemical absorption process (solvent removes CO_2 in the contactor at high pressure and preferably at low temperature. Exothermic - absorber and Endothermic – stripper) - Potassium carbonate process (For all the processes, the advantages and disadvantages are provided)	- The loading was observed to decrease with increase temperature. - Amine loading increase with increasing amine wt% in the solution. - The loading capacity decreases with increase in circulation rate. - CO_2 emission / present in the sweet gas and amine loss with the acid gas increases with solvent circulation rate.		polyethylene glycol) - Rectisol process (chilled methanol) - Fluor process (physical solvent propylene carbonate) Details of amine base solvents provided. DEA was chosen as solvent for this study bases on the provided justification.	er/prosjekt/Salako 2005.pdf 2005