

Simulation and Modelling of a Gas Separation System

By

Muhammad Faez Ezanee b. Mohamad @ Rusdi

15875

Dissertation report in partial fulfilment of
the requirements for the

Bachelor of Engineering (Hons)

Mechanical Engineering

FYP II JANUARY 2016

Universiti Teknologi PETRONAS
Bandar Seri Iskandar
32610
Perak Darul Ridzuan

CERTIFICATION OF APPROVAL

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Approved by:

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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 person.

MUHAMMAD FAEZ EZANEE B. MOHAMAD @ RUSDI

ABSTRACT

Natural gas processing is a very important field that is of great significance due to increasing demand for energy as well as separation of gas mixtures. Most of the natural gas produced in the world is coproduced with acid gases such as CO₂ which need to be removed to increase the caloric value of natural gas. The contaminants in natural gas are also need to be removed so that the natural gas will be an end product that is safe to be used by consumer. Thus, a comprehensive review of research efforts in CO₂ separation from natural gas is required to capture details of the current scientific and technological progresses on the development of Cryogenic system with better separation performance and more cost saving. A simulation has been done for this project in order to see the performance of a gas separation system by using ASPEN HYSYS software. The simulation of 70% CO₂ feed concentration at feed condition 50 barg and -25°C was done and at these conditions the percentage separation of the gas was found to be 98.48% of methane and 1.52% of CO₂ in the top product. The analysis proves that the proposed system can efficiently recover CO₂ from mixed gases, regardless of initial compositions as the CO₂ purity in the product could be as high as 99.9% under various circumstances. Results obtained from the model in this project has satisfied the requirement of LNG Specification and it is believed that this project will serve as a good reference for future work in design and development of gas separation equipment.

ACKNOWLEDGEMENT

All praises to Allah for guidance and blessings for giving an opportunity for the author to complete this Final Year Project as part of requirements for Bachelor of Engineering (Hons.) in Mechanical Engineering at Universiti Teknologi PETRONAS (UTP).

The author would like to express his most appreciation to the assigned supervisor for this project, A.P. Dr. Fakhruddin M. Hashim for his continuous guidance and support provided throughout the progression of his project and also Mr. Syed Ali Ammar Taqvi (Chemical Engineering) for the help with ASPEN HYSYS.

This acknowledgement would not be complete without giving credit to UTP especially Mechanical Engineering Department which has equipped students with essential skills for self-learning.

Many figures had provided immeasurable amount of guidance, ideas, assistance, support and advice. Without help from these people, this Final Year Project may not be a success. Greatest appreciation is expressed to them.

Finally, countless appreciation goes to the author's family and friends for their kind assistance and support throughout completing this project. They had been a wonderful source of encouragement and jot to the author and not to forget the fellow colleagues. Their help was a blessing gift to the author.

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CHAPTER 1 : INTRODUCTION

1.1 Background of Study

The development of alternative sources of energy even to the remote parts of the world, for example offshore, has been triggered by the high demand of energy throughout the world. For many thousand years, oil has been used worldwide for lighting purposes. During the old days, crude oil or gases were found in shallow reservoirs, and they may naturally develop. For example, the Chinese used to boil water by using natural gas in the years 500 B.C. [1].

Ever since 1859, the new era of energy sources begin when “Colonel” Edwin Drake started the sole purpose of finding oil when he successfully drilled the first oil well which is called the Drake Well. The well was located in north-western Pennsylvania, in the middle of a quiet farm country. Within few months, they completely transformed the landscape by building oil rigs across the field to extract oil and gas from reservoir up to 3000 meters down below by cable-tool drilling, and now rotary drilling [1].

Oil has been the engine of the world economy for over a century but hardly ever without an impact on the environment. Soon after, the search for oil and development of technologies to process petroleum began worldwide. A few decades ago, the major alternative source which is the energy from natural gas has been found and the energy also has less environmental effect. Natural gas normally contain some complex contaminants in it such as CO₂, CO, H₂S and Mercaptan (Acid Gs), which may hindered natural gas processes and may harm the environment greatly when get to atmosphere [2].

Natural gas has very high cost to be transported to the consumers who may be thousands of kilometers away from the natural source because natural gas content relatively low energy per unit volume. Gas is normally transported through pipelines but as the distance of sources to the shore increase, the cost to build pipelines started to become uneconomical. Therefore, gas is being processed to liquid and chemicals or also known as Liquefied Natural Gas (LNG) as a more viable option in contrary to pipelines [2].

The transformation of natural gas to the form of liquid is called liquefaction process. The process normally involves operation at pressure as low as atmospheric pressure, and very low temperature (-161°C). Before the liquefaction process, it is important to remove CO₂ from the natural gas because at these process conditions, CO₂ can reduce the plant or platform efficiency by freezing out at the plugging lines or exchanger surface. The removal of CO₂ is needed to prevent corrosion in the process equipment, to increase environmental performance and most importantly to meet the LNG product specifications [2].

There are many acid gas treating processes available for CO₂ removal from natural gas. These processes include Chemical Solvents, Physical solvents, Adsorption Processes Hybrid solvents and Physical separation (Membrane). The chemical solvents and physical solvents or combination of these two have been used extensively in existing base load LNG facilities. Cryogenics, which means very low-temperature liquefaction and separation of industrial gas has been discovered and fully developed in the 20th century and also is commonly used now in the industry [2].

Today, the world has widely used the software to do computer-aided simulation which has been the essential tools in process development. The software enables engineers to study the process alternative, new process technologies, to assess its feasibility and to simulate the process design in order to optimize the process equipment [3].

However, the content in the output gas of these systems still have certain percentage of CO₂. Thus, this project will simulate the process available to perform the CO₂ removal from natural gas in order to optimize the process to meet the LNG specifications of about 50-100 ppmv or 2-3% of CO₂ content in the downstream to prevent corrosion in pipelines and decreases in calorific value. Optimum process condition in the gas separation system that will reduce environmental effect will be input into the simulation, and the separation process will be simulated by using ASPEN HYSYS software [3].

Gas resources with CO₂ composition between 15%-80% is consider as sour gas resources that has high CO₂ content [4]. Some of the Malaysian natural gas reserve has CO₂ content that can goes up to 80%.and therefore is considered as sour gas resource. The following tables summarize all the high CO₂ gas fields in Malaysia [5].

Table 1: Peninsular Malaysia Gas Fields CO₂ Contents [5]

Peninsular Malaysia		
Holder	Field	CO ₂ Content
PETRONAS	Bujang	66%
PETRONAS	Sepat	60%
PETRONAS	Noring	60%
PETRONAS	Inas	60%
PETRONAS	Tangga Barat	32%
PCSB	Ular	50%
PCSB	Gajah	50%
PCSB	Bergading	40%
PCSB	Palas NAG	46%

Table 2: Sarawak Gas Fields CO₂ Contents [5]

Sarawak		
Holder	Field	CO ₂ Content
PETRONAS	K5	70%
PETRONAS	J5	87%
PETRONAS	J1	59%
PETRONAS	T3	62%
PETRONAS	Tenggiri Mm.	47%

Dehydration processes which are widely used are absorption and adsorption. On the other hand, CO₂ could be removed using methods such as adsorption, absorption, membrane separation and cryogenic separation. However, cryogenic separation is not comprehensively investigated, due to the perception of high energy cost. The advantage of cryogenic separation is that no chemical reaction is involved as well as has minimum footprint for offshore application. Recent finding shows that cryogenic separation is capable to separate water and CO₂ from natural gas at optimum energy requirements [6].

1.2 Problem Statement

The high content of contaminants in the natural gas especially CO₂ reduces the process efficiency. Natural gas must undergo processing to remove impurities in order to be used as a fuel. With the depletion of sweet gas reserves, Malaysian natural gas reserves that have high contents of CO₂ (up to 80%) need to be explored in order to meet the global demand. The presences of water contents and CO₂ in natural gas not only reduce the heating value but also cause pipelines corrosion and plugging. Existing methodology for CO₂ removal is not sufficient to remove high concentration of CO₂ in our natural gas supply. Thus, due to the compactness and economic attractiveness of Cryogenic system that has the ability to remove high concentration of CO₂, modelling and simulation of the system by ASPEN HYSYS needs to be done to predict its performance. By the study, we might be able to remove higher CO₂ content in natural gas supply.

1.3 Objectives

1. To model and simulate a given gas system for CO₂ gas separation from natural gas
2. To achieve required CO₂ content to meet the LNG specifications of about 50-100 ppmv or 2-3% of CO₂ in the downstream by using distillation column and addition of separator

1.4 Scope of Study

As outlined in the objectives, this project will be covering the investigation of the performance of gas separation system in separating carbon dioxide from natural gas whether it is meeting the required LNG specification. The scope of this project is to conduct a literature review on removal of CO₂ from natural gas stream using Cryogenic method. Prior to that, it is necessary to understand the theory of Cryogenic separation. Modelling of the separation process in the simulation software will also be done by using ASPEN HYSYS. The data to be ran into the model will be taken limitedly from the gas fields in Malaysia. Through this project student is exposed to explore research problems and build research objectives, applying appropriate methodology, analysing and interpreting data obtained from the simulation, troubleshooting any predicaments occur and also reporting the findings.

1.5 Relevancy of Study

In Chapter 2, the literature review in this report discuss on several methods of gas separation and the theory of each methods. These topics are relevant to the study of this project because in order to achieve CO₂ removal from natural gas, it is important to understand how the gas separation system behave. After identifying the specific factors for the process, the study can be more confined for the purpose of this project which is to achieve required CO₂ content to meet the LNG specifications of about 50-100 ppmv or 2-3% of CO₂ in the downstream.

1.6 Feasibility of Study

The project is scheduled for duration of 28 weeks altogether. For the first 14 weeks (FYP I), the project focuses on research activity to gather sufficient information in order to proceed with the second phase of the project (FYP II), which will focus on the modelling and simulation of gas separation system using ASPEN HYSYS software. The simulation work, the troubleshooting and the analysis of the results will be done in the duration of second phase of 14 weeks.

CHAPTER 2: LITERATURE REVIEW

2.1 CO₂ in Natural Gas

In the 21st century, the most sophisticated challenges in environmental protection are global warming which had worried a lot of parties for several years. This global warming phenomenon occurs because of the excessive amount of greenhouse gas emissions, especially CO₂. This matter has led to the study of removal of CO₂ in order to reduce the CO₂ emission to the environment. Carbon Capture and Storage (CCS) has been considered as one of the most significant methods in reducing [7] CO₂ since combustion of fossil fuels is reported to generate 90% of CO₂ emissions, which will be extensively used in the foreseeable future [8].

In the oil & gas industry, LNG has a certain specifications which require the gas to be processed. Before gas can be transported into pipelines to the end users, the various impurities in the natural gas must be removed. One of the main components in the natural gas is CO₂, which needs to be removed to an acceptable level prior to export. Previously, CO₂ is removed from natural gas a low pressure and being released to the atmosphere by convention removal technologies. Currently, some of the primary recovery and capture methods used are the Cryogenic or low temperature process, chemical and physical solvent processes, while in some cases, using membranes are also applicable [9-11].

2.2 Separation with Sorbents/Solvents

A few decades ago, a technology of amine scrubbing was established in the oil and chemical industries mainly for the CO₂ and H₂S removal from natural gas. Although practical experience is mainly in gas streams which are chemically reducing, the most commercially well-established methods available to remove CO₂ is amine scrubbing technology [12].

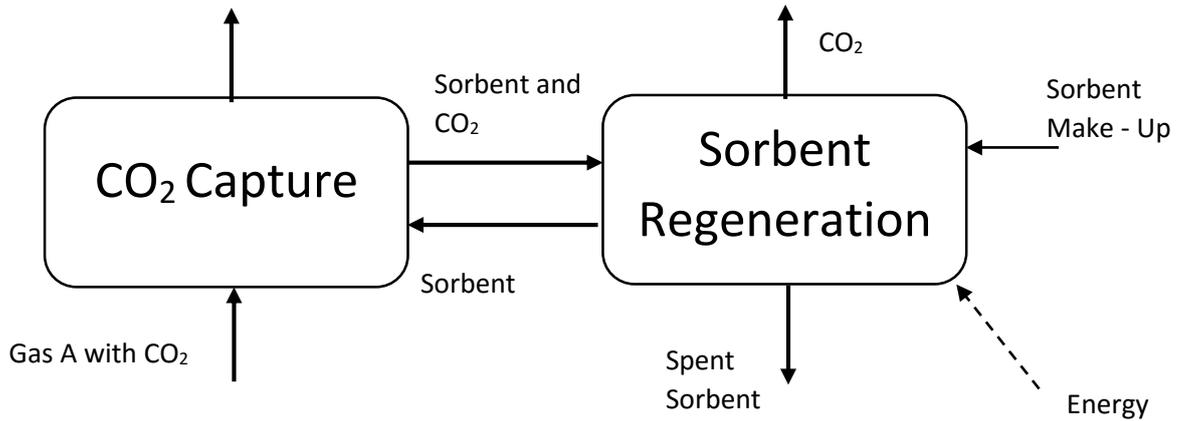


Figure 1: Schematic Diagram of Sorbent/Solvent Separations [12]

Today, there are several facilities to capture CO₂ from natural gas which uses amines. One of the amine type widely used is the Mono-Ethanolamine (MEA) which can produce CO₂ recovery rates of 98% and can achieve 99% of product purity in excess. However, the conventional MEA solvents are tend to be replaced with improved solvents which can reduce energy requirements by as much as 40%. These sterically hindered amines are claimed to have good desorption and absorption characteristics which can help in CO₂ removal process from natural gas [12].

Besides using the solvents, solid absorbent or commonly called as sorbents such as zeolites and activated carbon, also can be used to extract CO₂ from natural gas. There are two commercially used methods by using sorbents, which are Pressure Swing Absorption (PSA) and Temperature Swing Absorption (TSA). A packed bed of adsorbent at elevated pressure will be flown through with gas mixtures until equilibrium of desired gas concentration is reached in the PSA, and the bed will be regenerated by dropping the pressure. While in the TSA method, the adsorbent is regenerated by increasing its temperature [12].

2.3 Separations with Membranes

Gas separation by using membranes is also one of the common methods used in the industry. Membranes assist the gas separation by allowing one component in a gas stream to pass through faster than the others, therefore desired component such as CO₂ can be captured by the membranes [12].

The membranes are characterized by the permeability, selectivity and permeance of the components in order to determine its performance. Gas separation membranes consist of many types including palladium membranes, zeolites, polymeric membranes and porous inorganic membranes [12].

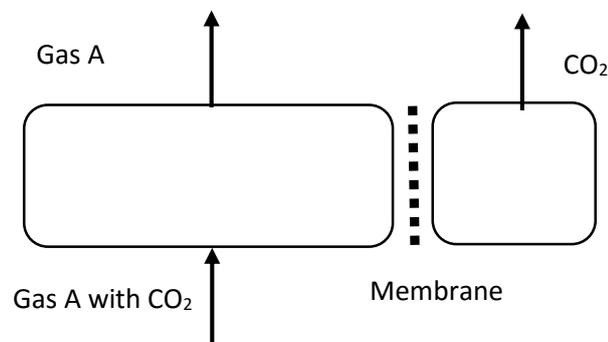


Figure 2: Schematic Diagram of Membrane Separation [12]

In certain cases, high purity CO₂ requires several types of membranes with different characteristics. Now, engineers and scientist are developing hybrid technologies of combining membranes and solvent scrubbing (solvent assisted membranes) in order to get the best features out of them and optimize the gas separation process. However, there is still much development needs to be done in order to enable the use of membranes on a large scale for gas separation process [12].

2.4 Cryogenics Separation

Cryogenic separation is a physical procedure that isolates CO₂ from natural gas under a great degree of low temperature. It empowers production of liquid CO₂ at a low pressure, so that the liquid CO₂ can be put away or sequestered by means of fluid pumping rather than compression of gaseous CO₂ to a high pressure, therefore compression energy can be saved [13-16]. During cryogenic division process, the segments of gas mixtures are captured by a progression of compression, refrigeration and detachment steps. Cryogenic separation process can be classified into three categories, namely conventional, non-conventional and hybrid cryogenic separation process. Non-conventional cryogenic separation process encourages the formation of solid CO₂ while conventional cryogenic separation process avoids the formation of solid CO₂. The hybrid cryogenic separation process includes both conventional and non-conventional cryogenic separation process.

Since all the steps are exceedingly develop advances in the technology of chemical industry, their operation and outline achievability can be ensured [16-18]. The cryogenic separation procedure requires no chemical agents, subsequently evading further optional contamination to the environment [13-18]. To the extent modern application is concerned, natural gas mixtures are generally made out of CO₂ and other different gases, and the boiling points of which are moderately low. These gases include Hydrogen (H), Nitrogen (N₂), Oxygen (O₂), Argon (Ar), and Methane (CH₄). These impurities influences bring down the phase transition temperature of CO₂, which can even drop to under -80°C. For this situation, the refrigeration energy penalty rises consequentially, and what's more, CO₂ freezing arrangement turns out to be very conceivable, therefore debilitating equipment safety [19]. Consideration should accordingly be paid to raising the phase transition temperature of CO₂ to enhance the cryogenic separation system and thus avoiding from equipment freezing issues and high energy penalty [20-23].

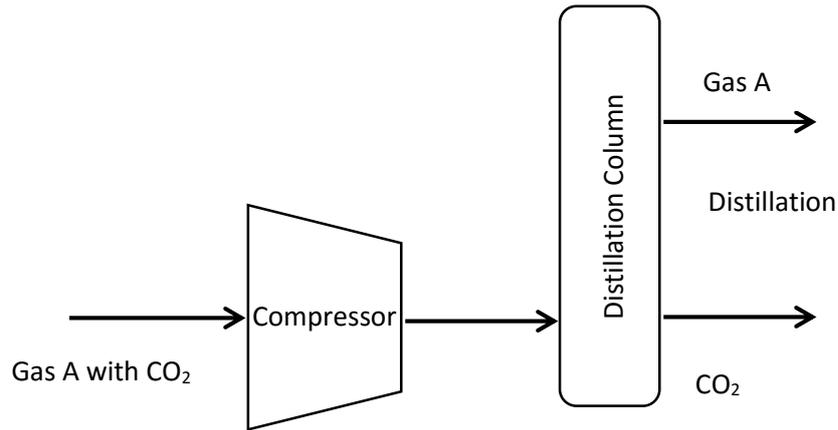


Figure 3: Schematic Diagram of Cryogenic Distillation Separation [12]

CO₂ can be separated from other gases by cooling and condensation. Cryogenic separation is generally utilized industrially for streams that as of now have high CO₂ concentrations (ordinarily > 90%) yet it is definitely not utilized for more dilute CO₂ streams. A noteworthy weakness of cryogenic separation of CO₂ is the measure of energy required to give the refrigeration required for the process, especially for dilute gas streams. Another stream is cooled, to prevent blockages. Cryogenic separation has the point of interest that it empowers direct generation of liquid CO₂, which is required for certain transport options, for example, transport by ship. Cryogenics would regularly only be applied to high concentration, high pressure gases, for example, in oxygen fired combustion or natural gas from deepwater wells [12].

2.5 CO₂ Purity Characteristics of the Cryogenic Separation Method

For the most part, a little measure of impurities dependably disintegrate in the liquid CO₂ separated under high pressure, and the higher the pressure of the separation, the bigger the measure of impurities [24]. From one viewpoint, the CO₂ separation proportion continuously increase with the augmentation of separation pressure, though the CO₂ purity in the item diminishes. Then again, diverse impurity composition affects the CO₂ purity differently in the output gas.

This is on account because of there exist critical contrasts in the physical properties of the diverse impurity gases, which influence the thermodynamic properties, for example, dew and bubble points, heat capacity, enthalpy and entropy of the CO₂ mixture, so the working conditions and separation execution of the purification procedure will therefore change appropriately, bringing about diverse CO₂ purity in the product [23]. Generally, if the physical properties of the impurity gas are recognized from those of the CO₂ (H₂ for instance), it is easier to separate them by high pressure cryogenic separation [25]. In any case, for gas mixtures comprising of CO₂, N₂, O₂, also Ar, the CO₂ purity in the product accomplished by high pressure cryogenic separation is too low to fulfil the necessities of most modern applications and also for transport and storage. Therefore, further purification measures ought to in this way be considered.

2.6 LNG Specification Standards

The table below are the details for LNG Specifications standard used for this project. The standard specifies the concentration of the component required to be achieved in any LNG processes.

Table 3: Typical LNG Product Specification [26]

Component	Limit (Maximum)
Hydrogen Sulfide	3 – 4 ppmv
Total Sulfur	30 miligrams per normal cubic meter
Carbon Dioxide	50 – 100 ppmv, 2-3 mol%
Mercury	0.01 micrograms per normal cubic meter
Nitrogen	1 mol%
Water Vapor	1 ppmv
Benzene	1 ppmv
Ethane	6-8 mol%
Propane	3 mol%
Butane and heavier	2 mol%
Pentane and heavier	1 mol%
High Heating Value	1050 Btu/Scf (Europe and USA) >1100 Btu/Scf (East Asia)

CHAPTER 3: METHODOLOGY

3.1 Work Flow Chart

The research methodology consists of the main project activities:

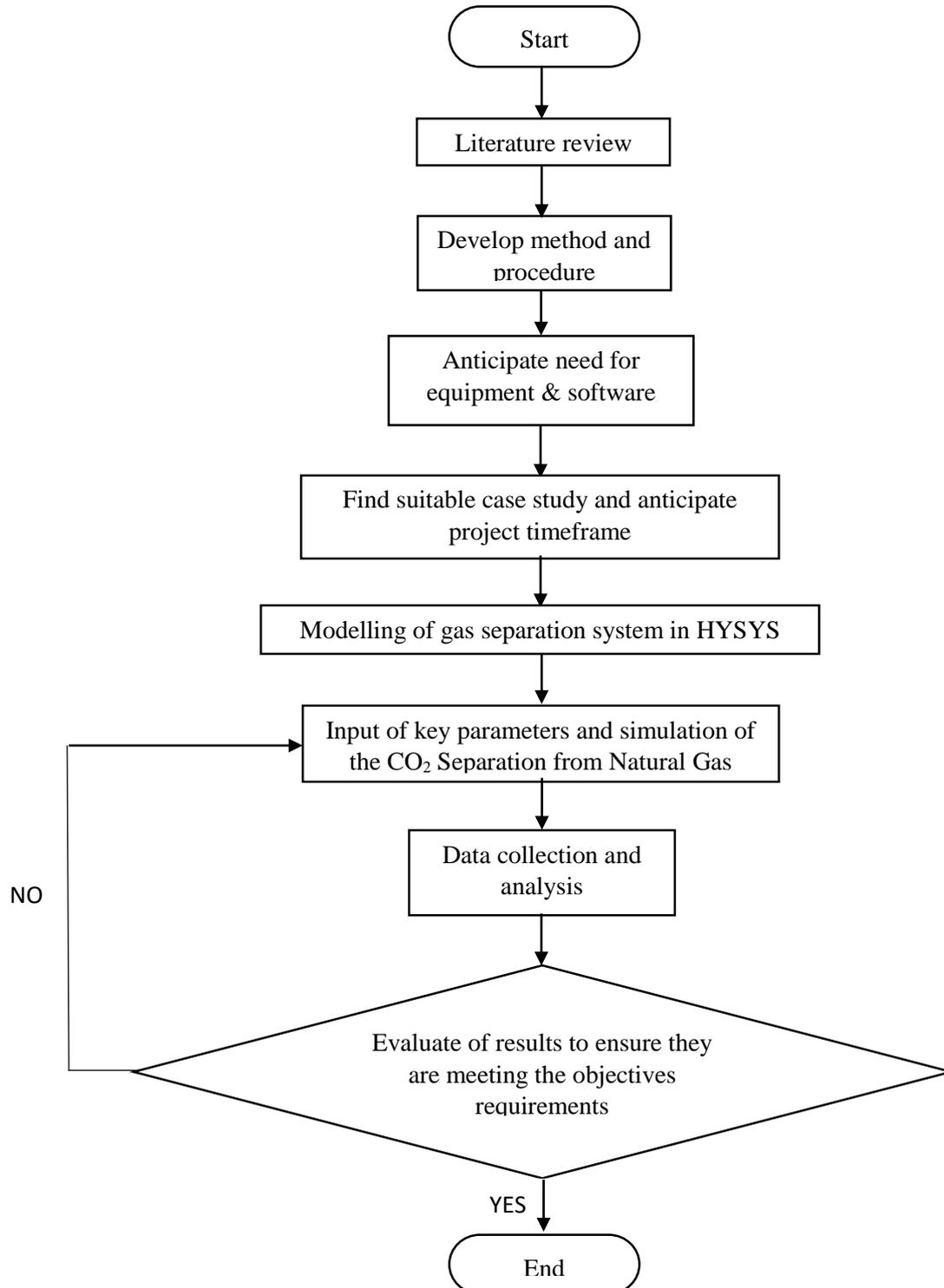


Figure 4: Flow Chart of Project Activities

3.2 Project Activities Flow Chart Description

The proposed model design for the gas separation system has been finalized and decided which is to use distillation column with condenser and reboiler as the first stage separation equipment and vertical separator as the second stage separation equipment. The design condition to be simulated with the model is shown in the Table 4. The results will later be analysed to ensure the system are meeting the LNG specifications of about 50-100 ppmv or 2-3% of CO₂ content in the downstream.

Table 4: Design Condition for Gas Separation Model [27]

Design Condition	
Flowrate	700 std L/min (0.0355 MMSCFD)
Operating Pressure	35 – 50 barg
Inlet Temperature	-30 to -10 °C
Top Product	< 20 mol % CO ₂
HC Loss	< 5 mol %
Feed Composition	CO ₂ : 60 – 80 mol % CH ₄ : 20 – 40 mol %

The inputs in the system are CO₂ and CH₄ because natural gas is assumed as Methane. This is because based on few studies worldwide, the composition of natural gas is on average with 95% Methane and the other 5% are non-Methane components depending on the location of the field.

As for the fluid properties package, Equation of State (EOS) model are proven to be very reliable in predicting the properties of most hydrocarbon based fluids over a wide range of operating condition. For this particular project, Peng-Robinson (PR) model has been chosen as its EOS. It is ideal for Vapor-Liquid Equilibrium (VLE) calculations as well as calculating liquid densities for hydrocarbon systems. Several enhancements to the original PR model were made to extend its range of applicability and to improve its predictions for some non-ideal systems.

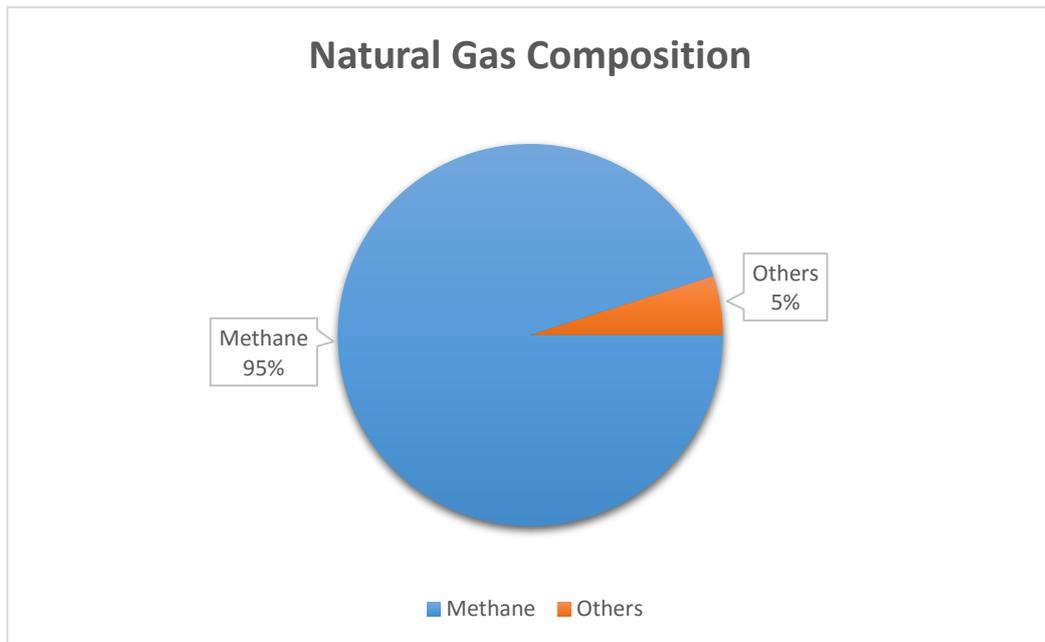


Figure 5: Natural Gas Composition [28]

The PR property package rigorously solves any single, two, or three-phase system with a high degree of efficiency and reliability and is applicable over a wide range of conditions which is suitable for this project, as follows:

- Temperature Range $> -271^{\circ}\text{C}$ or -456°F
- Pressure Range $< 100,000$ kPa or 15,000 psia

3.3 HYSYS Simulation Procedures

A base case was established using the following steps; the first step is to select the appropriate fluid package; in this project Peng-Robinson model is selected as in Figure 6 below. Figure 7 below shows another step in selecting component list.

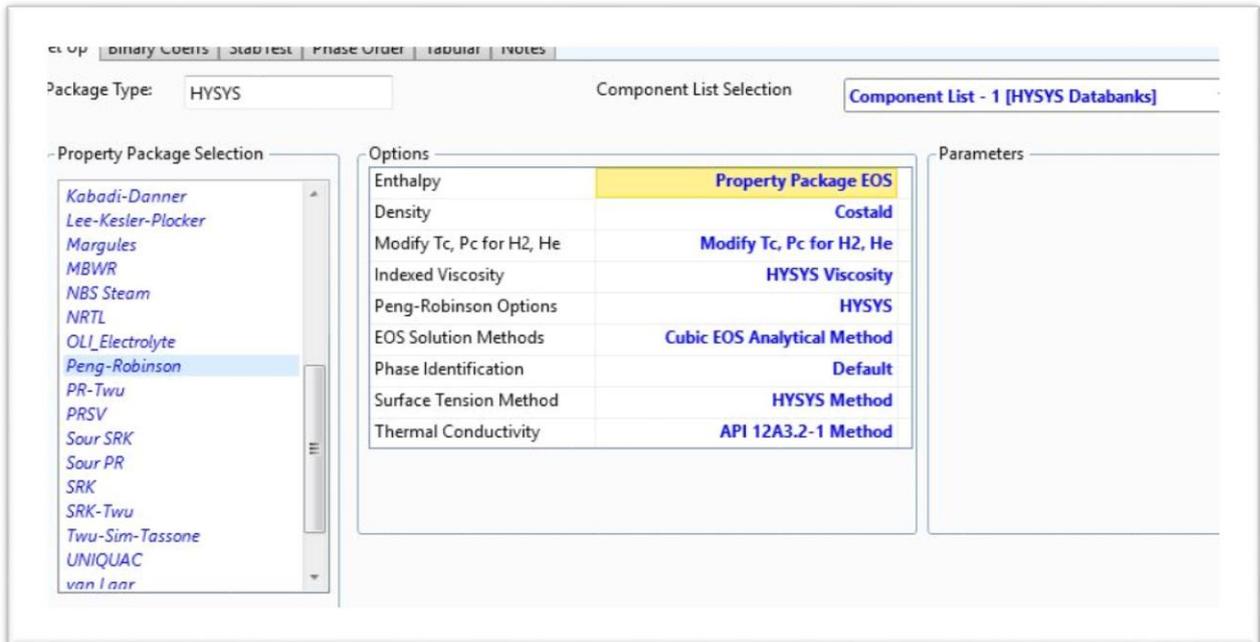


Figure 6: Fluid Package Basis Selection

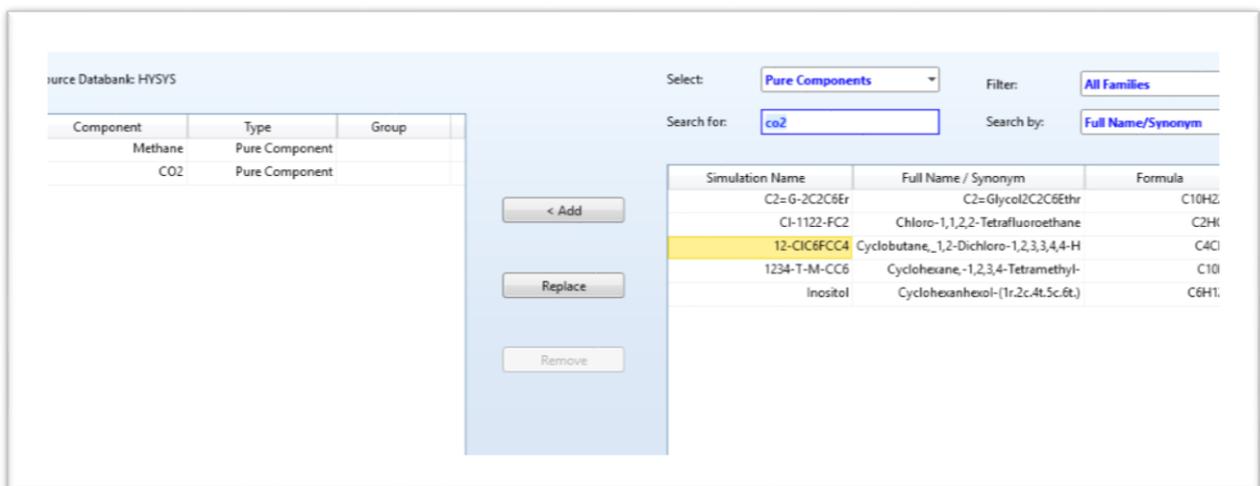


Figure 7: Dialog window used for components selection

After selecting the component of the fluid, the simulation environment is entered where the Process Flow Diagram (PFD) is built. The full simulation environment is shown in Figure 8 below.

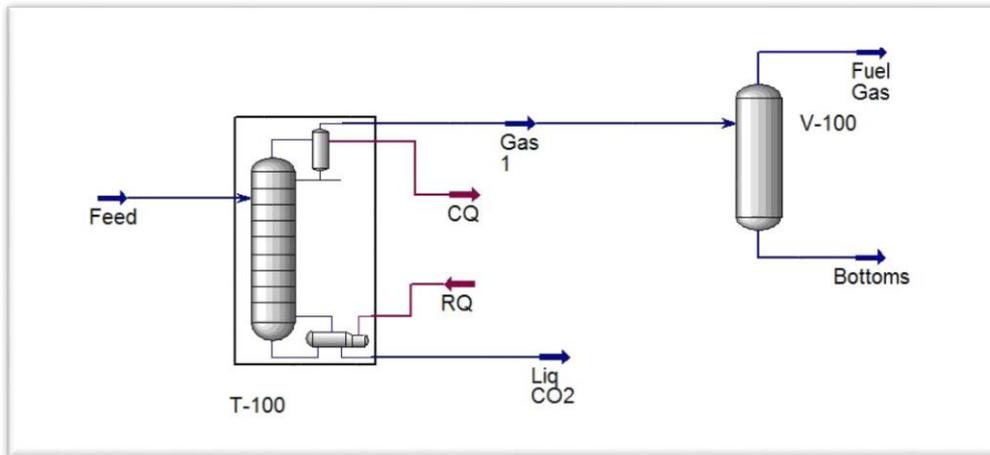


Figure 8: Process Flow Diagram

The simulation of the process begins with the simulation of the feed gas stream by specifying the gas temperature, pressure and flow rate and HYSYS calculate the remaining parameters as shown Figure 9 below.

Worksheet	Stream Name	Feed	Vapour Phase	Liquid Phase
Conditions	Vapour / Phase Fraction	0.3326	0.3326	0.6674
Properties	Temperature [C]	-25.00	-25.00	-25.00
Composition	Pressure [bar_g]	50.00	50.00	50.00
Oil & Gas Feed	Molar Flow [kgmole/h]	786.5	261.6	524.9
Petroleum Assay	Mass Flow [kg/h]	2.801e+004	7313	2.070e+004
K Value	Std Ideal Liq Vol Flow [m3/h]	42.00	13.99	28.01
User Variables	Molar Enthalpy [kJ/kgmole]	-3.086e+005	-2.149e+005	-3.554e+005
Notes	Molar Entropy [kJ/kgmole-C]	111.3	138.7	97.59
Cost Parameters	Heat Flow [kJ/h]	-2.427e+008	-5.620e+007	-1.865e+008
Normalized Yields	Liq Vol Flow @Std Cond [L/min]	<empty>	1.027e+005	2.058e+005
	Fluid Package	Basis-1		
	Utility Type			

Figure 9: Feed conditions entered in the simulation

One of the rigorous tasks in the convergence of the regenerator. By specifying the condenser and re-boiler pressure, the top temperature and bottom CO₂ composition required, the convergence is achieved.

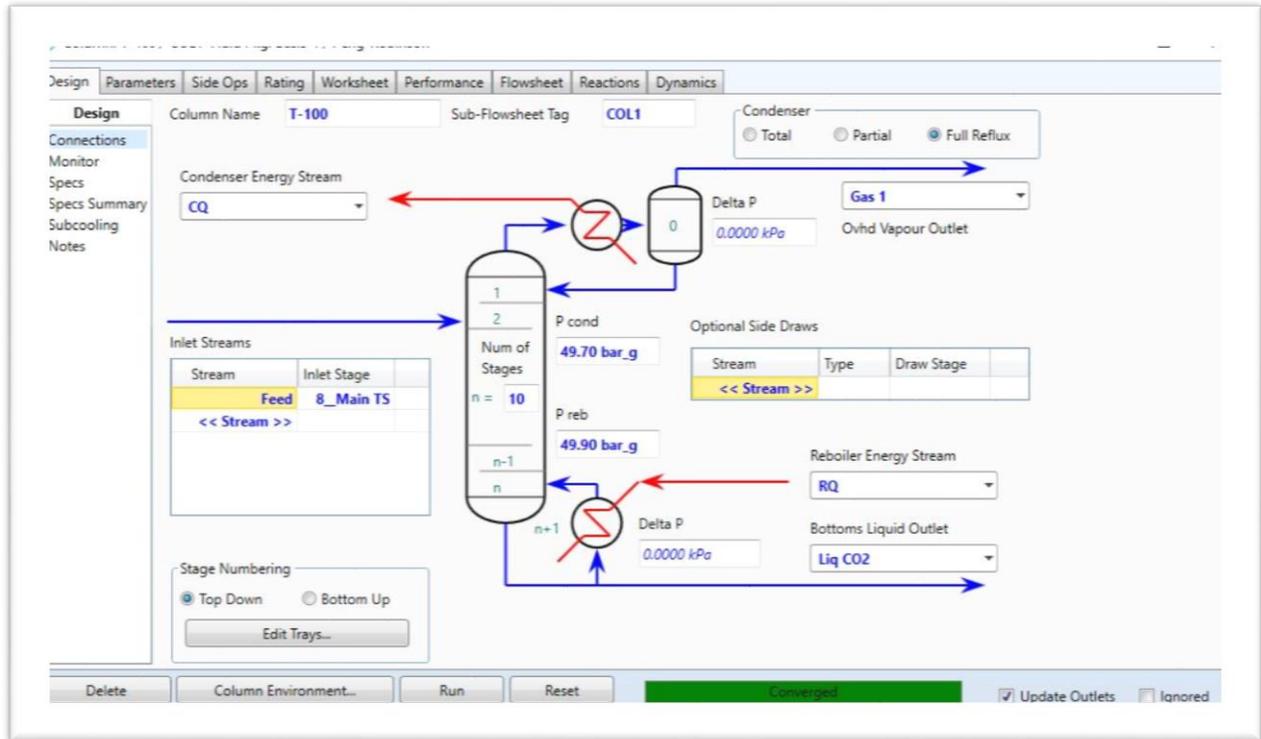


Figure 10: Converged windows for distillation column unit

With the convergence of the distillation column unit, a complete simulation for the base case was established. Optimization of the process was carried out by modification of some parameters to meet the project aims. Detail parameters for the base case and modified parameters are shown in tables of data.

CHAPTER 4: RESULTS

4.1 HYSYS Modelling of Gas Separation System

The model of separation process is as shown in Figure 11 where a feed of CH₄ and CO₂ enters the distillation column. There are a condenser placed at the top of the distillation column and reboiler placed at the bottom, both are working at a pressure of 49.7 barg and 49.9 barg respectively.

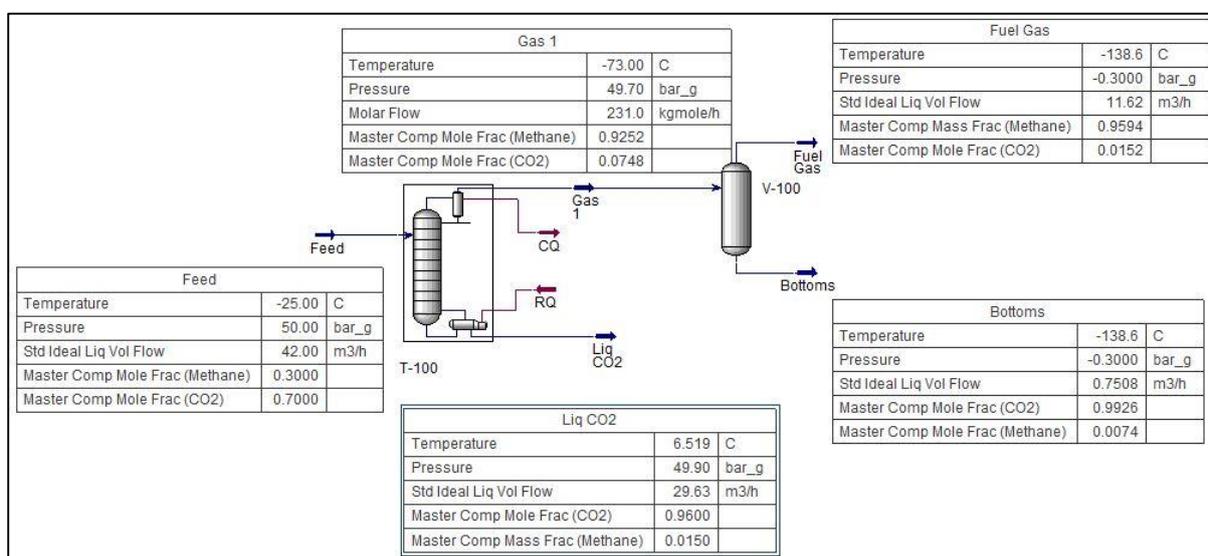


Figure 11: Layout of the Distillation Column in HYSYS Simulation

The condenser is used to cool down and condense the output gas into liquid state, and reboiler is a type heat exchanger typically used to provide heat to the bottom of the distillation columns. It boils the liquid from the bottom of the distillation column to generate vapours which are returned to the column to drive the distillation separation.

4.2 Data Tabulation and Analysis

All of the operating condition parameters needed for the simulation has be input. The findings are presented in the form of tables and graphs below.

Table 5: Distillation column data of the process simulation model

Name	Feed @Main	Liq CO2 @Main	Gas 1 @Main
Molecular Weight	35.62	42.89	18.13
Molar Density (kgmole/m ³)	8.345	19.44	7.763
Mass Density (kg/m ³)	297.3	833.8	140.8
Act. Volume Flow (m ³ /h)	94.24	28.57	29.76
Mass Enthalpy (kJ/kg)	-8665	-9164	-5819
Mass Entropy (kJ/kg-C)	3.124	2.389	6.916
Heat Capacity (kJ/kgmole-C)	90.28	156.7	390.9
Mass Heat Capacity (kJ/kg-C)	2.535	3.653	21.56
LHV Molar Basis (Std) (kJ/kgmole)	2.408e+005	3.211e+004	7.427e+005
LHV Mass Basis (Std) (kJ/kg)	6761	748.6	4.095e+004
Phase Fraction [Vol. Basis]	0.3330	1.918e-006	1.000
Phase Fraction [Mass Basis]	0.2611	1.795e-006	1.000
Partial Pressure of CO2 (kPa)	2174	4389	379.2

Table 6: Material Streams Condition and Distillation Column Product Composition

Material Streams						Fluid Pkg:	All
Name	Reflux	To Condenser	Boilup	To Reboiler	Fuel Gas		
Vapour Fraction	0.0000	1.0000	1.0000	0.0000	1.0000		
Temperature (C)	-73.00	-68.77	6.519	-1.903	-73.00		
Pressure (kPa)	5071	5071	5091	5091	5071		
Molar Flow (kgmole/h)	1272	1503	311.9	867.4	231.0		
Mass Flow (kg/h)	2.432e+004	2.851e+004	1.253e+004	3.635e+004	4189		
Liquid Volume Flow (m ³ /h)	68.10	80.47	16.64	46.27	12.37		
Heat Flow (kJ/h)	-1.507e+008	-1.721e+008	-1.103e+008	-3.316e+008	-2.438e+007		
Name	Liq CO2	Feed					
Vapour Fraction	0.0000	0.3326					
Temperature (C)	6.519	-25.00					
Pressure (kPa)	5091	5101					
Molar Flow (kgmole/h)	555.5	786.5					
Mass Flow (kg/h)	2.383e+004	2.801e+004					
Liquid Volume Flow (m ³ /h)	29.63	42.00					
Heat Flow (kJ/h)	-2.183e+008	-2.427e+008					
Compositions						Fluid Pkg:	All
Name	Reflux	To Condenser	Boilup	To Reboiler	Fuel Gas		
Comp Mole Frac (Methane)	0.8898	0.8952	0.1379	0.0752	0.9252		
Comp Mole Frac (CO2)	0.1102	0.1048	0.8621	0.9248	0.0748		
Name	Liq CO2	Feed					
Comp Mole Frac (Methane)	0.0400	0.3000					
Comp Mole Frac (CO2)	0.9600	0.7000					

Table 7 shows the mole fraction composition of Methane and CO₂ which are obtained from ASPEN HYSYS simulation results. The sets of data are plotted into Mole Fraction Composition vs Tray Position graph as shown in Figure 12 below. Methane's (red line) composition can be seen started to reduce as it moved across the distillation column from top to bottom while the CO₂ (green line) behaved oppositely as its mole fraction composition started to increase as the gas moved across the distillation column. At the top product, the composition is; Methane (0.8898) CO₂ (0.1102) and at the bottom; Methane (0.04) CO₂ (0.96).

Table 7: Mole Fraction Composition of Methane and CO₂ in Distillation Column

	Methane (Light Liq)	CO2 (Light Liq)
Condenser	0.8898	0.1102
1_Main TS	0.7719	0.2281
2_Main TS	0.3119	0.6881
3_Main TS	0.1767	0.8233
4_Main TS	0.1527	0.8473
5_Main TS	0.1476	0.8524
6_Main TS	0.1465	0.8535
7_Main TS	0.1463	0.8537
8_Main TS	0.1463	0.8537
9_Main TS	0.1129	0.8871
10_Main TS	0.0752	0.9248
Reboiler	0.04	0.96

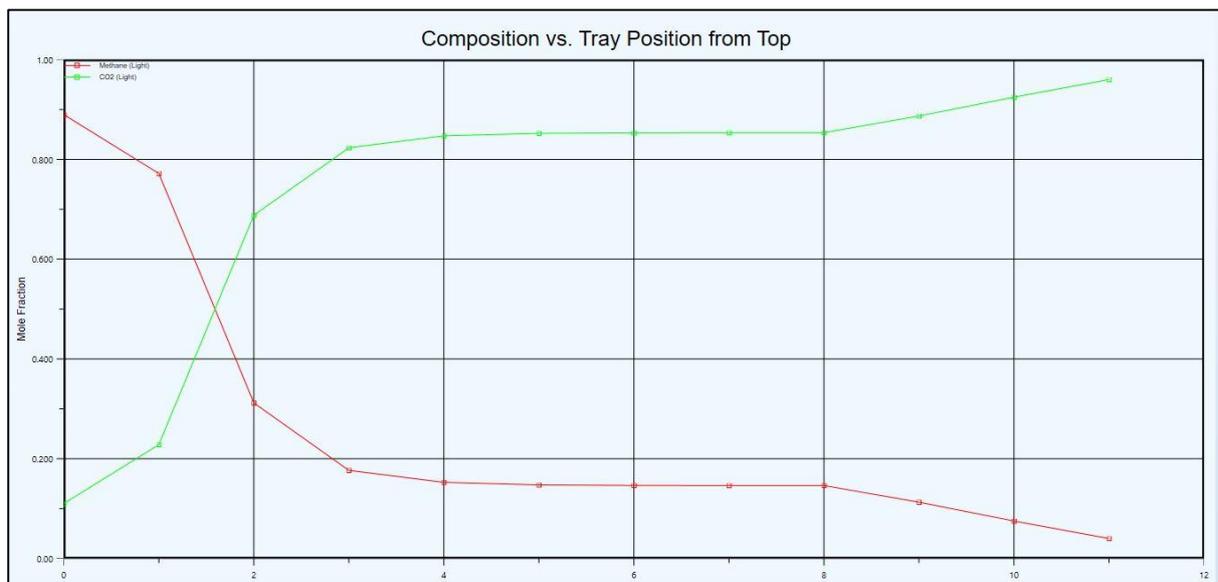


Figure 12: Mole Fraction Composition vs Tray Position from Top

Table 8 shows the temperature distribution in the distillation column which are obtained from ASPEN HYSYS simulation results. The sets of data are plotted into Temperature vs Tray Position graph as shown in Figure 13 below. The trend for the temperature is increasing as the gas moves downwards across the trays in the distillation column. The temperature is highest at the bottommost tray, as the heater is placed at the bottom of distillation column. The component which has higher boiling point ($\text{CO}_2 = -78.5^\circ\text{C}$) will be bottom product and component with lower boiling point ($\text{CH}_4 = -161.5^\circ\text{C}$) will be the top product.

Table 8: Temperature Distribution in Distillation Column

	Temperature [C]
Condenser	-73.00
1_Main TS	-68.77
2_Main TS	-53.70
3_Main TS	-28.79
4_Main TS	-22.49
5_Main TS	-21.09
6_Main TS	-20.77
7_Main TS	-20.69
8_Main TS	-20.66
9_Main TS	-11.68
10_Main TS	-1.903
Reboiler	6.519

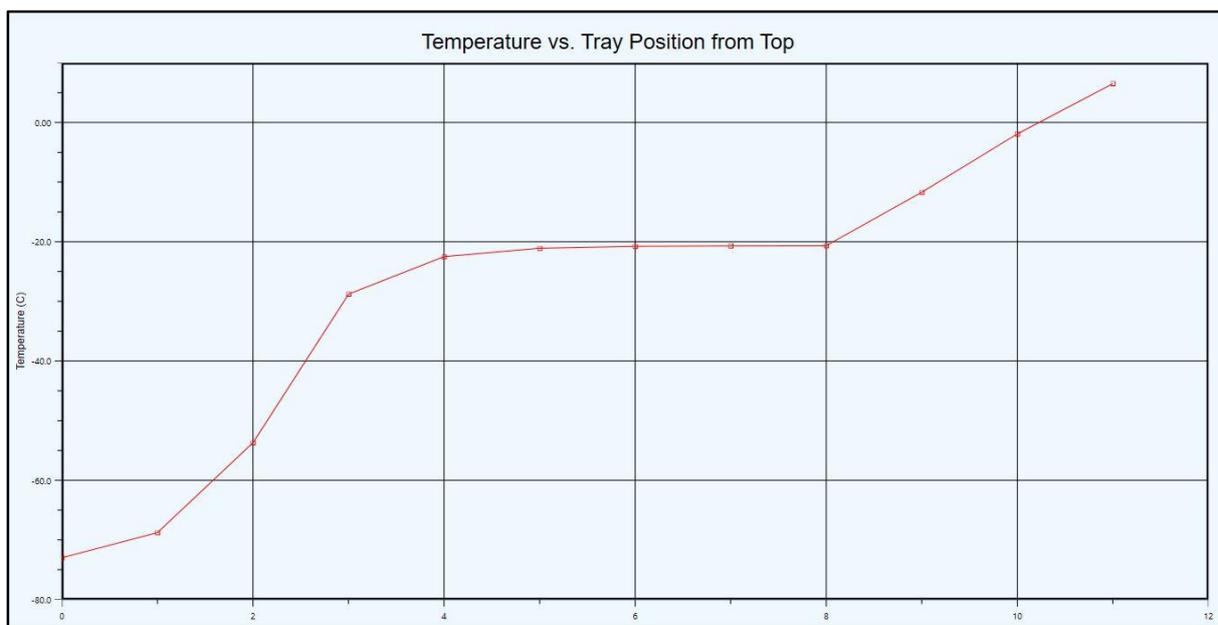


Figure 13: Temperature vs Tray Position from Top

Table 9 shows the pressure distribution in the distillation column which are obtained from ASPEN HYSYS simulation results. The sets of data are plotted into Pressure vs Tray Position graph as shown in Figure 14 below. The trend of the pressure is increasing as the gas moves downwards across the trays in the distillation column. The pressure is directly proportional to temperature. Temperature increased from top tray to the bottom tray therefore pressure increased along with the temperature. However there is not much pressure different between top tray and bottom tray, because the operating pressure at condenser (top) is 49.7 barg and operating pressure at reboiler (bottom) is 49.9 barg.

Table 9: Pressure Distribution in Distillation Column

	Pressure [bar_g]
Condenser	49.70
1_Main TS	49.70
2_Main TS	49.72
3_Main TS	49.74
4_Main TS	49.77
5_Main TS	49.79
6_Main TS	49.81
7_Main TS	49.83
8_Main TS	49.86
9_Main TS	49.88
10_Main TS	49.90
Reboiler	49.90

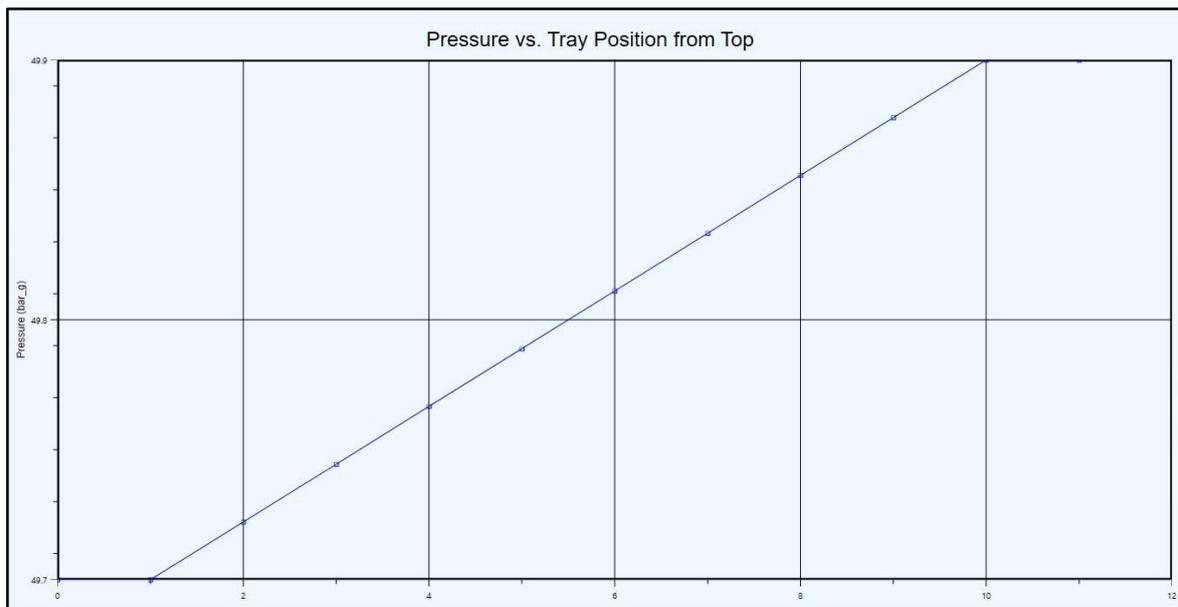


Figure 14: Pressure vs Tray Position from Top

4.3 Cryogenic Separation System

As shown in Figure 15, the feed entered the distillation column (T-100) at temperature of -25°C , pressure of 50 barg and flow rate of $42\text{ m}^3/\text{h}$ (700 std L/min). After the separation process, the product will be separated into top product and bottom product. The bottom product will be in the form of liquid. The properties of bottom product is as shown above which temperature of it is 6.519°C , pressure of 49.90 barg, flow rate of $29.63\text{ m}^3/\text{h}$, mole fraction of methane (0.0150/ or 1.5%) and the mole fraction of CO_2 (0.9600 or 96.0%). The condenser at the top is set to produce total reflux product (total vapour). The properties of top product is a shown in Figure 14 which temperature of it is -73°C , pressure of 49.70 barg, mole fraction of methane (0.9252 or 92.52%) and mole fraction of CO_2 (0.0748 or 7.48%). The top product already achieved composition of CO_2 less than 20% of total, however in order to meet the LNG specification requirement, second stage of separation is needed.

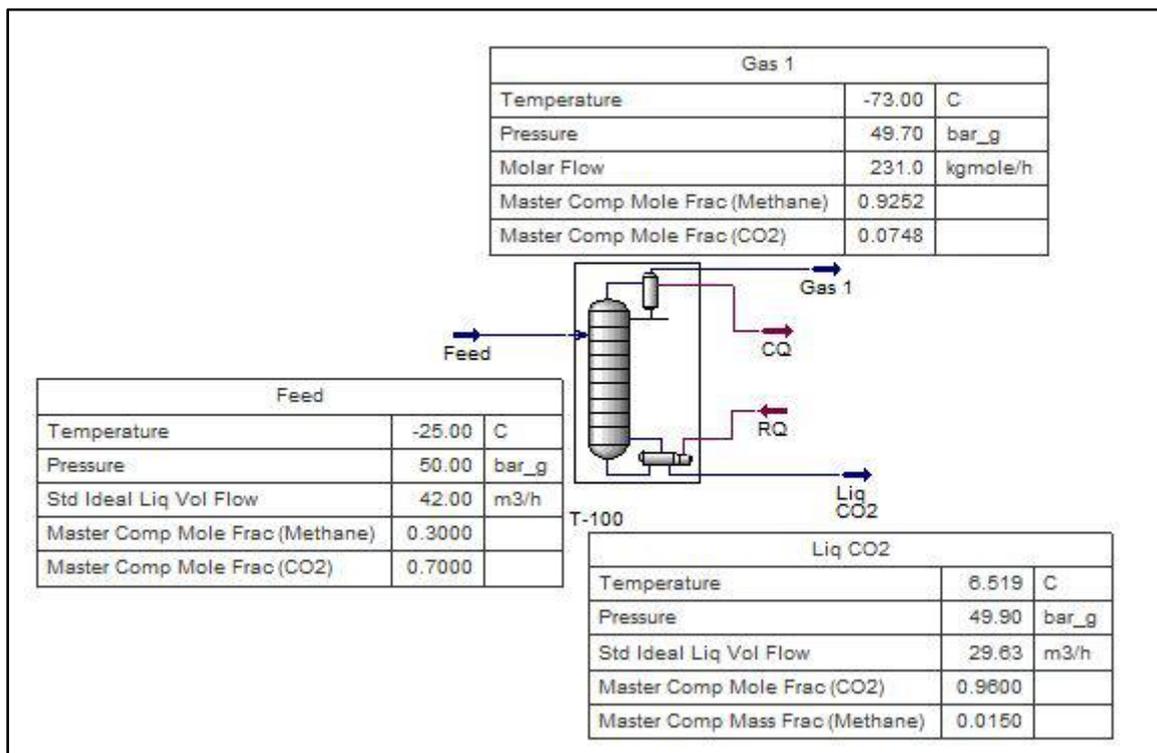


Figure 15: First stage separation in Distillation Column

As shown in Figure 16, the feed entered the vertical separator (V-100) is Gas 1, which is the top product from the separation in distillation column. In order to achieve the LNG specification requirement, the gas needs to undergo another separation process in the vertical separator. The vertical separator operating pressure is set at 50 barg. The top product is the Fuel Gas, which is ready to be exported because it has met the LNG specification requirement. The properties of the Fuel Gas; temperature of -138.6°C , flow rate of $0.7508\text{ m}^3/\text{h}$, mole fraction of methane (0.9848 or 98.48%) and mole fraction of CO_2 (0.0152 or 1.52%).

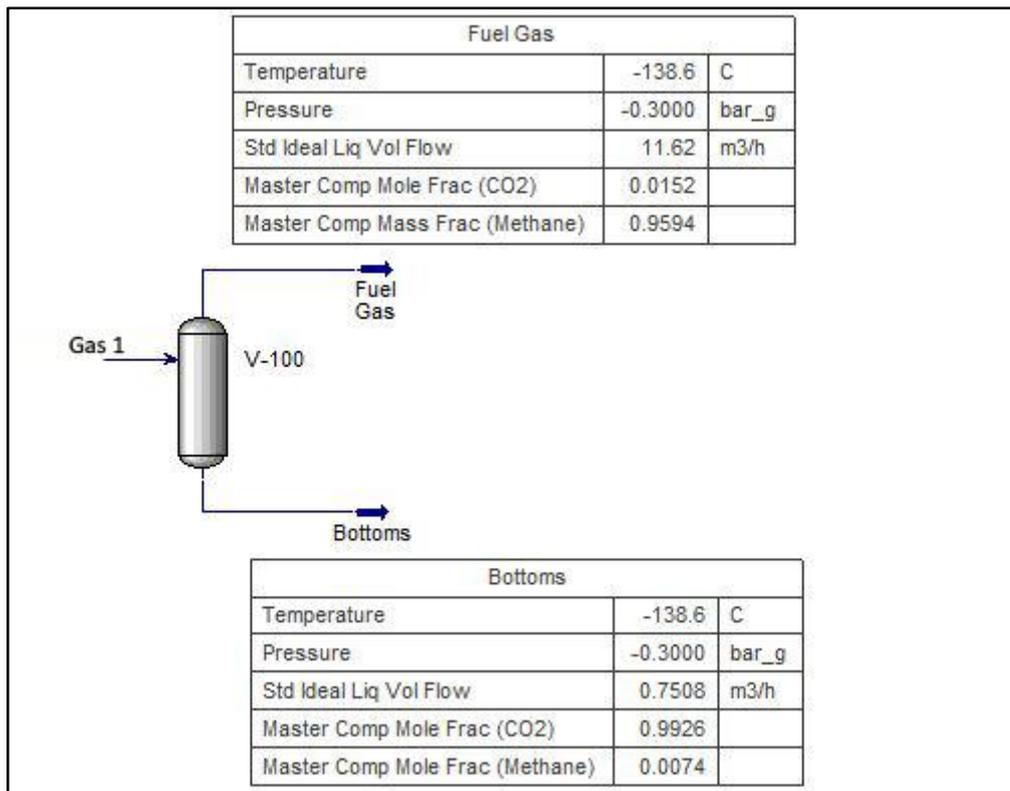


Figure 16: Second stage separation in Vertical Separator

4.4 Discussion of Results

The simulation objectives are to meet the LNG specifications of about 50 – 100 ppmv or 2-3% CO₂ concentration in the product stream, and then establish optimum conditions to reduce CO₂ emission and chemical loss. From Table 4, the composition of CO₂ of the feed gas used is 70 mol % which is above LNG CO₂ Specification of 2-3% as shown in Table 9 below.

Figure 11 shows the treatment of feed gas across the distillation column and the observation of % mole concentration of CO₂ and methane is shown in Figure 12. It was observed that as the temperature decreases, the % mole concentration of CO₂ in the product stream decreases.

The simulation of 70% of CO₂ feed concentration was done and the results are as shown above. However, the simulation of maximum feed concentration (80% CO₂ content) as given in the design condition was not successfully done due to simulation results that was not converging. The procedure for obtaining the relevant results for this project is quite complicated when programming in the ASPEN HYSYS since the author needs to key in a lot of input parameters and calculations. Some of the parameters are operating pressure, operating temperature, flowrate, component fraction, reflux rate, distillate rate, bottom production rate and etc. The author still needs to do more validation to see whether the simulation gives the correct result of every variable or not. In order to do that, a lot of experiments must be done in the future.

CHAPTER 5: CONCLUSION AND RECOMMENDATION

5.1 Conclusion

The separation of carbon dioxide from methane is very challenging in terms of process and technology. Considering the large difference between the physical properties of CO₂ and other impurities, the distillation process is conducted under high pressure. Consequently, the CO₂ purity in the product significantly increases to more than 98%. In this study, the optimal operating conditions for Cryogenic separation by distillation column are investigated. A detailed simulation study of the system was done.

The proposed system has superior performance in recovering CO₂ from mixed gases with high initial CO₂ concentration. The simulation of 70% CO₂ feed concentration at feed condition 50 barg and -25°C was done and at these conditions the percentage separation of the gas was found to be 98.48% of methane and 1.52% of CO₂ in the top product. The analysis proves that the proposed system can efficiently recover CO₂ from mixed gases, regardless of initial compositions as the CO₂ purity in the product could be as high as 99.9% under various circumstances. The present study showed results that are meeting the worldwide LNG specifications, however more research work needs to be done in order to assess the system and be able to separate higher concentration of CO₂ in the feed input.

5.2 Recommendations

Since distillation is such an important process used throughout multiple industries a wider analysis would be useful to determine the proper reflux ratio for a given quality of a product at a given flow rate. Future work on this project should do a research into how present distillation columns can be optimized. There are ongoing research endeavours to improve distillation. Future work should focus on how to make distillation columns more efficient in order to conserve the massive amounts of energy needed to perform this kind of separation. Work on methods for stricter controls on temperature should also be focused. This is helped by advances in thermal insulation as well as new more efficient packing for the columns. As technology improves so does the possibilities and outlook for distillation.

REFERENCES

1. H. Devold, *Oil and Gas Production Handbook : An Introduction to Oil and Gas Production, Transport, Refining and Petrochemical Industry*, 3rd. ed., Oslo : ABB Oil and Gas, 2013. pp. 1-2.
2. S. A. Ebenezer, “*Removal of Carbon Dioxide from Natural Gas for LNG Production*”, Institute of Petroleum Technology, Norwegian University of Science and Technology, Trondheim, Norway, 2005. pp. 1.
3. S. A. Ebenezer, “*Removal of Carbon Dioxide from Natural Gas for LNG Production*”, Institute of Petroleum Technology, Norwegian University of Science and Technology, Trondheim, Norway, 2005. pp. 2.
4. Burgers, W. F. J., Northrop, P. S., Kheshgi, H. S., & Valencia, J. A. (2011). Worldwide development potential for sour gas. *Energy Procedia*, 4(0), 2178-2184.
5. Darman, N. H., & Harun, A. R. B. (2006). Technical Challenges and Solutions on Natural Gas Development in Malaysia. Proceedings of the Petroleum Policy and Management (PPM) Project- 4th Workshop of the China-Sichuan Basin Case Study, 30 May - 3 June, 2006, China.
6. Abulhassan. A., Maqsood. K., Syahera, N., Shariff, A., Ganguly S.(2014). Minimization of Energy Consumption In Counter Current Switched Cryogenic Paced Beds during Purification of Natural Gas with High Carbon Dioxide Content, *Chemical Engineering & Technology*, 37(10), 1-12.
7. Working Group III of the Intergovernmental Panel on Climate Change (IPCC). *IPCC Special Report on Carbon Dioxide Capture and Storage*; Cambridge University Press: Cambridge, UK, 2005.
8. Working Group III of the Intergovernmental Panel on Climate Change (IPCC). *IPCC's Fourth Assessment Report (AR4): Mitigation of Climate Change*; Cambridge University Press: Cambridge, UK, 2007.
9. Ma'mun, S.; Svendsen, H.F.; Hoff, K.A.; Juliussen, O. Selection of new absorbents for carbon dioxide capture. *Energy Convers. Manag.* **2007**, 48, 251–258.
10. Saha, A.K.; Biswas, A.K.; Bandyopadhyay, S.S. Absorption of CO₂ in a sterically hindered amine: Modeling absorption in a mechanically agitated contactor. *Sep. Purif. Technol.* **1999**, 15, 101–112.

11. Mandal, B.P.; Guha, M.; Biswas, A.K.; Bandyopadhyay, S.S. Removal of carbon dioxide by absorption in mixed amines: Modeling of absorption in aqueous MDEA/MEA and AMP/MEA solutions. *Chem. Eng. Sci.* **2001**, *56*, 6217–6224.
12. CO₂ Capture Project. (2008). Three Basic Methods to Separate Gases. [Online]. Available : <http://www.co2captureproject.com/pubsearch.php>
13. Pierce, W.F.; Riemer, P.; William, G.O. International perspectives and the results of carbon dioxide capture disposal and utilisation studies. *Energy Convers. Manag.* **1995**, *36*, 813–818.
14. Wang, B.Q. *Process Mechanism and System Synthesis for CO₂ Capture in IGCC System*; Chinese Academy of Sciences: Beijing, China, 2004.
15. Wang, B.Q.; Jin, H.G.; Han, W. IGCC system with integration of CO₂ recovery and the cryogenic energy in air separation unit. In *Proceedings of ASME Turbo Expo*, Vienna, Austria, 14–17 June 2004; GT-2004-53723.
16. Wang, B.Q.; Jin, H.G. A novel IGCC system with H₂/O₂ cycle and CO₂ recovery by ASU cryogenic energy. In *Proceedings of the 7th International Conference on Greenhouse Gas Control Technologies*, Vancouver, BC, Canada, 5–9 September 2004.
17. Deng, S.; Jin, H.; Cai, R. Novel cogeneration power system with LNG cryogenic exergy utilization. *Energy* **2004**, *29*, 497–512.
18. Zhang, N.; Lior, N. A novel near-zero CO₂ emission thermal cycle with LNG cryogenic exergy utilization. *Energy* **2006**, *31*, 1666–1679.
19. Song, C.F.; Kitamura, Y.; Li, S.H. Evaluation of Stirling cooler system for cryogenic CO₂ capture. *Appl. Energy* **2012**, *98*, 491–501.
20. Kanniche, M.; Gros-Bonnivarda, R.; Jauda, P.; Valle-Marcosa, J.; Amann, J.M.; Boualloub, C. Pre-combustion, post-combustion and oxy-combustion in thermal power plant for CO₂ capture. *Appl. Therm. Eng.* **2010**, *30*, 53–62.
21. Zanganeh, K.E.; Shafeen, A. A novel process integration, optimization and design approach for large-scale implementation of oxy-fired coal power plants with CO₂ capture. *Greenh. Gas Control* **2007**, *1*, 47–54.
22. Zanganeh, K.E.; Shafeen, A.; Salvador, C. CO₂ capture and development of an advanced pilot-scale cryogenic separation and compression unit. *Energy Procedia* **2009**, *1*, 247–252.
23. Li, H.; Yan, J.; Yan, J.; Anheden, M. Impurity impacts on the purification process in oxy-fuel combustion based CO₂ capture and storage system. *Appl. Energy* **2009**, *86*, 220–213.

24. Besong, M.T.; Maroto-Valer, M.M.; Finn, A.J. Study of design parameters affecting the performance of CO₂ purification units in oxy-fuel combustion. *Int. J. Greenh. Gas Control* 2013, 12, 441–449.
25. Xu, G.; Li, L.; Yang, Y.P.; Tian, L.H.; Liu, T.; Zhang, K. A novel CO₂ cryogenic liquefaction and separation system. *Energy* 2012, 42, 522–529.
26. Union Gas. *Union Gas Material Safety Data Sheet (WHMIS)*. [Online]. Available : <https://www.uniongas.com/about-us/about-natural-gas/Chemical-Composition-of-Natural-Gas>
27. David, C., Kellogg, B., and Pankaj, S. (2003). LNG A Proven Stranded Gas Monetization Option, SPE Paper. (84252), pp 3.
28. Gas Separation Research Centre. *Cryomin Design Condition for Gas Separation Technology*. Universiti Teknologi PETRONAS: Perak, Malaysia, 2015.

APPENDIX A

Semester		FYP 1														FYP 2															
Week		1	2	3	4	5	6	7	8	9	10	11	12	13	14	1	2	3	4	5	6	7	8	9	10	11	12	13	14		
Literature Study / Data Gathering	Literature Review																														
	CO ₂ in Natural Gas																														
	Separation with Sorbents/Solvents																														
	Separation with Membranes																														
	Cryogenics Separation																														
	CO ₂ Purity Characteristics of the Cryogenic Separation Method																														
Project Execution	Project Planning																														
	Develop method and procedure																														
	Anticipate need for equipment & softwares																														
	Equipment & softwares research																														
	Test Project																														
	Find suitable case study																														
	Anticipate project time frame																														
	Conduct Project																														
	Modelling of Gas Separation System																														
	Simulation of the whole Gas Separation System																														
Results analysis and discussion																															

 key milestones