

DYNAMIC MODEL OF CO₂
REMOVAL USING ASPEN
HYSYS

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DYNAMIC MODEL OF CO₂ REMOVAL USING ASPEN HYSYS

MOHD FARIDHWAN BIN MOHAMAD ZULKAPLI

Report submitted in partial fulfilment of the requirements for the award of the degree
of Bachelor of Chemical Engineering

Faculty of Chemical & Natural Resources Engineering
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JULY 2013

SUPERVISOR'S DECLARATION

I hereby declare that I have checked this project and in my opinion, this project is adequate in terms of scope and quality for the award of the degree of Bachelor of Chemical Engineering.

Signature

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STUDENT'S DECLARATION

I hereby declare that the work in this project is my own except for quotations and summaries which have been duly acknowledged. The project has not been accepted for any degree and is not concurrently submitted for award of other degree.

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ABSTRAK

Objektif kajian ini adalah untuk merangsang proses penyingkiran CO₂ dengan menggunakan HYSYS Aspen. Metodologi kajian ini terbahagi kepada dua fasa. Fasa pertama adalah berkaitan dengan pembangunan model keadaan mantap dan fasa kedua yang berkaitan dengan simulasi dinamik. Dalam fasa pertama, reka bentuk data yang dikumpul daripada industri. Keputusan simulasi ini kemudiannya dibandingkan dengan data reka bentuk yang ada. Fasa kedua pada asasnya melibatkan peralatan saiz yang perlu dijalankan sebelum model dinamik maju. Pengesahan model dinamik dan data tumbuhan sebenar dipertimbangkan berdasarkan keadaan biasa. Simulasi tidak normal kemudian dijalankan dengan memperkenalkan gangguan dan atau kekurangan dalam proses. Sebagai kesimpulan, simulasi ini boleh digunakan sebagai latihan dan pembelajaran alat untuk jurutera dan pengendali, untuk memahami ciri-ciri dinamik proses penyingkiran CO₂ dan juga boleh menggunakan simulasi untuk prestasi yang lebih baik daripada proses penyingkiran CO₂.

ABSTRACT

The objective of this study is to simulate CO₂ removal process by using Aspen HYSYS. The methodology of this study is divided into two phases. The first phase relates to the model development of steady state and the second phase related to dynamic simulation. In the first phase, the design data are collected from an industry. The simulation results are then compared to the available design data. The second phase basically involves equipment sizing that should be conducted before the dynamic modeling is developed. Validation of dynamic model and real plant data is considered based on normal condition. The abnormal simulation is then conducted by introducing disturbances and or faults in the process. As the conclusion, this simulation can be used as training and learning tools for engineers and operator, to understand the dynamic characteristic of CO₂ removal process and also be able to use the simulation to improved performance of the CO₂ removal process.

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LIST OF SYMBOLS

%	percentage
kPa	kilopascal
psi	pounds per square inch pressure
°C	degree celcius
kg	kilogram
m ³	volume

LIST OF ABBREVIATIONS

CO	Carbon monoxide
CO ₂	Carbon dioxide
DEA	Diethanolamine
DGA	Diglycolamine
DIPA	Diisopropanolamine
CH ₄	Methane
H ₂	Hydrogen
H ₂ S	Hydrogen Sulphide
MDEA	Methylethanolamine
MEA	Monoethanol amine
N ₂	Nitrogen
H ₂ O	Water

CHAPTER 1

1.0 INTRODUCTION

1.1 Background of Proposed Study

The process of carbon dioxide removal starts from the absorber which the lean amine enter upper steam to the absorber whereas the natural gas enter from lower of the absorber. The reaction occurs and amine absorbs carbon dioxide from natural gas which is called rich amine. Rich amine then transfer to the stripper which released the carbon dioxide from amine. Then amine is feedback to absorber, and used all over again. Almost all industries that involve natural gas as a raw material must go through CO₂ removal process before proceeding to further process of natural gas. The amount of carbon dioxide contents in the natural gas can vary from 4% to 50% depending on the gas source. Before the transportation of natural gas, it must be pre-processed in order to meet the typical pipeline specification of 2–5% carbon dioxide. Aspen Hysys has been used since 2000 to simulate CO₂ removal from gas based power plants. Aspen Hysys is use in order to calculate permeate and retentate of the system with any number of modules, allowing complex process simulations. The programme has the possibility to use ASPEN HYSYS capabilities to calculate mass and energy balances and combine in the process model. The important process parameters are flow rates, temperatures,

compositions, pressure ratio (between the upstream pressure and downstream pressure over the membrane) and stage cut (ratio of permeate to feed flow rate).

1.2 Problem Statement

When an abnormal occurs and we want to find the source of the problem, to do trial and error to the real plant will cause harmful to the workers, effect the purity of the product and also lost time, energy and material.

1.3 Research Objective

1.3.1 To develop dynamic simulation using Aspen HYSYS.

1.3.2 To understand the characteristics of CO₂ removal.

1.3.3 To control the dynamic simulation of CO₂ removal.

1.3.4 To improve the performance of CO₂ removal.

1.4 Research Questions

1.4.1 How to develop dynamic simulation?

1.4.2 Can the performance of CO₂ removal be improved by using dynamic simulation?

1.5 Scope of Proposed Study

The scope of the study is the CO₂ removal by amine absorption from a gas based power plant and also simulation using Aspen HYSYS or Aspen Plus.

1.6 Expected Outcomes

The expected outcomes for this proposed study are to use simulation as training and learning tools for engineers and operator, to understand the dynamic characteristic of CO₂ removal process and also be able to use the simulation to improved performance of the CO₂ removal process.

1.7 Significance of Proposed Study

The training and learning simulation of CO₂ removal can be developed and to become the bench mark for the CO₂ removal industries.

1.8 Conclusion

Dynamic simulation uses software in order to make a process that can be used in a bigger plant and also can be used to improve the process without disturbing the real process. Software process simulation modeling is beginning to be used to address a variety of issues from the strategic management of software development, to supporting process improvements, to software project management training. As a conclusion, dynamic simulation gave a lot of benefits to human to make life easier.

CHAPTER 2

2.0 LITERATURE REVIEW

2.1 Introduction

The research is about dynamic simulation of carbon dioxide removal using Aspen HYSYS. Aspen HYSYS is a computer program that simulates chemical processes. Using a computer for a process simulation takes a fraction of the time it takes to do it by hand. The speed of a computer simulation allows the user to observe quickly the effect of changes in a simulation. For example, using HYSYS, it easily compares the amount of product produced using different ratios of starting materials. Doing this comparison with hand calculation would be a long and tedious task. The objective of this research is to develop the dynamic simulation of carbon dioxide removal by control, operational management, process improvement, technology adoption, understanding, training and learning.

2.2 Carbon Dioxide Removal Process

Gas sweetening process often referred to the removal of acid gases (CO₂, H₂S and other sulfur components) from natural gas. Carbon dioxide present in the natural gas

need to be removed in other to; increase the heating value of the gas, prevent corrosion of pipeline and gas process equipment and crystallization of CO₂ during cryogenic process (liquefaction process). The removal of carbon dioxide can be accomplished in a numbers of ways. Varieties of processes and (improvement of each) have been developed over the years to treat certain types of gas with the aim of optimizing capital cost and operating cost, meet Gas specifications and for environmental purpose (Tennyson et .al 1977). The major processes available can be grouped as follows (Maddox, 1982);

- Absorption Processes (Chemical and Physical absorption)
- Adsorption Process (Solid Surface)

The flow diagram of CO₂ removal simulation of amine process is shown in Figure 2.1. The natural gas is feed into the absorber than the CO₂ in the natural gas is absorbed by lean amine. Natural gas without CO₂ is then use for further process. The focusing process is CO₂ removal which happens in two processes which is absorber and stripper. In the absorber, the natural gas is feed from lower part of the absorber then the lean amine (amine without CO₂) is feed from upper side of the absorber. Then the absorption occurs between natural gas and amine. Amine absorbs CO₂ that carry by natural gas then amine leave the absorber carrying CO₂. The rich amine (amine with CO₂) then move to the stripper where the CO₂ is removes from amine. Then from rich amine, it becomes lean amine which is used over again for removing CO₂ in the absorber.

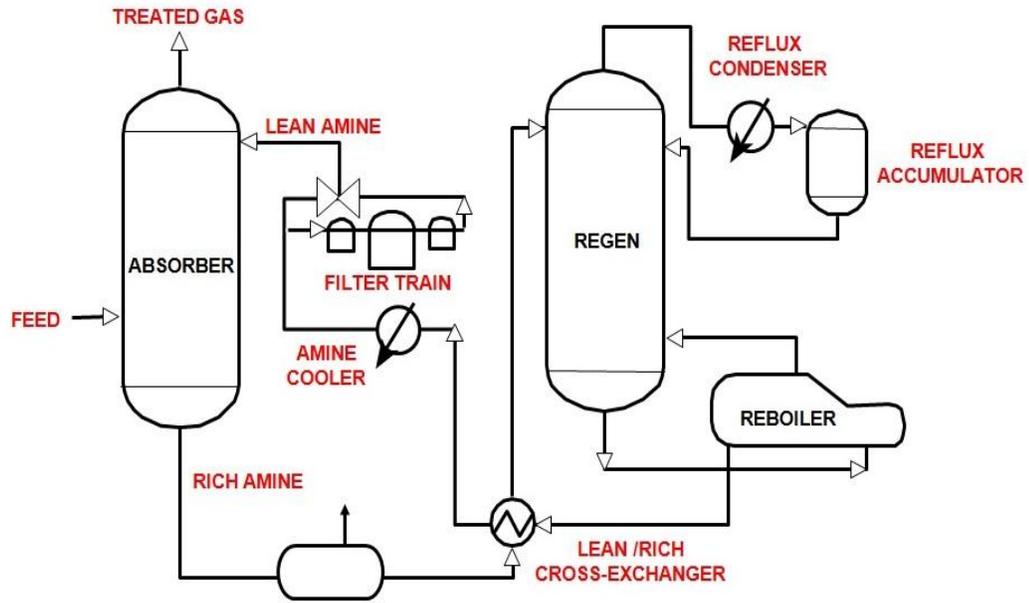


Figure 2.1: The flow diagram of CO₂ removal simulation of amine process

An absorption and desorption process for CO₂ removal with an aqueous MDEA solution had been simulated. The exhaust gas from the power plant model is used as the feed to this model. The absorption column is specified with 30 stages each with a Murphree efficiency of 0.25. (An estimated HETP (Height Equivalent to a Theoretical plate) of 4 meter, is about equivalent to 0.25 efficiency for each meter of packing.) Traditional concentrations, temperatures and pressures are used in the base case simulation. The thermodynamics for this mixture is described by an Amines Property Package available in Aspen HYSYS. The Kent Eisenberg [10] model is selected in the Amines Property Package. Specifications for the calculation are listed in table 2. The Aspen HYSYS CO₂ removal model is presented in figure 5. Different versions of this model have been developed in several student projects. The version in figure 5 is based on a Master Project work by Trine Amundsen. (Amundsen, T., 2007).

Table 1: Data from industry

Inlet gas temperature	46°C
Inlet gas pressure	674.7 kPa
Inlet gas flow	58934 Kg/hr
CO ₂ in inlet gas	0.10 mole %
Water in inlet gas	0.015 mole %
Lean amine temperature	60°C
Lean amine pressure	655.1 kPa
Lean amine rate	5088.39 kgmole/hr
MDEA content in lean amine	0.96 mole %
CO ₂ in lean amine	0.036 mole %
Number of stages in absorber	30

2.2.1 Physical Absorption Processes

Physical solvent processes use organic solvents to physically absorb acid gas components rather than react chemically. Physical absorption processes of removing CO₂ are based on the solubility of CO₂ within the solvents. CO₂ solubility depends on the partial pressure and on the temperature of the feed gas. Higher CO₂ partial pressure and lower temperature favors the solubility of CO₂ in the solvents as absorbent, at these conditions complete removal of acid gas from natural gas is possible. Regeneration of the spent solvent can be achieved by flashing to lower pressure or by stripping with vapor or inert gas, while some is regenerated by flashing only and require no heat (Dimethyl ether of Polyethylene Glycol).

Selection of physical processes for the removal of CO₂ from natural gas is favored on the following conditions;

- i. The partial pressure of the CO₂ in the feed should be 50 psi or higher
- ii. The concentration of heavy hydrocarbon in the feed should be low.
- iii. Only bulk removal of acid gas is required.
- iv. Selective removal of CO₂ is required.

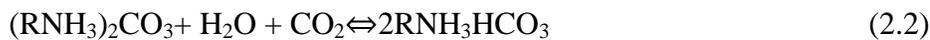
2.2.2 Chemical Absorption Process

Chemical absorption processes are based on the exothermic reaction of the solvent to remove the CO₂ that present in the gas stream. In this case, reactive material (solvent) remove CO₂ in the contactor at high pressure and preferably at low temperature and most chemical reaction are reversible. The reaction is then reversed by endothermic reaction using the stripping process at high temperature and low pressure. Chemical absorption processes are particularly applicable where acid gas (CO₂) partial pressure are low and for low level of acid gas requirement in the residue gas. The solvent more suitable for feed sour gas rich in heavy hydrocarbon because of the water content of the solution minimize the heavy hydrocarbon absorption. Most of chemical solvent processes use either an amine or carbonate solution.

2.3 Amine Base Process Facilities

The alkanolamines are generally accepted and widely used of the various available solvents for removal of CO₂ from natural gas stream (Bottom, 1930). Monoethanolamine (MDEA) and Diethanolamone (DEA) have made the solvent achieved a pinnacle position in the gas processing industry because of their reactivity and availability at low cost especially.

Formation of carbonate bicarbonate:



Formation of carbamate:



The reactions above shown the reaction proceed to the right at low temperature and to the left at a higher temperature, thus making CO₂ to be absorbed at ambient temperature. The reaction is reversed that is backward reaction is favored at elevated temperature (as obtained in the stripper column) where the carbonate salt formed is decomposed to release the acid gas absorbed, therefore stringent control of stripper column temperature should be adopted to reduce the release of carbonate salt. Reaction (2.1) and (2.2) are slow reaction because carbon dioxide must form carbonic acid with water (slow reaction) before reacting with amine. Elimination of selectivity of hydrogen sulfide is impossible because of reaction (2.3) which predominate when MEA is involved is relatively fast. Methyldiethanolamine (MDEA) and diethanolamine (DEA) are today the most tertiary amines for acid gas removal (Rejoy et.al., 1997).

Diglycoamine, diisopropanolamine and methyldiethanolamine are other amine solutions that can be used for this purpose.

Monoethanolamine (MEA); the concentration of MEA in solution is usually about 10-15% by weight. MEA is very reactive and can absorb CO_2 and H_2S simultaneously. MEA however reacts with COS, CS_2 and mercaptans. Its relatively high vapour pressure causes greater losses compared with other amines. For this reason it is used for intensive purification, with fairly low H_2S concentrations for a gas containing no COS or CS_2 .

Diethanolamine (DEA) helps to overcome the limitation of MEA, and can be used in the presence of COS and CS_2 . The application of DEA to natural gas processing was described by Berthier in 1959 (Kohl and Riesenfeld, 1985). Operating with solutions containing 25-30% by weight of DEA can be used to process natural gas with even high acid gas contents.

Diglycolamine (DGA) exhibits similar properties with monoethanolamine, but is less volatile, and therefore can be used in much higher concentration (40 – 60%). This helps to reduce the circulation rate, thus increasing the economics of the process.

Diisopropanolamine (DIPA) is used, in relatively high concentration from (30 – 40%) by the “Adip Process (Shell International Petroleum Company) (Klein, 1970). This solution is mostly used in processing of refinery gas or liquid with high COS.

Methylethanolamine (MDEA) allows the selective absorption of H_2S in the presence of CO_2 , but can be used effectively to remove CO_2 from natural gas in the presence of additives (Meisner and Wager, 1983). The reaction between CO_2 and MDEA solution is presented as follows;



The normal range of acid gas pickup, mol/ mol of amine (MDEA) is from 0.2 – 0.55(Perry, 1974).

Amine solutions are basic and hence non-corrosive but they are sometime use as corrosion inhibitors. Significant corrosion may occur at points where the concentration and temperature of acid gas is high in the presence of acid gases. The application of primary solution requires the use of corrosion inhibitors and the unit may be made of special steels because primary amines are the most corrosive (DuPart et al., 1993). Foaming is a frequent problem in these installations due the following;

- Suspended solids
- Condensed hydrocarbon
- Amine-degradation products.
- Foreign matter from corrosion inhibitors.

The foaming tendency in these installations can be prevented by good design and operation; also anti-foaming agents can be used (Kohl and Riesenfeld, 1985). Filtration of the solvent recycled to the absorber step is essentially important. The recommended filter that will retain particle sizes is larger than 10 μm (Pauley et al., 1989). Degradation of amine solvents occur when get in contact with the air or oxygen, and the oxidation products often cause corrosion. Oxidation can be reduced by placing the amine solutions under an inert gas blanket in the storage tanks.

2.4 Absorption and Reaction Mechanisms

The details of the mechanisms of CO₂ absorption into an amine solution in an absorption column are complicated. There are a lot of references about the chemistry involved in the process, and many references and models comprising mass transfer mechanisms and chemical reaction kinetics. The first step is CO₂ has to be transported from the gas to the liquid surface, and then it is absorbed in the liquid solution. The gas liquid interface area a (in m²/m³) and liquid holdup h (in m³/m³) are main parameters in describing such mechanisms. The CO₂ may react chemically with other components in the liquid.

The following reactions are assumed to take place when CO₂ reacts in a primary amine like MEA (monoethylamine) in an aqueous solution. In the case of MEA (NH₂C₂H₂OH), R is C₂H₂OH.



According to equation (2.5) and (2.6), two moles of MEA are necessary to absorb one mole of CO₂. A simple overall description of the combined absorption and reaction process is simply



The CO₂ is not 100 % removed from the gas. The percentage of CO₂ removal is limited both by low absorption and reaction rates and also by the equilibrium conditions. If the kinetics in the reactions should be calculated, more details about the intermediate reactions in equation (2.5) and (2.6) should be included. This is done in the MEA property insert model in Aspen Plus. The simulation program Aspen HYSYS is mainly

based on equilibrium calculations. In that case, equation (2.7) is sufficient to calculate the absorption process. (Lars Erik, 2007).

2.5 Simulation Using Aspen HYSYS

The commercial process simulation tools such as ProVision, ProMax or Aspen Plus can also be used to simulate the process as Aspen HYSYS. Aspen Plus has the possibility to calculate rate expressions on an ideal mixing stage (simulating a column plate). This has the advantage of taking into account the reaction rates for different reactions simultaneously. It is possible to include rate expressions of absorption (transport of CO₂ from the gas to the liquid phase) in such a model but it is difficult to be done. It is also a question whether this kind of a mixing stage model is a good model for continuous countercurrent operation as in structured packing. On the other hand, the presented Aspen HYSYS model is based on a specified Murphree efficiency for each stage (or height of packing). It is possible to make this efficiency a function of rate expressions for the absorption rate and the reaction rates. It is of course possible to simulate CO₂ removal processes without using commercial process simulation programs. It is however necessary to include at least one reliable and robust equilibrium calculation model and one robust column model. It is difficult to compete with the commercial process simulation programs in these two matters. The commercial programs also normally have very good input and output facilities. A problem with the commercial process simulation programs, at least from an academic point of view, is that some of the models of interest are not documented accurately. (Lars Erik, 2007).

A simulation model is a computerized model which possesses the characteristics described above and that represents some dynamic system or phenomenon. One of the main motivations for developing a simulation model or using any other modeling method is that it is an inexpensive way to gain important insights when the costs, risks or logistics of manipulating the real system of interest are prohibitive. Simulations are generally employed when the complexity of the system being modeled is beyond what static models or other techniques can usefully represent.

Complexity is often encountered in real systems and can take any of the following forms that are system uncertainty and stochasticity, dynamic behavior, feedback mechanisms. System uncertainty and stochasticity is the risk or uncertainty of the system is an essential feature to consider. Bounds on this uncertainty and the implications of potential outcomes must be understood and evaluated. Analytical models have constraints on the number and kind of random variables that can be included in various types of models. Simulation provides a flexible and useful mechanism for capturing uncertainty related to complex systems without these restrictive constraints. Dynamic behavior is a system behavior can change over time. For example, key variables such as productivity and defect detection rates can change over time. A dynamic model is necessary when accounting for or controlling these changes is important. However, analytic techniques such as dynamic programming can become intractable when the system being modeled becomes overly complex. Dynamic simulation models are very flexible and support modeling of a wide variety of system structures and dynamic interactions. Feedback mechanisms is a behavior and decisions made at one point in the process impact others in complex or indirect ways and must be accounted for. For example, in a software development process the decision to hire or

not to hire a new employee has multiple impacts and implications over the entire course of the project. The decision to inspect requirements or not also has many implications. For complex feedback or feed forward systems, analytic models may not be useful or even possible. Simulation enables a more usable alternative. (Marc I. Kellner, 1998).

2.6 Process Description

The general process flow diagram of an amine CO₂ removal process is shown in figure 16. The natural gas enters the bottom of the absorber in countercurrent contact with aqueous lean amine solution. Sweet gas leaves the top of the absorber while lean amine that flow downward counter currently to the natural gas and absorbed the CO₂ constituent and become rich solution. The rich solvent from the bottom of the absorber then pass through amine-amine heat exchanger to the stripper where the acid gas absorbed is stripped off at a very high temperature and low pressure. The acid gas then leaves the top of the stripper column. The lean amine from the bottom of the reboiler attached to the stripper flow through amine-amine heat exchanger and through a water air cooler before being introduced back to the top of the absorber.

The amine-amine heat exchanger serves as a heat conservation device.. The reminder of the rich solution flows downward through the stripper in countercurrent contact with vapour generated in the reboiler; which strips the acid gas from the rich solution. The stripper overhead products (acid gas and steam) pass through a condenser where the steam is condensed and cooled and returned to the top of the stripper as a reflux, while the acid gas is separated in a separator and sent to the flare or compressed for sequestration process.

2.7 Conclusion

The conclusion for this literature review, the dynamic simulation has become increasingly important as processes become more complex and are designed and operated closer to constraints. The use of intermediate buffer tanks has been greatly reduced because of environmental and safety concerns. Increasing yields and suppressing the formation of undesirable and environmentally unfriendly by-products are often achieved by using complex flowsheets with many recycle streams. Increasing energy costs keep pushing design engineers towards more heat integration. All of these trends make dynamic control more difficult and dynamic simulation more important.

CHAPTER 3

METHODOLOGY

3.1 Introduction

In this section, the details explanation about the process flow and the manual usage of Aspen HYSYS simulation is important. The data from industry is needed in order to run this simulation. In this chapter will explain about the equipment used in this simulation and also the procedure of CO₂ removal process in simulation. The process of making this study is shown in Figure 3.1 below.

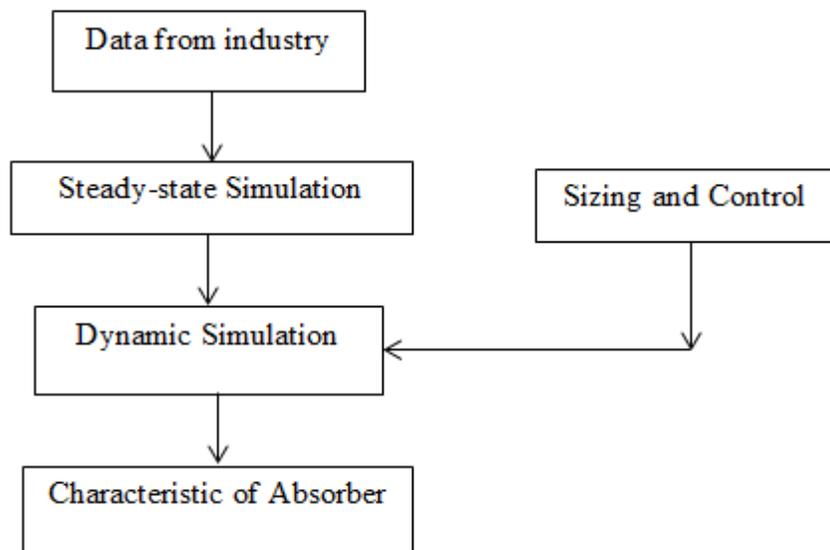


Figure 3.1 Process flow

3.2 Description of Process Equipment

Most often, amine unit operating problems can be traced to contaminants brought in with the gas from the pipeline. Pipeline contaminants can be in the form of “down-hole” corrosion inhibitors or other “treating” chemicals, liquid slugs caused by pipeline volume surges or line pigging, well “workover” fluids sent to the pipeline, and compressor lubricating oils. These contaminants are prevented from getting into the units by slug catcher. For the CO₂ removal units the following is a brief description of the major equipment necessary for successful simulation of amine unit and to operate environmental acceptable units. Here fictitious units such as mixer will not be discussed.

- a) MDEA ABSORBER; The absorber allows counter-current flow of lean amine from the top and sour gas from the bottom. Here the amine solvent absorbed CO₂ and rich amine is flow to the bottom while the sweet gas is collected at the top for further processing.
- b) AMINE-AMINE HEAT EXCHANGER; The rich/lean exchanger is a heat conservation device where hot lean solvent preheats cooler rich solvent. In this project Shell-and-tube TEMA type E exchanger is used in the simulation. The shell and tube side pressure drop is set to 542 kpa and heat loss/leak is assumed zero. The heat exchanger helps to raise the rich amine solvent temperature before entering the stripper. Thus reduce re-boiler work load.
- c) AMINE DISTILLATION COLUMN; Depending upon the solvent type, this is normally a 20-tray or equivalent packed tower. Here 30- trays were sufficient to strip the CO₂ from the rich solvent. Physical solvents can require fewer trays. Trays diameter is about 4m with 0.5 spacing. Liquid and jet floods in the 65-75%

range with a 75% foam factor. It is assumed that the trays in the upper third, be stainless steel due to the corrosivity of the environment.

- d) AMINE COOLER, REFLUX CONDENSER; Air-cooled, forced draft with automatic louvers for temperature control. Cold climate service may require airrecirculation and/or preheat media on fans/coils. Condenser tubes should be made of stainless steel, as this is a wet, acid gas environment and sloped to the outlet side.
- e) REFLUX ACCUMULATOR: This vessel separates the reflux water and watersaturated acid gases. The water is pumped back to the still and the acid gases are directed to vent, incinerator, or sulfur recovery unit. A reflux accumulator with a 4" to 8" thick mist pad is used.
- f) SOLVENT REBOILER: This is either a direct-fired fire tube type or cabin heater, or indirect hot oil or steam heated unit. Typically heat flux rate should be kept in the 7500 to 10,000 Btu/hr/ft² range to assure no surface burning of the solvent. This exchanger provides the steam necessary to heat and strip the solvent back to a "lean" condition.
- g) COOLER; The lean amine solvent from the re-boiler through amine-amine heat exchanger is further cool here before entering the absorber again, since absorbers operate more efficiently at relatively low temperature.
- h) PUMPS: The reflux and booster centrifugal pump is installed to maintain the recycle lean solvent at the desired operating pressure of the absorber. The main circulation pump choice depends upon contactor operating pressure and solvent flow rates. Centrifugal pump considered in this project is set to 75% adiabatic efficiency for low head cases and large volume, high head cases which is

specifically design for amine service and have non-lubricated packing/system seal with ceramic or hard coated fluid parts.

3.3 HYSYS Simulation Procedures

A base case was established using the following steps; the first step is open selection component window by selecting view in the component-list show in Figure 3.2. Figure 3.2 shows dialog window is use for components selection

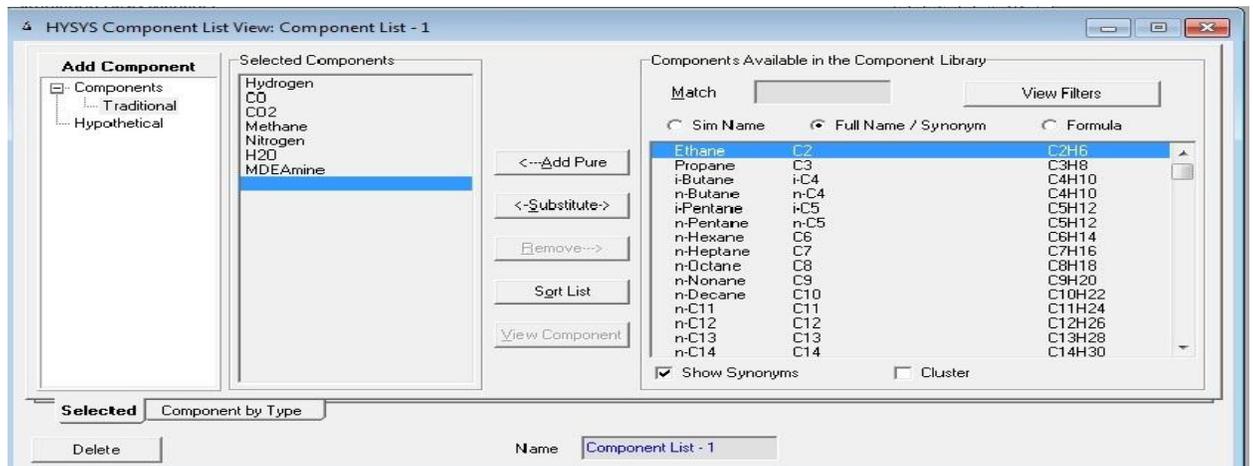


Figure 3.2: Component selection windows.

Then select the appropriate fluid package; here amine fluid package and Kent-Eisernberg model is selected as in Figure 3.3 below;

The simulation of the process begins with the simulation of the feed natural gas stream by specifying the gas temperature, pressure and flow rate (Blue colour) and HYSYS calculate the remaining parameters (Black colour) as shown in figure 4 below;

Property	Value
Stream Name	natural gas
Vapour / Phase Fraction	1.0000
Temperature [C]	46.00
Pressure [kPa]	674.7
Molar Flow [kgmole/h]	5738
Mass Flow [kg/h]	5.893e+004
Std Ideal Liq Vol Flow [m3/h]	192.2
Molar Enthalpy [kJ/kgmole]	9529
Molar Entropy [kJ/kgmole-C]	169.6
Heat Flow [kJ/h]	5.468e+007
Liq Vol Flow @Std Cond [m3/h]	<empty>
Fluid Package	Basis-1
Utility Type	

Figure 3.5: Natural Gas specification windows

Other streams specifications made are; the regenerated feed out of the amine-amine heat exchanger temperature to control the exchanger. MDEA to Contactor temperature pressure and flow rate, make up water temperature and MDEA to recycle temperature. With these specifications made, HYSYS make use of its flexibility of calculating forward and backward to completely simulate the process. One of the rigorous tasks is the convergence of the absorber and the regenerator, to converge the absorber the absorber top and bottom temperature and pressure was specified and run, Figure 3.6.

While the regenerator is converged by specifying the condenser and re-boiler pressure, the reflux ratio and the vent rate, the column is then run, Figure 3.7.

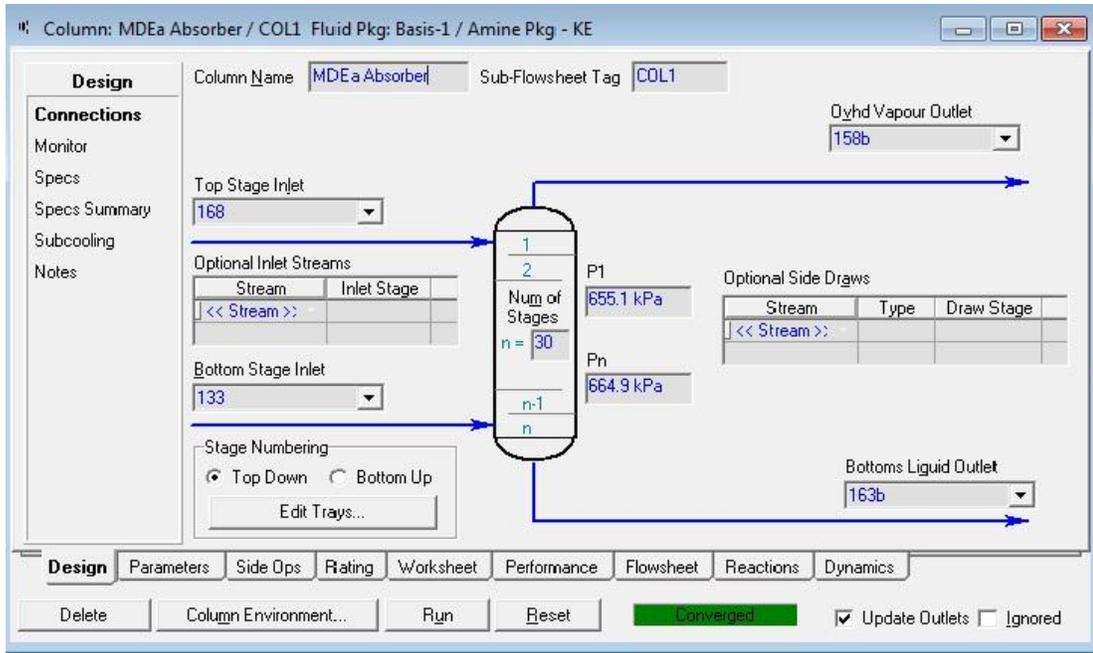


Figure 3.6: Converged window of the Absorber

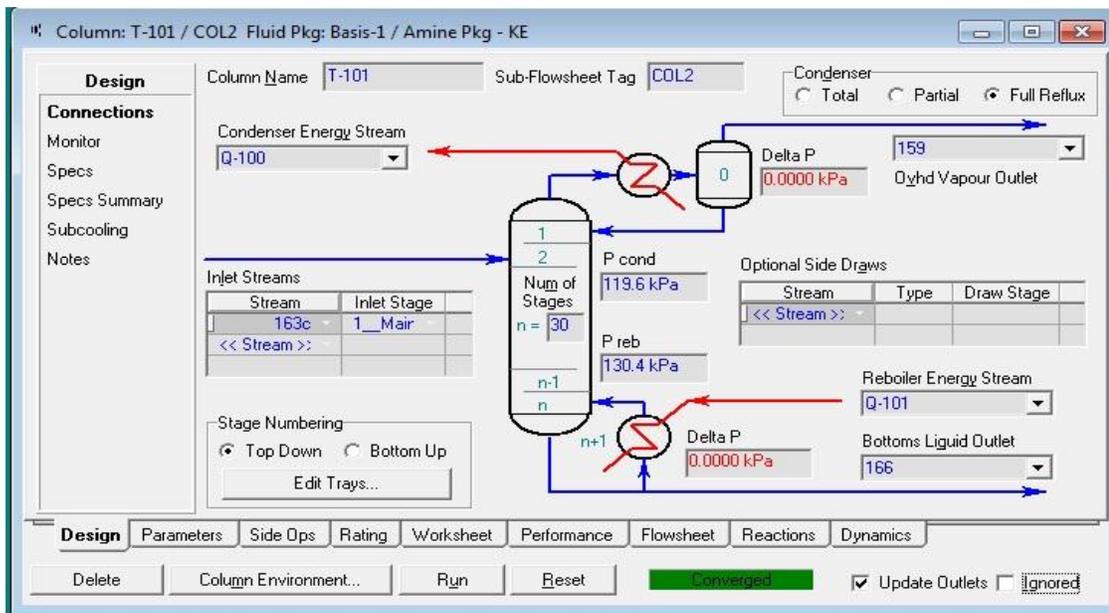


Figure 3.7: Converged windows for regenerator unit

With the convergence of the absorber and the regenerator units a complete amine simulation for the base case was established as shown in Figure 3.8. 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.

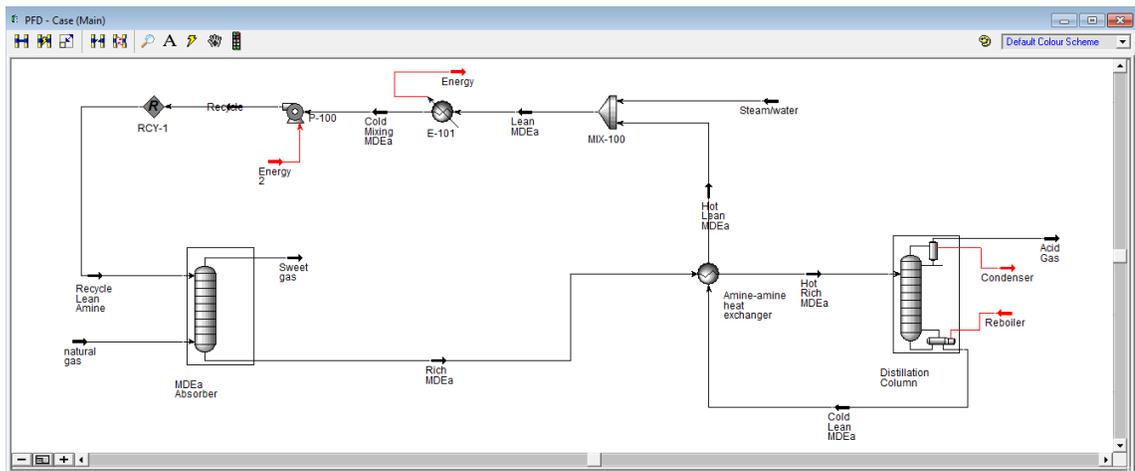


Figure 3.8: Complete Simulations Unit

3.4 Moving from Steady-State to Dynamic Simulations

The steady-state simulation does not need information that has no effect on steady-state results. These items include column diameters, sizes of all surge vessels, sizes of control valves, etc. However, the dynamic simulation does need this information because the dynamic response of a process unit depends on the size of the equipment. The capacitance of the system (its time constant) dictated by its size (volume or mass) relative to the flux (flowrate, heat-transfer rate, etc.). Therefore all equipment must be sized (at least approximately) before dynamic simulation can be performed.

The other important aspect of the flowsheet that must be specified in order to conduct a dynamic simulation of a process is the plumbing. This includes installing pumps, compressors and control valve.

3.4.1 Sizing Equipment

In order to conduct dynamic simulations, all equipment must be sized. This sizing does not have to include all the detailed mechanical design. At the conceptual design level, we only need to have approximate estimates of equipment volumes.

In this study, only absorber unit is considered in dynamic simulation. The process is arranged as shown in Figure 3.9 below.

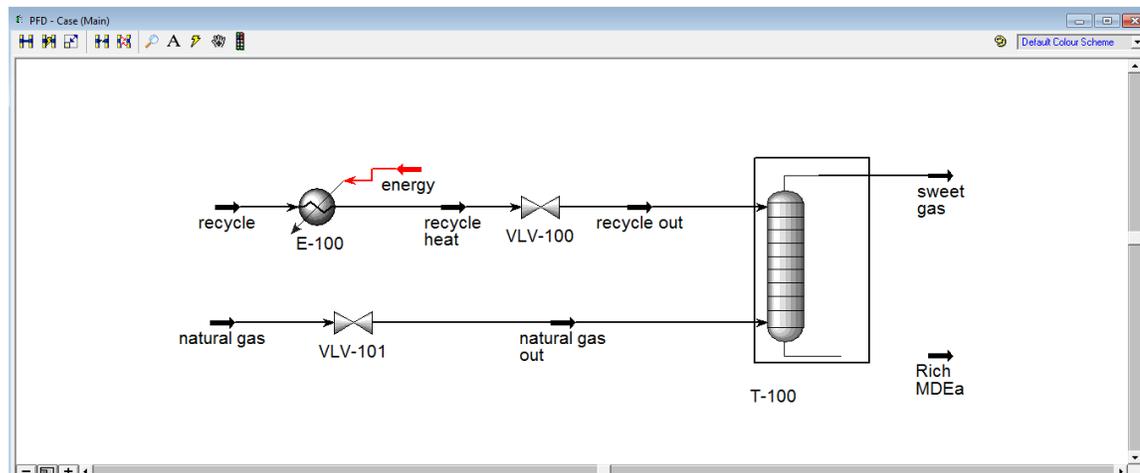


Figure 3.9: Absorber Flowsheet

Name	recycle amine	natural gas	sweet gas	rich amine
Vapour Fraction	0.0000	0.9997	1.0000	0.0000
Temperature [C]	40.00	46.00	60.61	64.42
Pressure [kPa]	700.0	700.0	655.1	674.6
Molar Flow [kgmole/h]	2.162e+004	8368	8170	2.182e+004
Mass Flow [kg/h]	5.928e+005	8.596e+004	7.444e+004	6.043e+005
Liquid Volume Flow [m3/h]	586.2	280.3	265.9	600.6
Heat Flow [kJ/h]	-5.097e+008	7.964e+007	8.142e+007	-4.691e+008
Name	v1out	heat out	v2out	*** New ***
Vapour Fraction	0.0000	0.0000	1.0000	
Temperature [C]	40.00	60.00	45.63	
Pressure [kPa]	655.1	655.1	674.6	
Molar Flow [kgmole/h]	2.162e+004	2.162e+004	8368	
Mass Flow [kg/h]	5.928e+005	5.928e+005	8.596e+004	
Liquid Volume Flow [m3/h]	586.2	586.2	280.3	
Heat Flow [kJ/h]	-5.097e+008	-4.673e+008	7.964e+007	

Figure 3.10: Workbook Stream Conditions

3.4.1.1 Absorber

Absorbers are tanks that have both liquid and vapor streams leaving the unit. The vapor velocity must be kept low enough so that liquid entrainment is small. The F-Factor can be used to calculate the minimum diameter of the vessel. Use a more conservative F-Factor (0.5 in English Engineering units) so effective absorber of the two phases is achieved.

$$F - Factor \equiv V_{max} \sqrt{\rho_v}$$

The liquid holdup must be checked if it is adequate. The normal heuristic is to provide at least five minutes of holdup. This means the volume of liquid in the tank

(normally with the interface at 50% of the tank height, assuming a vertical vessel) should be five times the volumetric flowrate of the liquid leaving the tank.

To illustrate the calculations, an absorber operating at 60°C and 655.1 kPa. The vapor leaving the tank is 4.807×10^4 kg/hr (1.06×10^5 lb/hr) with a vapor density of 2.047 kg/m³ (0.1278 lb/ft³). The liquid leaving the tank is 6.036×10^5 kg/hr (1.331×10^6 lb/hr) with a liquid density of 1036 kg/m³ (64.66 lb/ft³). The tank is a vertical cylindrical vessel with an aspect ratio (length-to-diameter ratio) of two.

First, calculate the required diameter based on the vapor velocity. The maximum vapor velocity, using a 0.5 F-Factor, is

$$V_{max} = \frac{F - Factor}{\sqrt{\rho_v}} = \frac{0.5}{\sqrt{0.1278}} = 1.39864 \text{ ft/sec}$$

$$\begin{aligned} \text{volumetric flowrate of vapor} &= 1.06 \times 10^5 \frac{\text{lb}}{\text{hr}} \times \left(\frac{1 \text{ ft}^3}{0.1278 \text{ lb}} \right) \times \left(\frac{1 \text{ hr}}{3600 \text{ sec}} \right) \\ &= 230.395 \frac{\text{ft}^3}{\text{sec}} \end{aligned}$$

Therefore, the cross-sectional area of the tank is

$$\text{Area} = \frac{230.395 \text{ ft}^3/\text{sec}}{1.39864 \text{ ft/sec}} = 164.992 \text{ ft}^2$$

Thus the tank diameter must be at least

$$D = \sqrt{\frac{4(164.992)}{\pi}} = 14.49 \text{ ft}$$

Then check the liquid holdup requirements. The volumetric flowrate of liquid is

$$\begin{aligned} \text{volumetric flowrate of liquid} &= 1.331 \times 10^6 \frac{\text{lb}}{\text{hr}} \times \frac{1 \text{ ft}^3}{64.66 \text{ lb}} \times \frac{1 \text{ hr}}{60 \text{ min}} \\ &= 343.08 \text{ ft}^3/\text{min} \end{aligned}$$

To have five minutes holdup of liquid with the tank half full, the volume of the tank should be

$$\text{volume of absorber} = 2 \times 5 \text{ min} \times 343.08 \text{ ft}^3/\text{min} = 3430.8 \text{ ft}^3$$

With the aspect ratio of two, the relationship between volume and diameter is

$$\text{Volume} = \frac{\pi}{4} D^2 L = \frac{\pi}{4} D^2 (2D) = \frac{\pi}{4} D^3$$

Therefore the diameter is

$$\text{Diameter, } D = \sqrt[3]{\frac{2(3430.8)}{\pi}} = 12.97 \text{ ft}$$

Since the larger diameter is calculated from F-Factor, the diameter of absorber was specify with 15 ft and length of 30 ft.

3.4.1.2 Control Valve Sizing

Once the locations of all control valves have been established, their sizes must be specified. This boils down of setting their percent opening and their pressure drop under design conditions.

The design can be for a small pressure drop over the valve or a large pressure drop over the valve. The former is favored by steady-state economics. The pump or

compressor head is lower, a smaller motor can be used and motor energy consumption is less. The higher the design pressure drop, the larger the achievable flowrate changes. This translates into a better dynamic control because larger changes in the flowrates of manipulated variables can be rejected disturbance more quickly.

A simple equation describing the flow through a control valve is

$$F = f_{(x)} C_V \sqrt{\Delta P_V}$$

where F= flowrate through the valve, $f_{(x)}$ = fraction of the valve opening, C_V = valve size coefficient and ΔP = valve pressure drop. The control valve (C_V) is sized at design conditions.

$$C_V = \frac{F}{f_{(x)} \sqrt{\Delta P_V}}$$

Then, find out how much the flow through this system can be increased by finding the maximum flowrate, F_{max} . the pressure drop is proportional to the square of the flowrate.

$$\Delta P_{@F} = \Delta P_{@F_{design}} \left(\frac{F}{F_{design}} \right)^2$$

So at the maximum flowrate the pressure drop will be

$$\Delta P_{@F_{max}} = \Delta P_{@F_{design}} \left(\frac{F_{max}}{F_{design}} \right)^2$$

The pressure drop over the control valve will be

$$\Delta P_{V @ F_{max}} = \left(\frac{F_{max}}{f_{(x)} C_V} \right)^2$$

Solving for the maximum flowrate. The larger the valve pressure drop selected, the better the control.

Double click the valve icon and go to Dynamic page tab Figure 3.11A and Figure 3.11B show this for two valve. Specify the percentage open (usually 50% unless higher flowrate are required), check the Check Valve button and click the Size Valve button. This will calculate the C_v size coefficient for the valve.

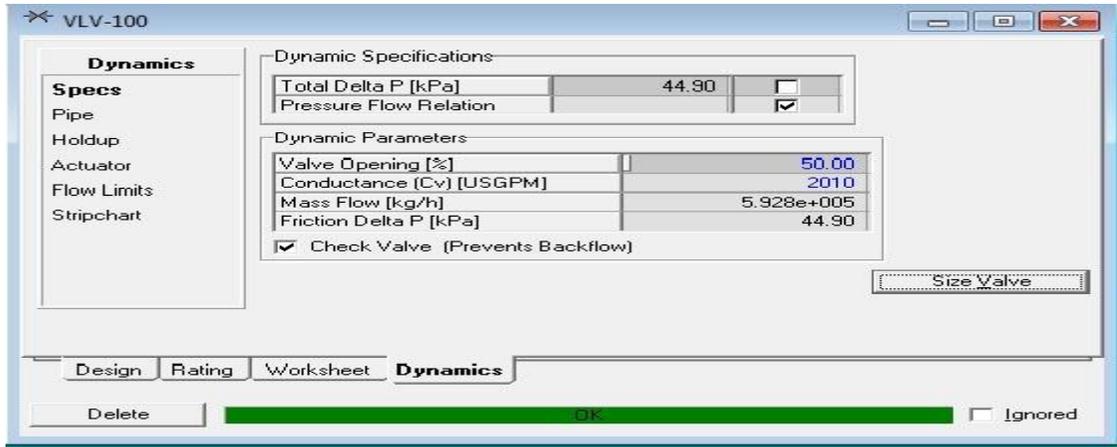


Figure 3.11A: Valve VLV-100

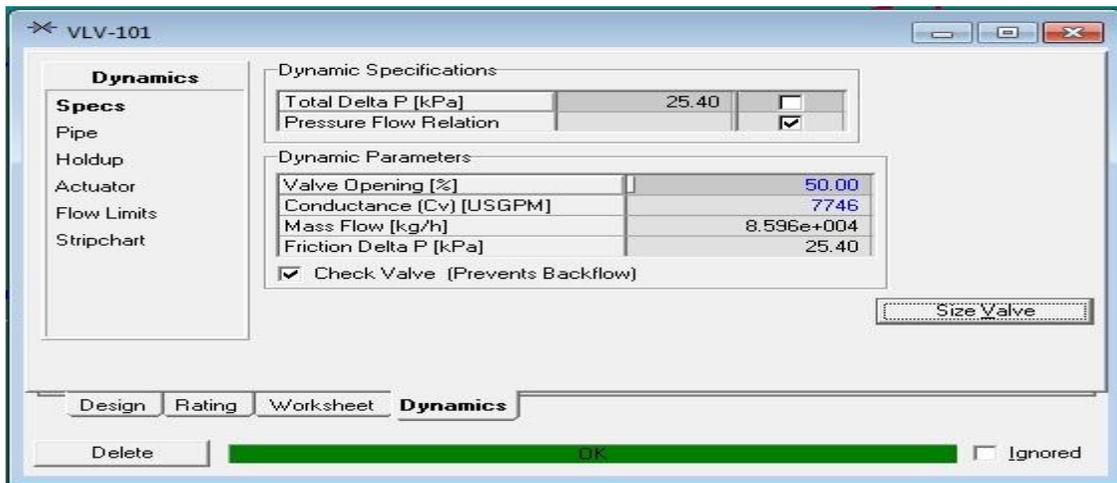


Figure 3.11B: Valve VLV-100

The dynamic specification for the heater must also be specified. Double click the heater icon and click the Dynamic page tab (Figure 3.11C). Click the Overall k buttons then Calculate k buttons.

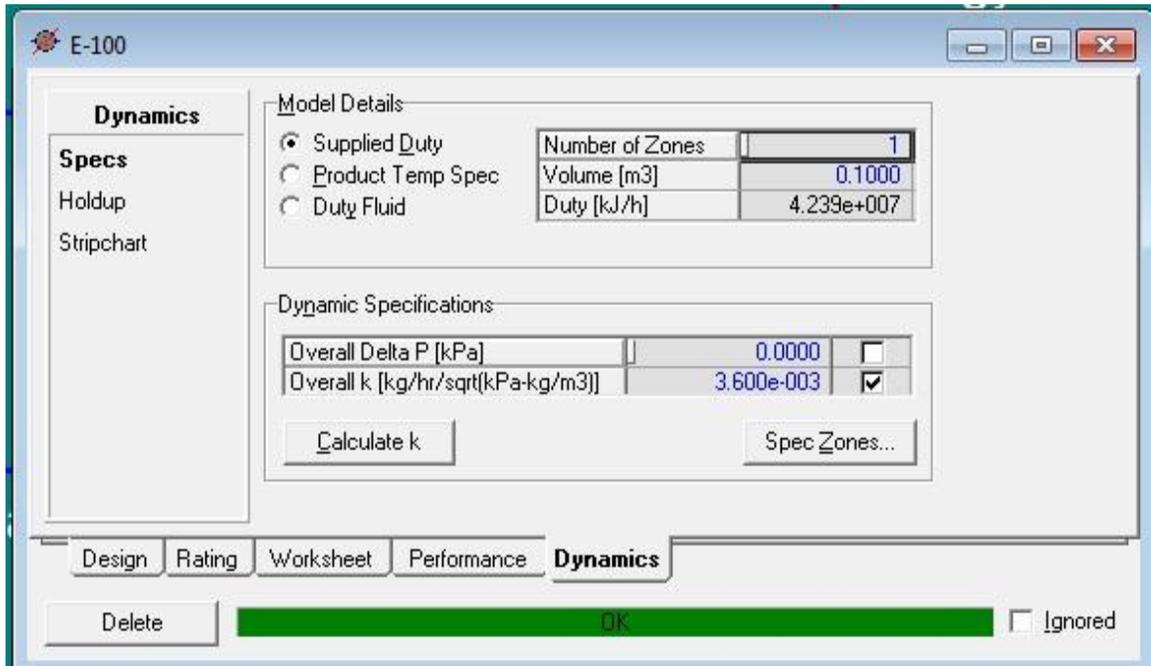


Figure 3.11C: Heater E-100

3.4.2 Switching to Dynamics

When the steady state is converged and the plumbing has been specified click the Dynamic buttons on top of tool bar (Figure 3.12). The dynamic assistant will suggest that some changes be made in some specifications so that the flow-driven simulation is correctly set-up, as shown in Figure 3.13.

The control structure chosen for this system is:

- I. Flow control the recycle amine with valve VLV-100
- II. Flow control the natural gas with valve VLV-101
- III. The temperature of feed to absorber with heater E-100

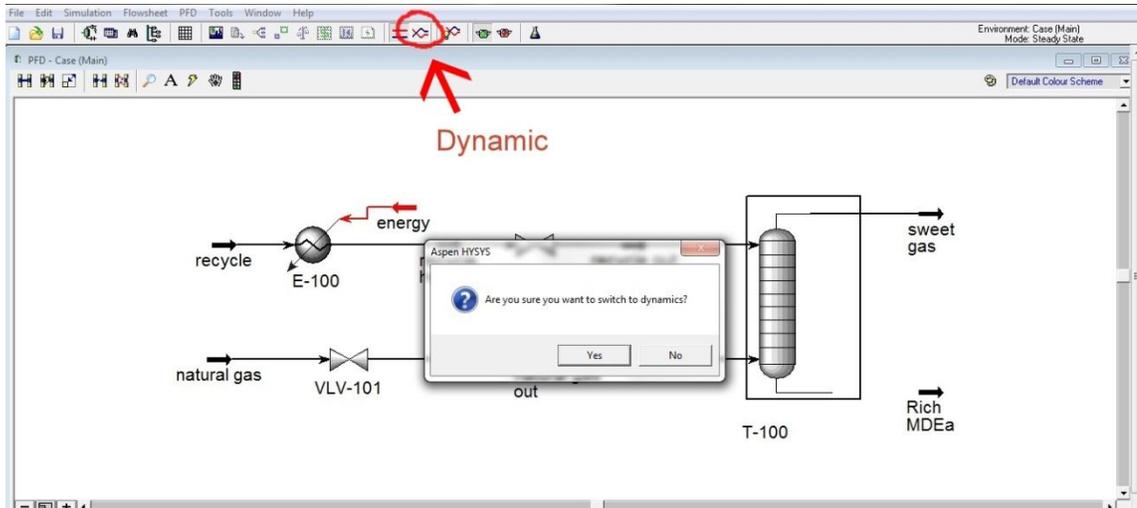


Figure 3.12: Dynamic Assistant Changes

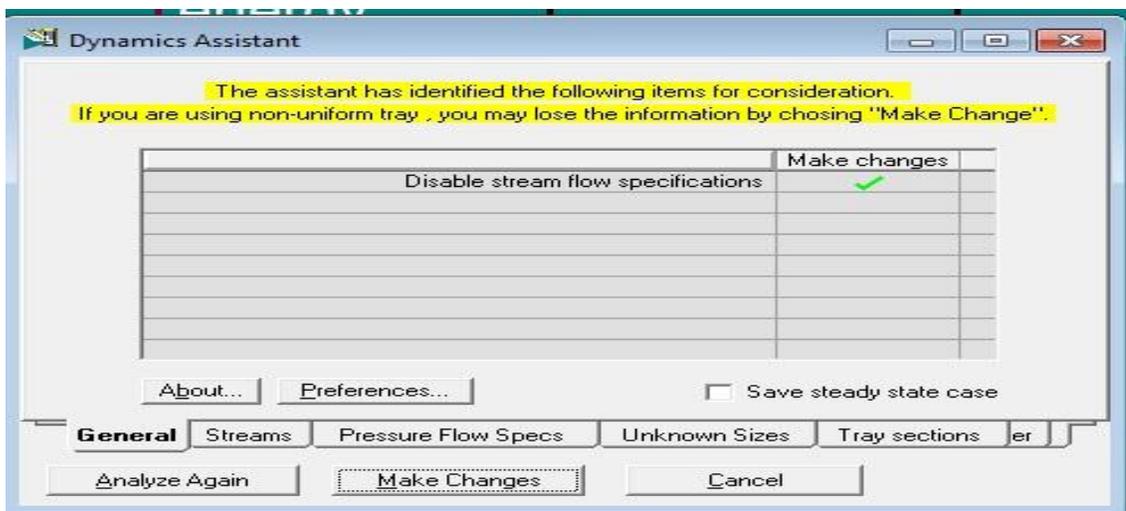


Figure 3.13: Dynamic Assistant Changes

3.4.2.1 Tuning Controllers

A typical plant has dozens of controllers, all of which must be specified (which algorithm to use: P, PI, PID, MPC, nonlinear, etc.) and tuned (selecting controller tuning parameters, for example gain, integral time, derivative time, etc.). The algorithm selection and tuning of some of these loops is trivial. For others this is not the case and these are the controllers that require a logical, effective controller-tuning procedure, which is also applied. In this simulation, considers only conventional linear PI controllers in a decentralized (single-input-single-output) environment. While there have been many industrial applications of model predictive control (MPC) and enumerable academic papers published in the area of MPC, the use of conventional PI controllers is still widespread. Many of the MPC proponents now take the position that MPC should be applied on top of basic regulatory PI control structure.

There is important consideration in simulation work concerning the use of derivative action. It is more conservative to only use PI controllers in the simulation. The simulation is an approximation of the real plant. If high performance controllers are required to get good dynamics from the simulation, the real plant may not work well. On the other hand, if a low-performance PI controller works well on the simulation but does not work as well in the plant, we still have the flexibility to go to PID control to improve things. The basic philosophy is to make conservative estimates and approximations in the model and simulation so that the real plant will operate well.

3.4.2.2 Flow Controllers

The tuning of flow controllers is usually a no-brainer. The majority of the flow control loops feature an orifice-plate sensor, a differential-pressure transmitter, a PI controller and a control valve. The dynamics of flow measurement are fast. The time constants for moving control valve are small (several seconds unless very large valves are involved). Therefore, the controller can be tuned with a small integral or reset time constant τ_1 . A value of $\tau_1=0.3$ minutes works in most flow controllers.

The value of controller gain should be kept modest because flow measurement signals are sometime noisy due to the turbulent flow through the orifice plate. A value of controller gain of $K_c=0.5$ is often used. Derivative action should not be used.

In a real plant application, filtering of the flow signal is also recommended because of the noise. In a simulation, noise is not a problem. However, the equation-based integrator in AspenDynamics appears sometimes to have stability problems in flow control loops unless a small amount of filtering is used.

3.4.3 Installing Controllers

The procedure for adding a controller is outlined below.

1. Click the Controller icon on the pallet and, with the right mouse button held down; drag it on the PFD. (see Figure 3.14).

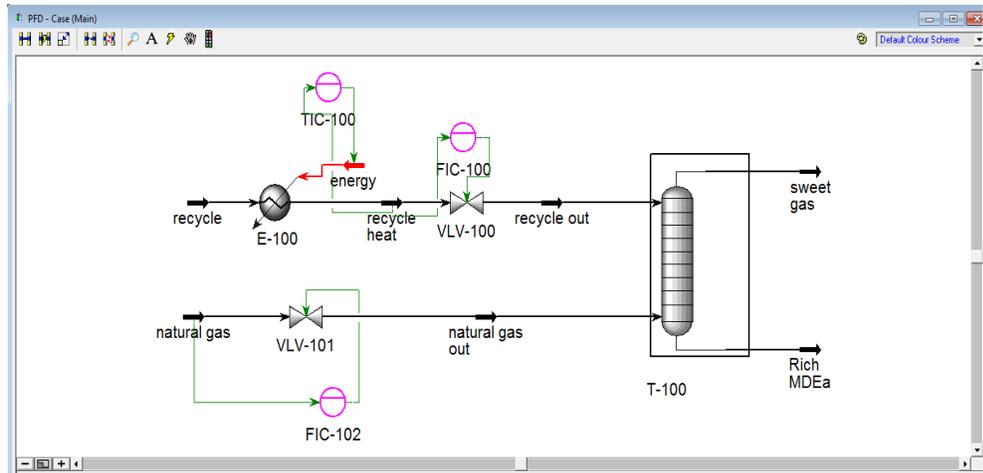


Figure 3.14: Absorber Flowsheet with Controller

2. Double clicking on the controller icon brings up the controller window. The first page tab is Connections, show in Figure 3.15.

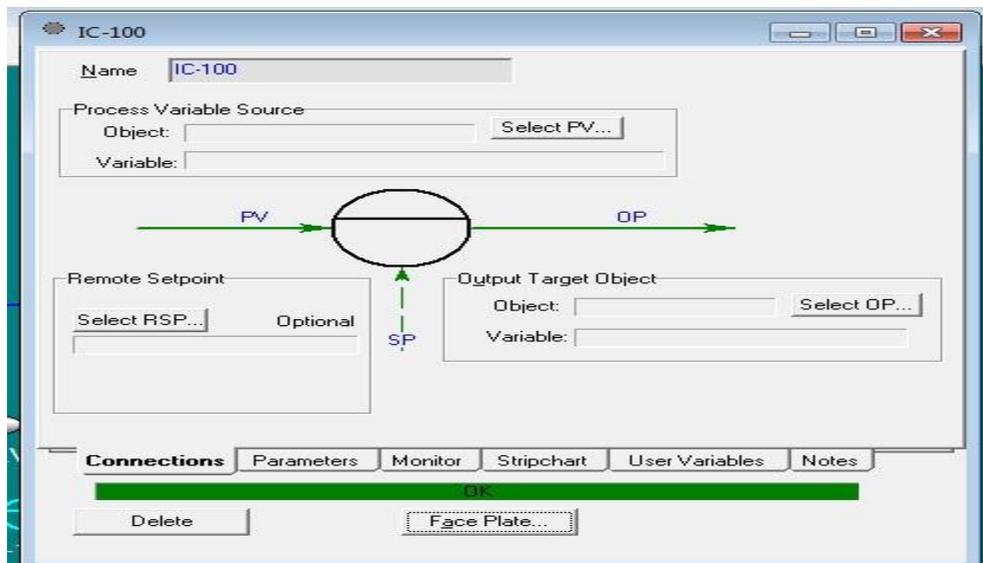


Figure 3.15: Controller Connections Page Tab

3. Click the Select PV button to specify the unit or stream and the variable to control (see Figure 3.16).

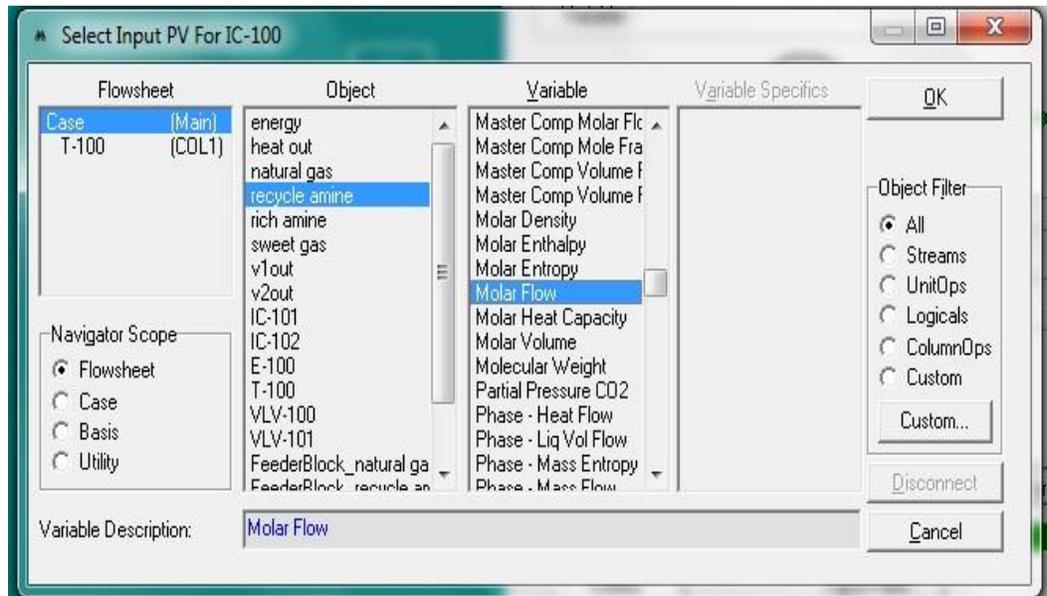


Figure 3.16: Selecting PV Source

4. Select the target of the OP signal (the place where the controller output is sent).
Figure 3.17 shows the OP signal goes to VLV-100. Figure shows the connections page view with both the PV and OP connections specified.

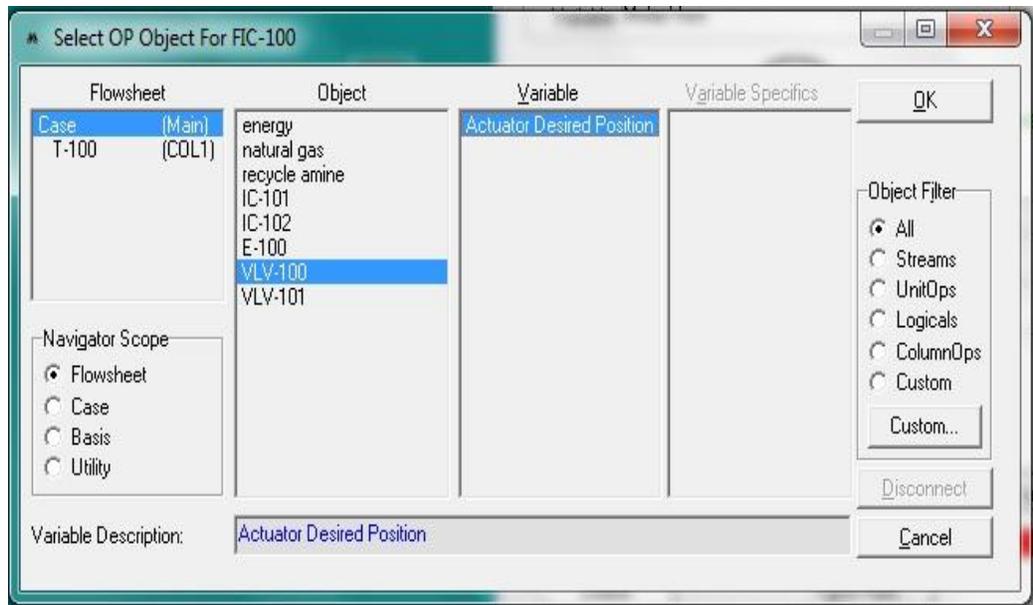


Figure 3.17: Selecting OP Target

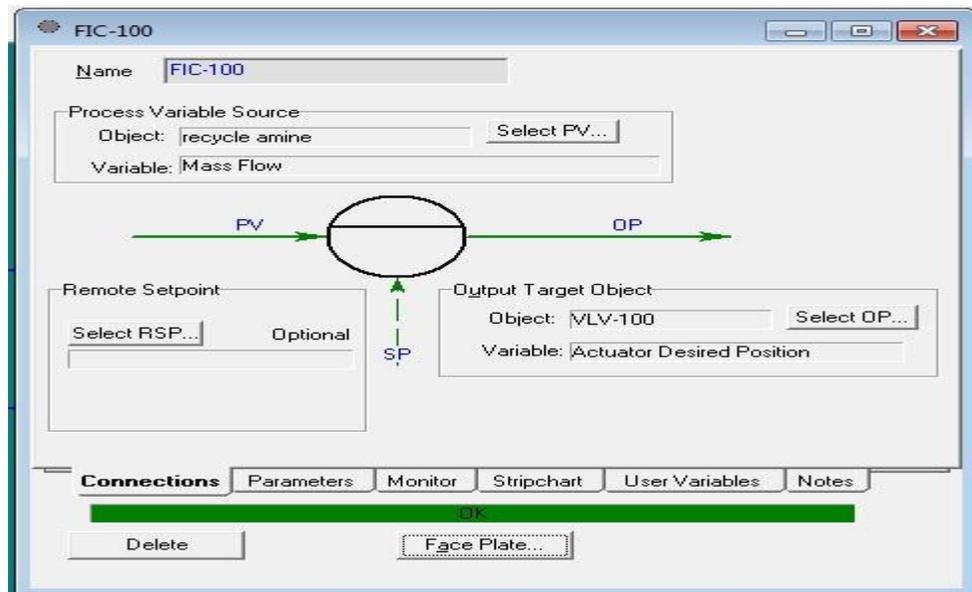


Figure 3.18: Connection Parameter Page Tab with PV and OP Selected

5. The second page tab is Parameters and is shown in Figure.
6. Specify the range of the sensor/transmitter.

7. Check the values of the process variable, the setpoint and the percent valve opening.

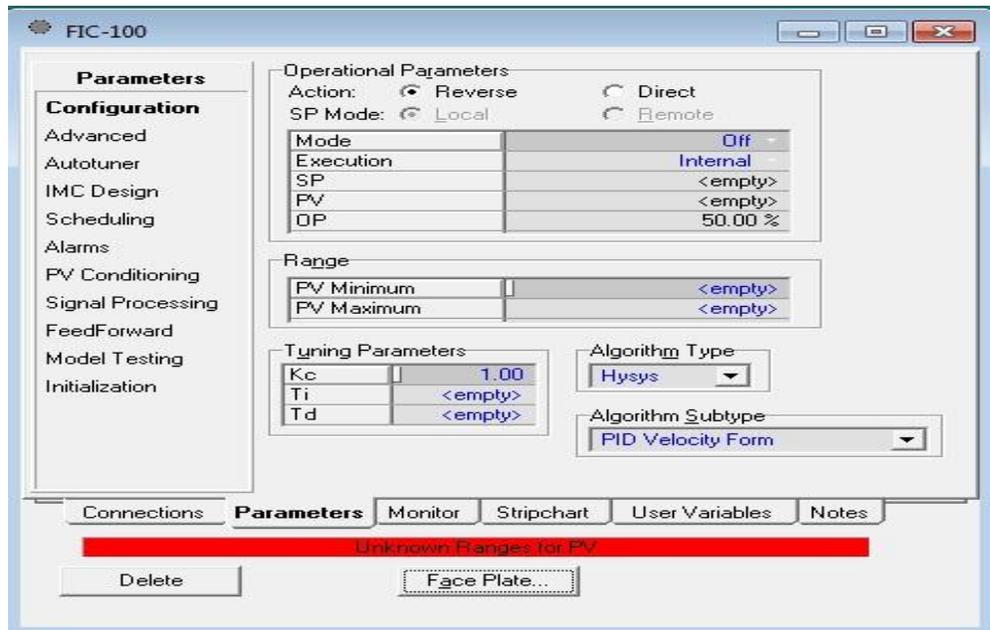


Figure 3.19: Controller Parameter Page

8. Specify the controller tuning constants: gain K_C , integral time τ_I and derivative time τ_D . to achieve a proportional-only controller, delete whatever number is in the integral box (“empty” should appear). For the flow controller, specify a gain of 0.5 and an integral time of 0.3 minutes (see Figure 3.20).

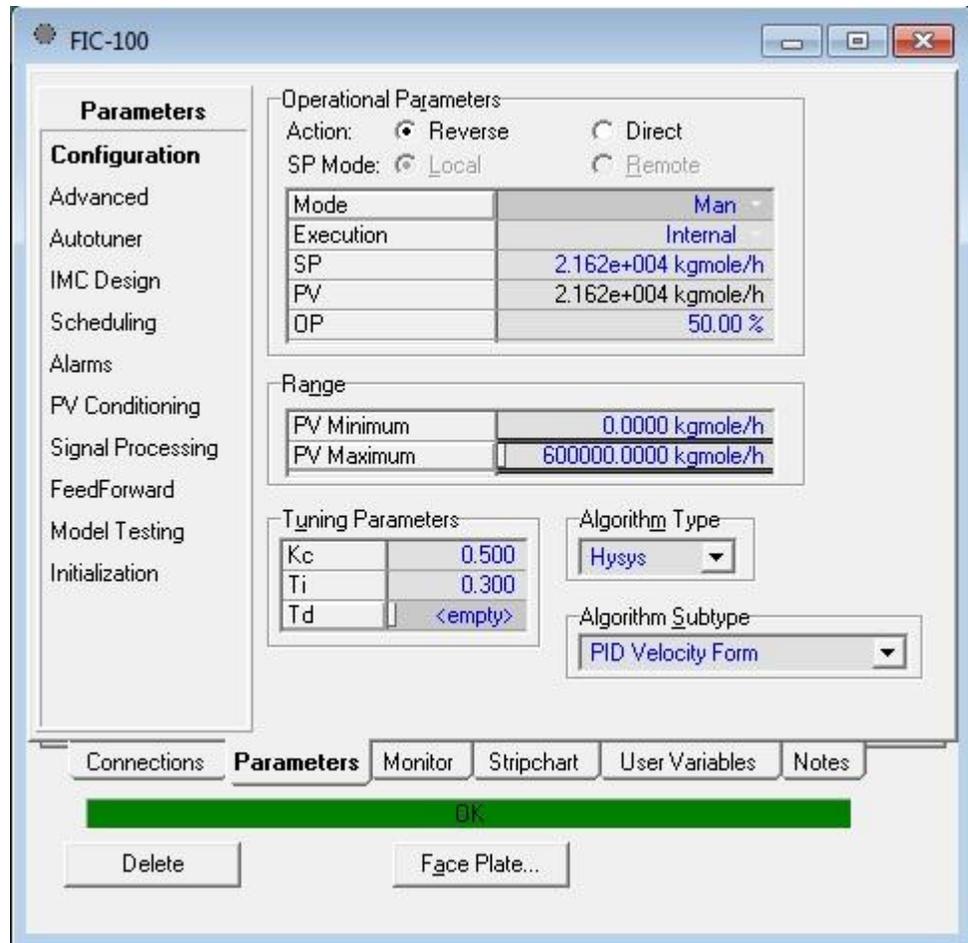


Figure 3.20: Flow Controller Tuning

9. Put the controller into manual or automatic.
10. The final step is to click the faceplate button at the bottom of the window. This places a faceplate on the workspace, as shown in Figure 3.21.



Figure 3.21: Controller Faceplate

The faceplate indicates if the controller is on manual or automatic, and the controller can be switched from one to the other by using the dropdown arrow, as illustrated in Figure 3.21. Clicking the Tuning button on the faceplate opens up the window showing the parameters page tab. From this view the tuning constants can be changed.

For heater controller, the step is the same as flow controller. But the different is, for heater, Direct Q is needed in order to heat or cool the flow. Click the Control Valve buttons on under the Controller page; specify the minimum Direct Q and maximum Direct Q (see Figure 3.22). Then the steps after that is the same as flow controller.

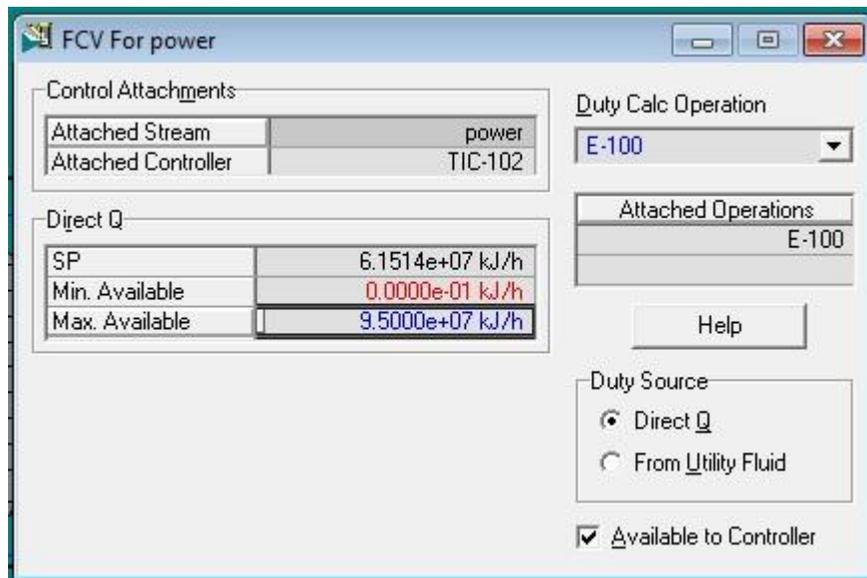


Figure 3.22: Heating Controller Direct Q

3.4.4 Installing Recorders

Strip-chart recorders or data-loggers are useful for recording the data changing with time. The steps for installing and defining the properties of recorder are:

1. Click Tools on the top menu bar and click DataBook (see Figure 3.23).
2. On the Variables page tab, click Insert. Select the variable to be recorded. Then click the OK after selected the variable that want to be recorded.
3. Click the Strip Chart page tab. This opens the view shown in Figure 3.26.
4. Click Add button. This installs a data logger.
5. Specify which variables in the list that wants to be recorded on this strip chart (see Figure 3.27).
6. Clicking view brings up the strip-chart window.
7. Right click on the strip chart window and select Graph Control. This opens the window shown in Figure 3.28. The properties of the strip chart can be adjusted: colors, scales, labels, etc. Figure 3.28 shows the General page tab in which the colors can be specified.
8. Figure 3.29 shows that the time axis can be specified.

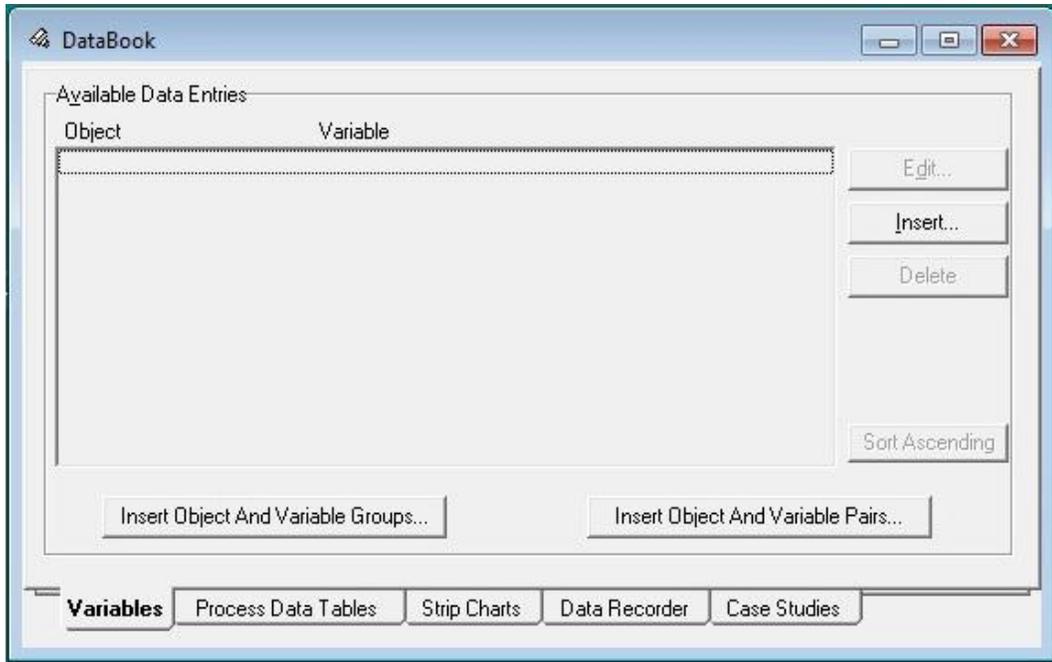


Figure 3.23: DataBook

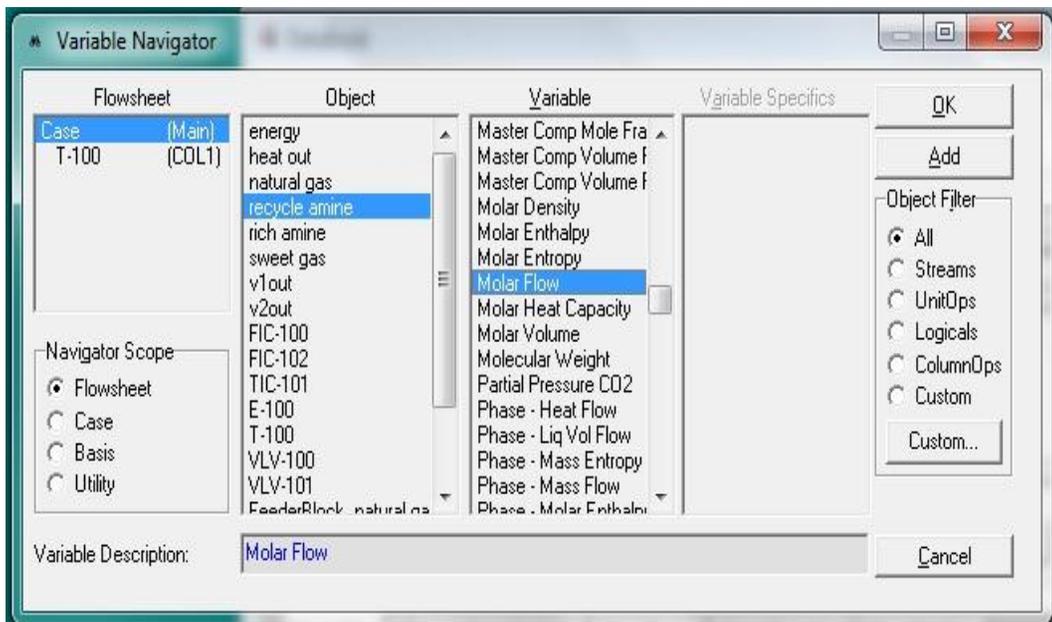


Figure 3.24: Inserting Flowrate Variable

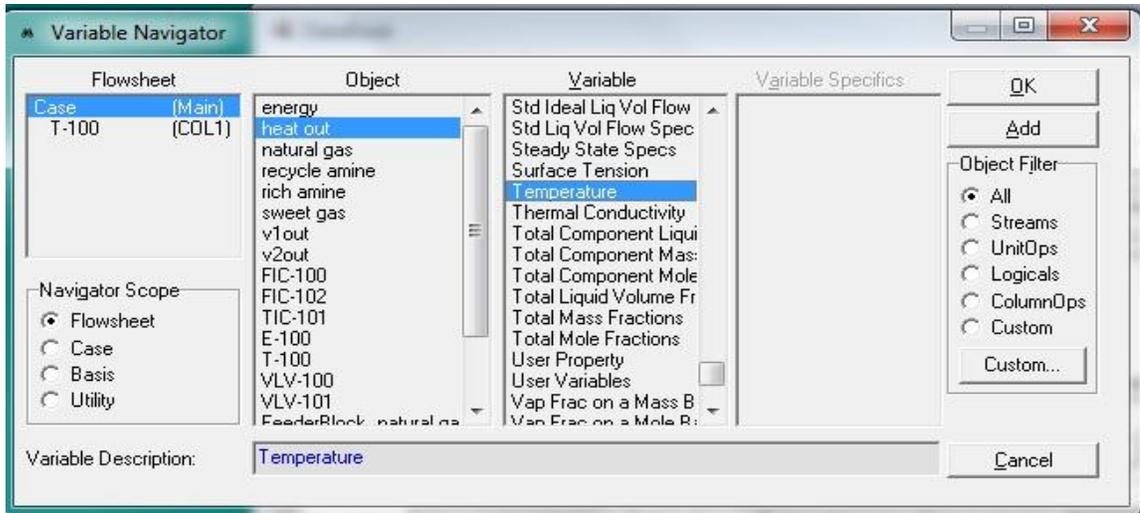


Figure 3.25: Inserting Temperature Variable

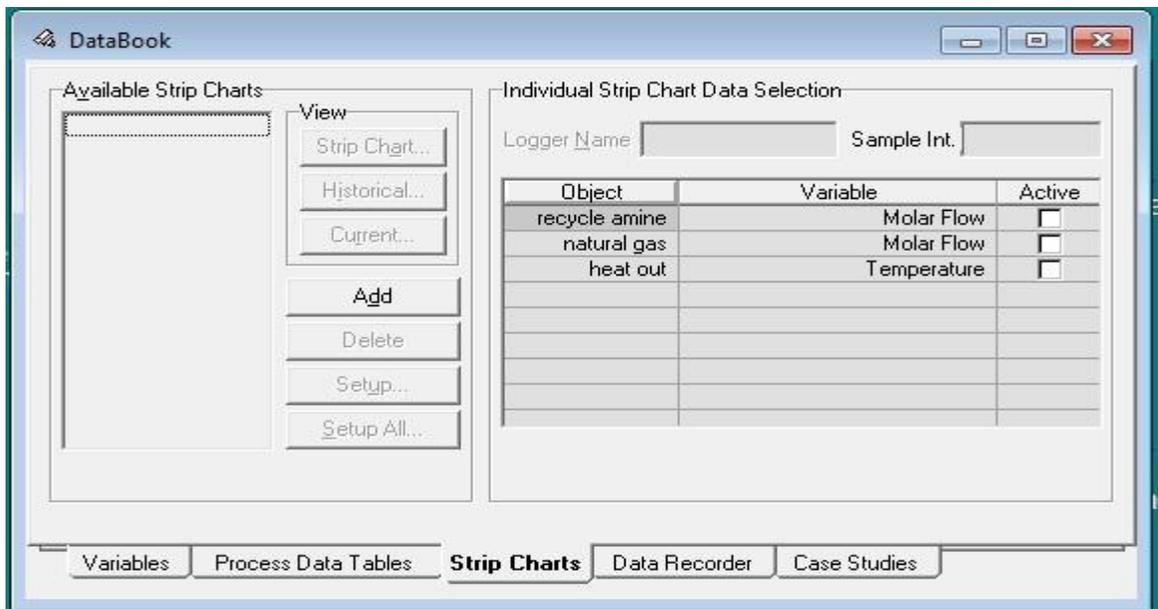


Figure 3.26: Add Strip Chart

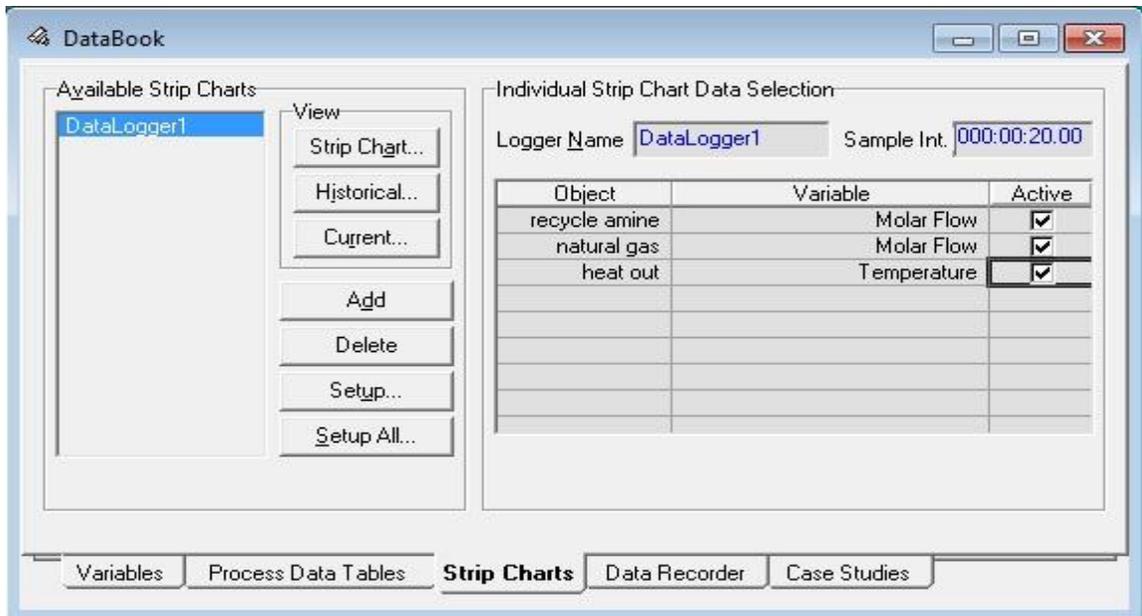


Figure 3.27: Check Active Variables

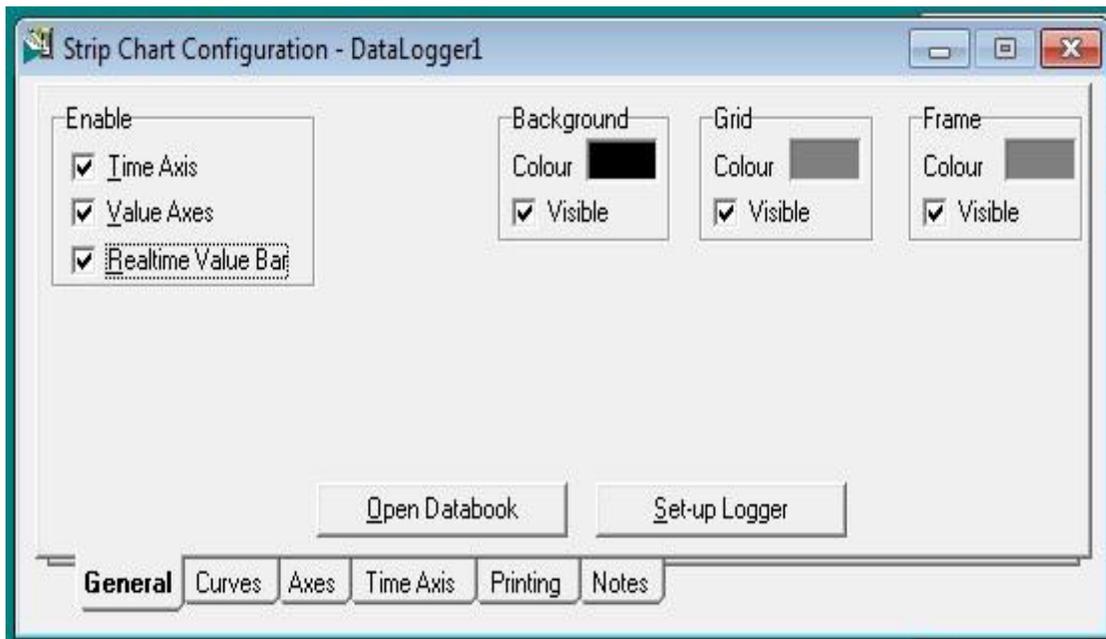


Figure 3.28: General Page Tab of Graph Control

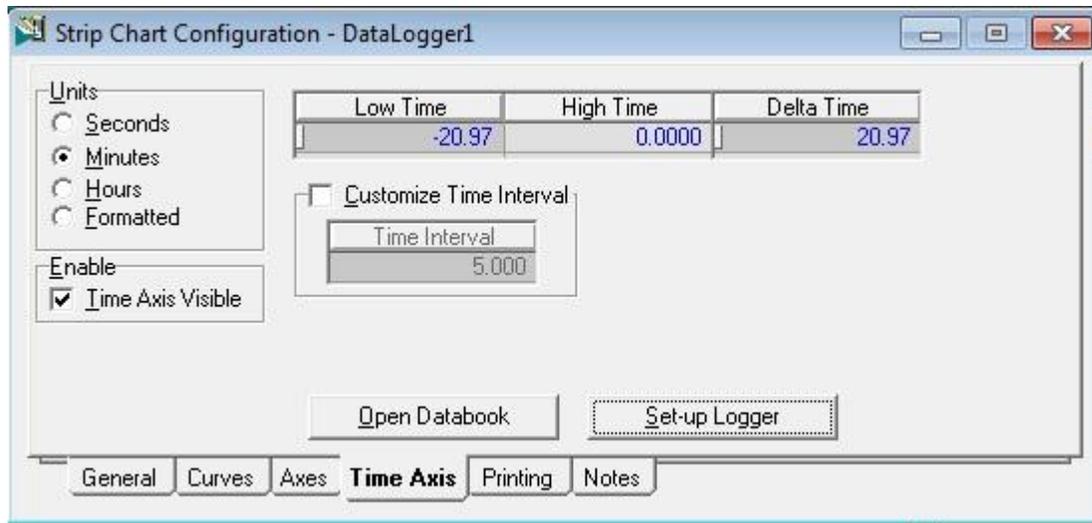


Figure 3.29: Setting Time Axis

In addition to seeing the data from dynamic run on strip chart, these data can be saved in a file and exported to some other program for plotting or analysis.

3.4.5 Running the Simulations

Now that all the elements are ready to go, the integrator can be started. Clicking the green button on the top tool bar starts the integrator. The strip-chart will show as in Figure 3.30.

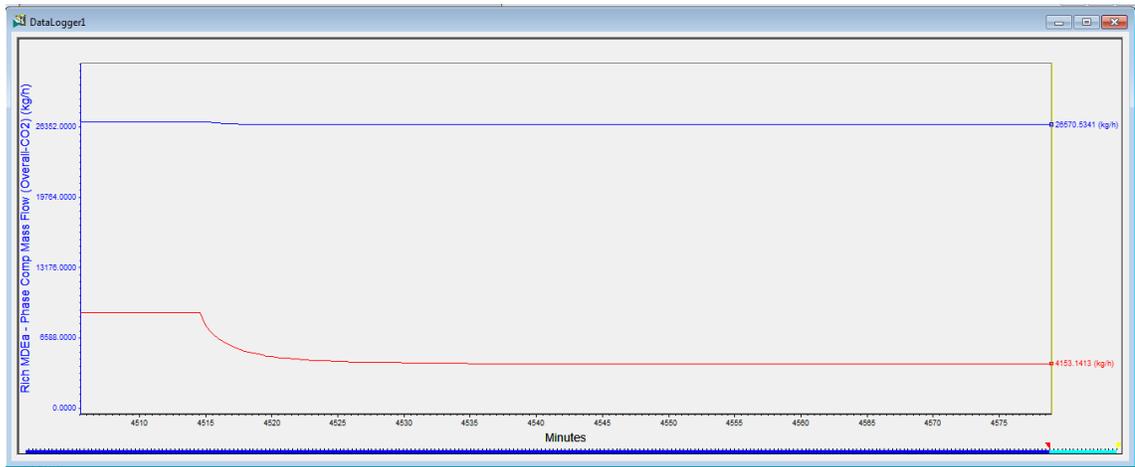


Figure 3.30: Graph

3.5 Conclusion

In this chapter, all the basic steps and methods in steady-state, moving from steady state to dynamic simulation and dynamic simulation procedure has covered. Providing the equipment size data, adding controllers and installing strip charts are essential steps required. By changing the setpoint of the flow, the changes can be illustrated in the strip-chart in dynamic simulation. The purpose of this simulation is to see the changes in the process if one or more variable is change. The simulation is successful and can be illustrated.

CHAPTER 4

RESULT AND DISCUSSION

4.1 Introduction

In this chapter, the results of steady-state and dynamic simulation of CO₂ removal by using Aspen HYSYS are presented. In this study, dynamic simulation only applied at absorber because at this equipment, absorption process to remove CO₂ from natural gas is occurs. Steady-state and dynamic process flow diagram can be seen in Figure 4.1 and Figure 4.2at the appendix.

4.2 Steady-state Simulation Result

Table 2: Data Generated from the Simulation Model

Flow Name	Natural gas	Lean MDEA	Recycle Lean Amine	Sweet gas	Rich MDEA	Cold Lean MDEA	Hot Rich MDEA
Vapour Fraction	1.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
Temperature (°C)	46.00	84.65	60.00	60.29	66.78	109.66	88.00
Pressure (kPa)	674.70	119.64	119.64	655.08	664.89	130.43	122.89
Molar Flow (kgmole/h)	5737.68	24043.11	24043.15	5441.91	24338.91	21878.15	24338.91
Mass Flow (kg/h)	58934.00	631733.47	631738.63	44173.73	646498.90	592731.47	646498.90
Liquid Volume Flow	192.20	623.56	623.57	174.01	641.76	584.48	641.76
Heat Flow (kJ/h)	54675067	-481365885	-540343341	54056982	-539817535	-359866502	-483660641

Table 2: “Continued”

Flow Name	Hot Lean MDEA	Steam/water	Cold Mixing MDEA	Recycle	Acid Gas
Vapour Fraction	0.0000	0.0000	0.0000	0.0000	1.0000
Temperature (°C)	85.32	76.00	60.00	60.00	100.06
Pressure (kPa)	119.64	119.64	119.64	119.64	119.64
Molar Flow (kgmole/h)	21878.15	2164.96	24043.11	24043.11	2460.76
Mass Flow (kg/h)	592731.47	39002.00	631733.47	631733.47	53767.43
Liquid Volume Flow	584.48	39.08	623.56	623.56	57.28
Heat Flow (kJ/h)	-416023396	-65342489	-540342493	-540342493	30494253

Table 3: Component Composition

Name	natural gas	Recycle Lean Amine	Lean MDEA	Sweet gas	Rich MDEA	Cold Lean MDEA	Hot Rich MDEA
Methane	0.07	0.00	0.00	0.07	0.00	0.00	0.00
Hydrogen	0.71	0.00	0.00	0.76	0.00	0.00	0.00
Nitrogen	0.01	0.00	0.00	0.01	0.00	0.00	0.00
Carbon monoxide	0.10	0.00	0.00	0.11	0.00	0.00	0.00
Carbon dioxide	0.10	0.00	0.00	0.02	0.02	0.00	0.02
Water	0.01	0.92	0.92	0.03	0.90	0.91	0.90
MDEA	0.00	0.08	0.08	0.00	0.08	0.09	0.08

Table 3: “Continued”

Name	Hot Lean MDEa	Steam/water	Cold Mixing MDEa	Recycle	Acid Gas
Methane	0.00	0.00	0.00	0.00	0.00
Hydrogen	0.00	0.00	0.00	0.00	0.00
Nitrogen	0.00	0.00	0.00	0.00	0.00
Carbon monoxide	0.00	0.00	0.00	0.00	0.00
Carbon dioxide	0.00	0.00	0.00	0.00	0.18
Water	0.91	1.00	0.92	0.92	0.82
MDEA	0.09	0.00	0.08	0.08	0.00

Table 4: Equipment Energy

Component name	Heat Flow (kJ/h)
Condenser	314858613.18
Reboiler	465925637.17
Cooling energy	56189180.54
Pump energy	0.00

4.3 Steady-state Simulation Discussion

Natural gas feed to the absorber from bottom because the gas will countercurrent with recycle lean amine (MDEA) and absorb CO₂ from natural gas. The number of stages used for absorber is 30 stages while the optimum stages used for CO₂ absorption is 20 trays. The pressure different in the absorber also give an effect on the efficiency of CO₂ absorption. The parameter that is needed for this absorber is pressure and input flow. Input flow parameter for natural gas and recycle MDEA is obtained from industrial data.

The absorption of CO₂ in the natural gas is not 100% absorb because of many factors. In order to increase the efficiency of CO₂ removal, the number of tray need to be increase. But by increasing the number of tray will increase the height of the absorber. Other than tray, pressure also gives an important role in giving a better efficiency of removing CO₂ in natural gas.

Amine-amine heat exchanger is used to increase the temperature of rich MDEA entering stripper and to cold lean MDEA that leave stripper. Stripper used 30 trays to release CO₂ from plant and MDEA used is recycles back to the absorber. The difficulties are face when the stripper used did not converge. A lot of parameters used in order to converge this equipment for example, bottom flow rate, reflux ratio which is assume 3.0 and the temperature output. Other parameter that is needed in order to run this stripper is input parameter, pressure and temperature. The pump is used to keep the flow forward entering absorber.

4.4 Result and Discussion of Dynamic Simulation

4.4.1 CO₂Flow Rate Trend with $\pm 10\%$ Recycle Amine Flow Rate Stream

In dynamic simulation, an input of flow rate stream is given by increasing and decreasing the flow rate of recycle amine flow rate. The trend or characteristic of CO₂ removal can be observed from the graph in Figure 4.1 and Figure 4.2 below.

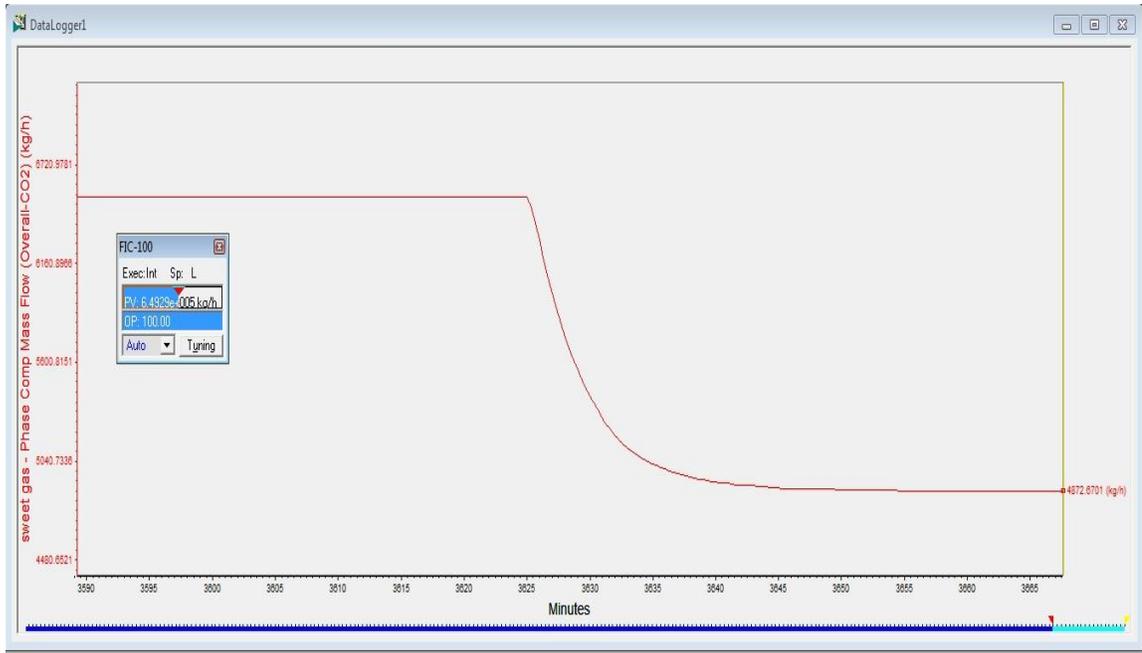
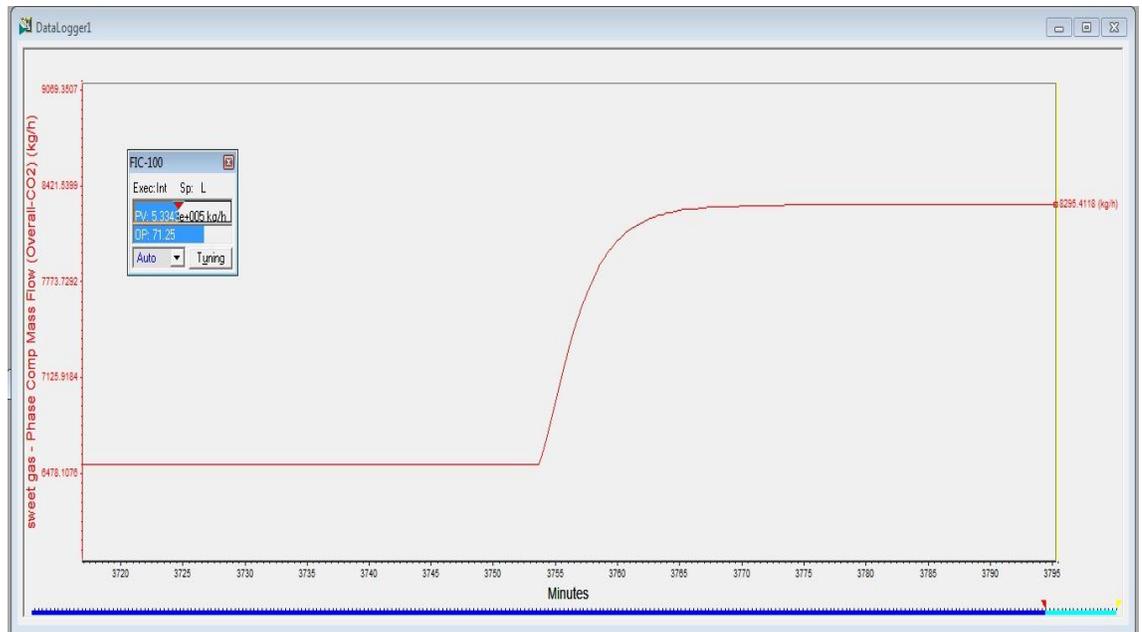


Figure 4.1: Flow rate of CO₂ in sweet gas stream with 10% increase of recycle amine flow rate stream.



The graph in Figure 4.1 shows the flow rate of CO₂ in sweet gas stream after the flow rate of recycle amine at the inlet of the absorber is increased. From the graph, it shows that the flow rate of CO₂ is decreased from 6538.03 kg/hr to 4872.88 kg/hr after an input is applied. From this observation, it can be concluded that, by increasing the recycle amine flow rate, the amount of CO₂ in the sweet gas is less and the efficiency of CO₂ removal is increased by increasing the amount of amine (MDEA) entering the absorber.

The graph in Figure 4.2 shows the flow rate of CO₂ in sweet gas stream after the flow rate of recycle amine is decreased. The trend shows the increasing in the amount of CO₂ from 6538.03 kg/hr to 8296.91 kg/hr in the sweet gas stream. By observing this trend, it can be concluded that, if the amount of recycle amine entering the absorber is less, the amount of CO₂ in the sweet gas is more.

An input that is applied at the recycle amine stream not only affects the sweet gas stream but also the rich amine stream. Figure 4.3 and Figure 4.4 show the CO₂ flow rate trend in the rich amine stream after the disturbance is applied.

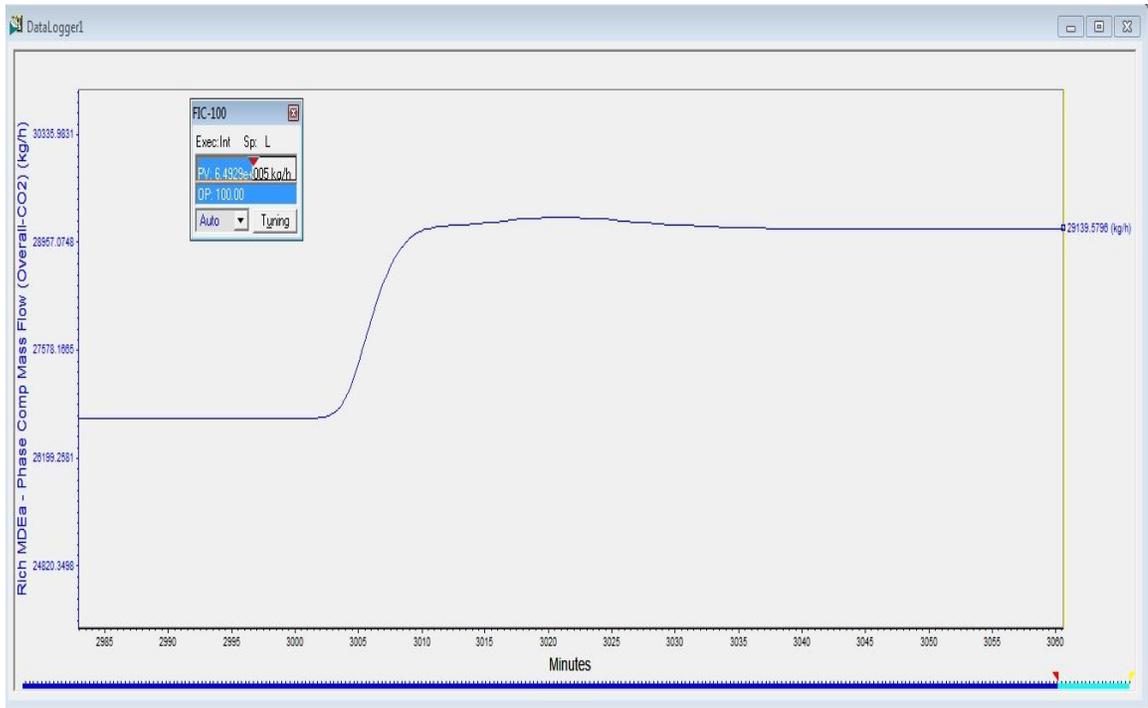


Figure 4.3: Flow rate of CO₂ in rich amine stream with 10% increase of recycle amine flow rate stream.

Figure 4.3 shows the flow rate of CO₂ in rich amine after the flow rate of recycle amine is increased. From the observation, it shows that the amount of CO₂ in the rich amine is increased after the flow rate of recycle amine is increased from 26714.76 kg/hr to 29139.58 kg/hr. This can be conclude that, by increasing the flow rate of recycle amine, the amount of CO₂ absorb from the natural gas is increased. The efficiency of the CO₂ is increased.

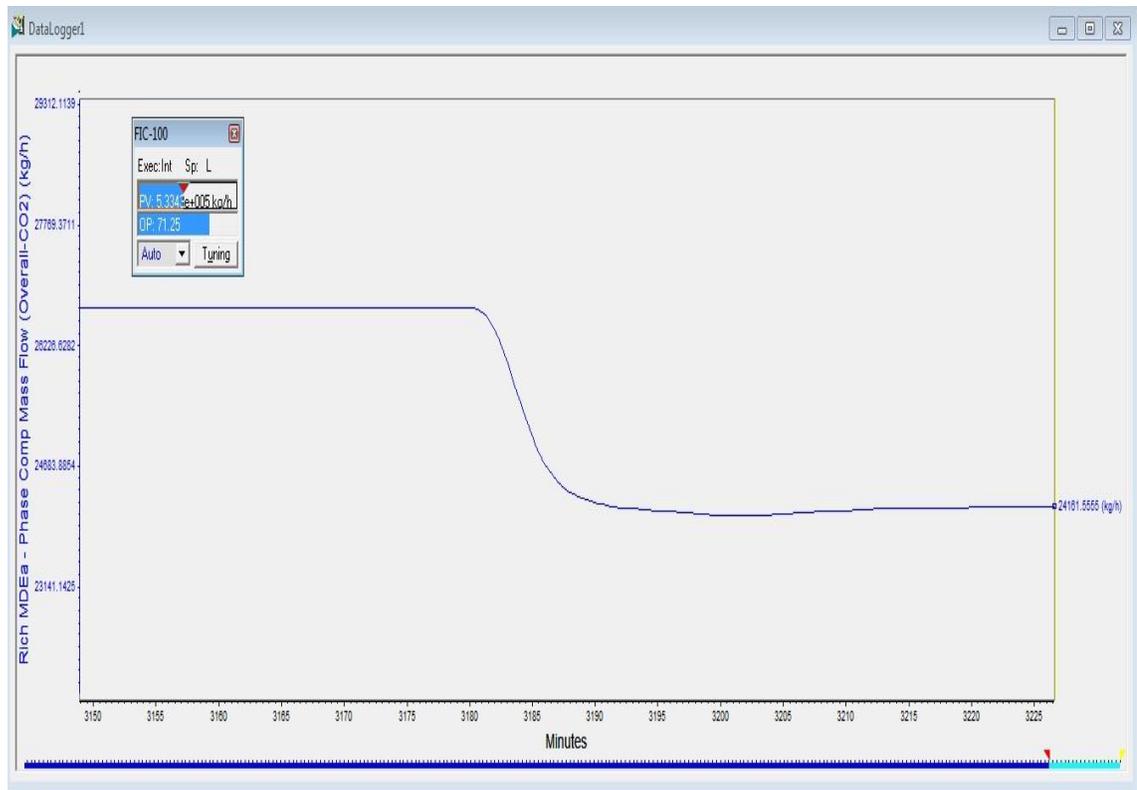


Figure 4.4: Flow rate of CO₂ in rich amine stream with 10% decrease of recycle amine flow rate stream.

In Figure 4.4 shows that the amounts of CO₂ in rich amine steam after the flow rate of recycle amine is decreased. From the observation of Figure 4.4, it shows that the amount of CO₂ in the rich amine stream is less from 26714.76 kg/hr to 24181.56 kg/hr. The CO₂ is more in the sweet gas stream and the efficiency of removing CO₂ from the natural gas is less.

4.4.2 CO₂ Flow Rate Trend with ±10% Natural Gas Flow Rate Stream

An input is given at the natural gas stream is to see if by applied the changes in at the flow rate of natural gas would effects the CO₂ removal. An input that has been applied is by increasing and decreasing the flow rate of natural gas entering the absorber.

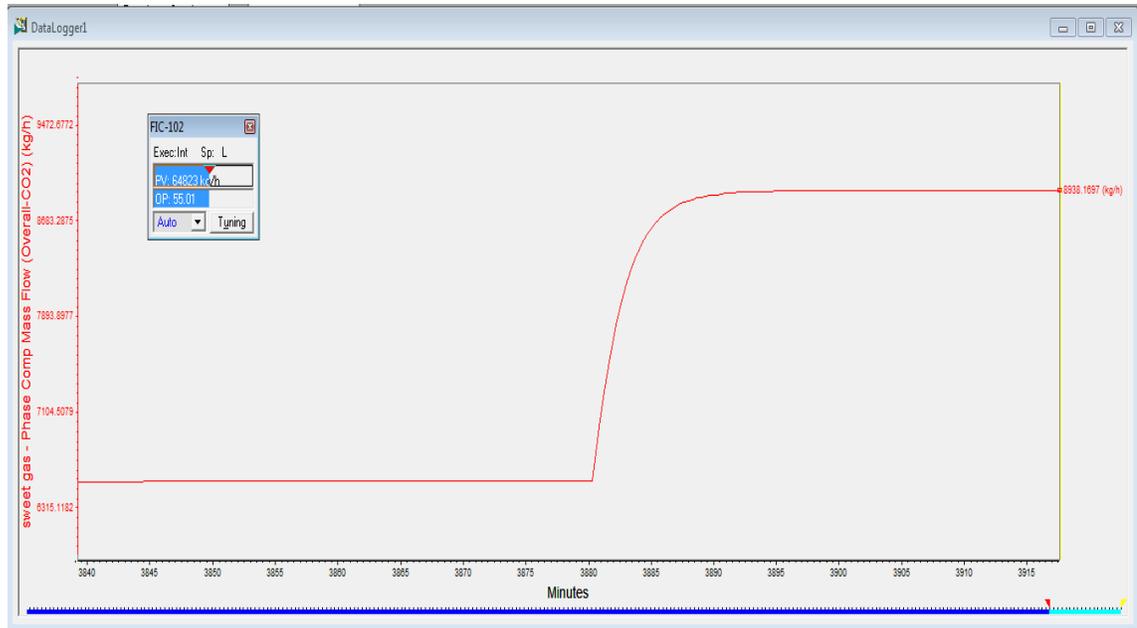


Figure 4.5: Flow rate of CO₂ in sweet gas stream with 10% increase of natural gas flow rate stream.

Figure 4.5 shows the flow rate of CO₂ in sweet gas stream after the flow rate of natural gas is increased. From the observation of Figure 4.5 above, it shows that the increasing in amount of CO₂ in sweet gas from 6538.03 kg/hr to 8938.25 kg/h after an input is made. This can be conclude that, by increasing the flow rate of natural gas, the efficiency of CO₂ is less.

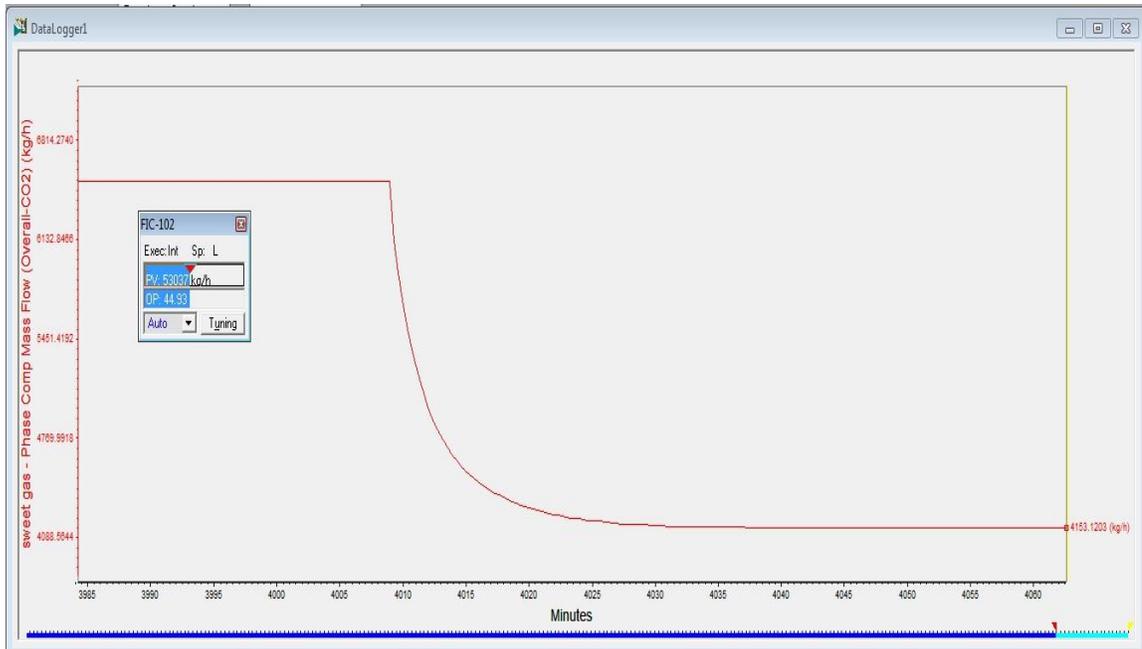


Figure 4.6: Flow rate of CO₂ in sweet gas stream with 10% decrease of natural gas flow rate stream.

Figure 4.6 above shows the flow rate of CO₂ in sweet gas after the flow rate of natural gas is decreased. It shows that, the amount of CO₂ in the sweet gas stream is decreased after the flow rate of natural gas is decreased from 6538.03 kg/hr to 4153.12 kg/hr. If the natural gas stream inlet is less, the amount of CO₂ at the sweet gas stream is also less.

The observation is not only made at the sweet gas stream, it also made at the rich amine stream where the CO₂ is absorbed. The characteristics of CO₂ at the rich amine recorded at the result.

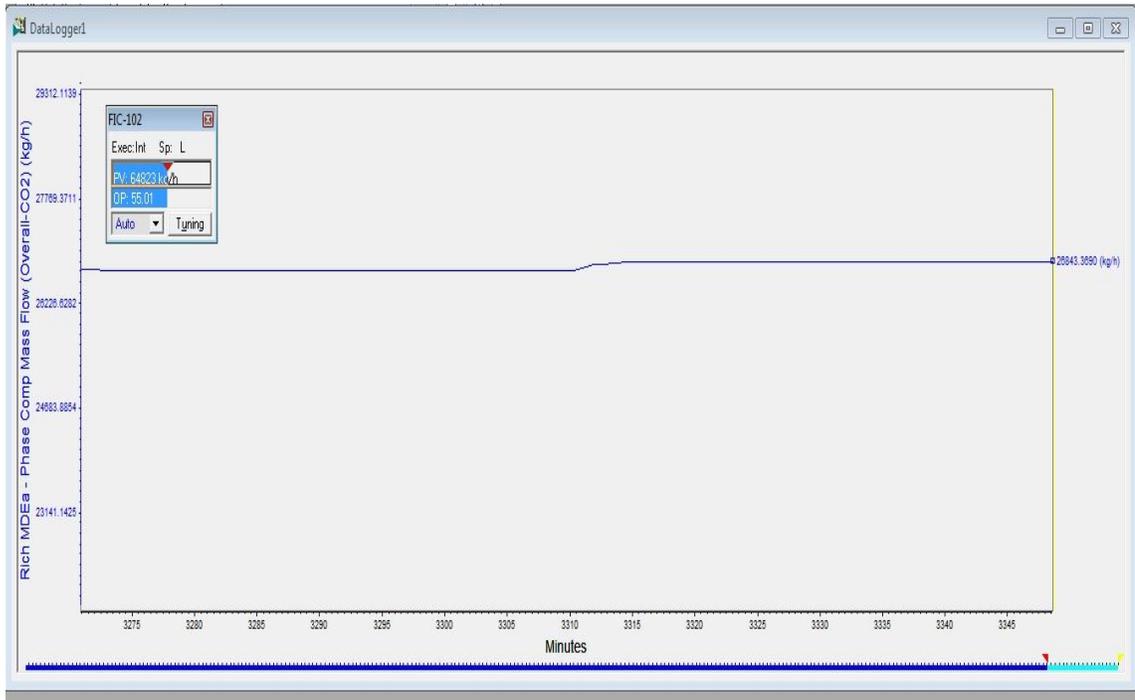


Figure 4.7: Flow rate of CO₂ in rich amine stream with 10% increase of natural gas flow rate stream.

Figure 4.7 above is the trend of CO₂ in the rich amine stream after the flow rate of natural gas is increased. The change observed from the Figure 4.7 is the amount of CO₂ in the rich amine stream is slightly increased from 26714.76 kg/hr to 26843.85 kg/hr after an input is made. This can be conclude that, by increasing the natural gas flow rate, the CO₂ absorbed is not much. The effect of removing CO₂ is less.

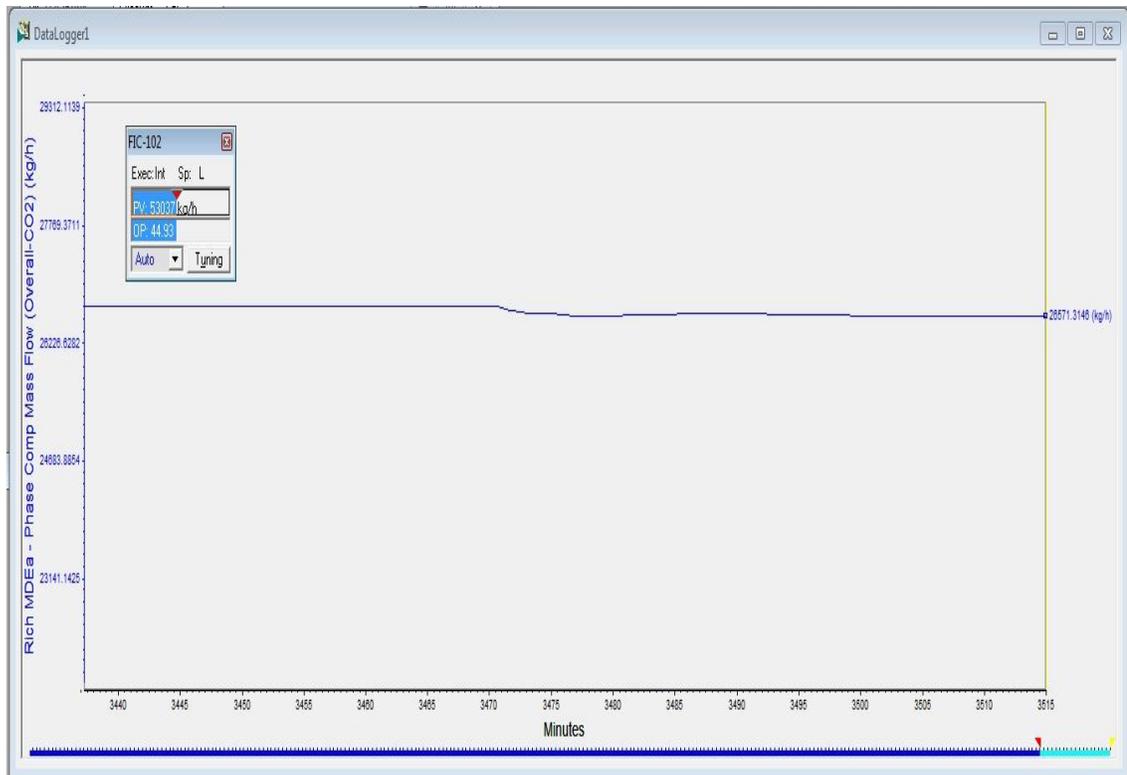


Figure 4.8: Flow rate of CO₂ in rich amine stream with 10% decrease of natural gas flow rate stream.

Figure 4.8 shows the flow rate of CO₂ in rich amine stream after the natural gas flow rate is decreased. The CO₂ in the rich amine stream is slightly decreased from 26714.76 kg/hr to 26571.32 kg/hr after the change is made. After the observation of Figure 4.8, it can be concluded that, by decreasing the natural gas flow rate, it did not give an effect on CO₂ absorption.

4.6 Summary

The simulation objectives are to develop dynamic simulation using Aspen HYSYS, to understand the characteristics of CO₂ removal, to control the dynamic simulation of CO₂ removal and also to improve the performance of CO₂ removal. The dynamic simulation can be developed after steady-state simulation is completed. The characteristics of CO₂ removal can be understood by conducting steady-state and dynamic simulation. Removal of CO₂ by absorption processes are based on solubility of CO₂ within the solvents. The solubility of CO₂ depends on the partial pressure and on the temperature of the feed gas. The dynamic simulation is done for absorber by controlling the flow rate of amine and natural gas entering the absorber. The compressor is used in order to increase the flow rate of natural gas while pump is used to increase the flow rate of amine liquid. Valve is used in each flow to increase or decrease the flow rate. By increasing the flow rate of recycle amine, the CO₂ removal is increased. As a conclusion, the characteristic of CO₂ removal from natural gas can be observed by using dynamic simulation in Aspen HYSYS.

CHAPTER 5

CONCLUSION AND RECOMMENDATION

5.1 Conclusion

Based on the literature reviewed and the results from simulation model the following conclusions can be made:

- a) The dynamic simulation can be developed using Aspen HYSYS. In this simulation, the component used in real plant is existed and have the same function.
- b) The characteristics of CO₂ removal can be understand from this simulation.
- c) The dynamic simulation can be used to control CO₂ removal.
- d) The performance of CO₂ removal can be improved by using dynamic simulation.

In the future, this simulation can be used widely to obtain the result of the plant process before a real plant can be build. The characteristic of the process can be easily understood by implementing the simulation process and hope that undergraduate student can learn this simulation more in the study.

5.2 Recommendation

In this study, there are some recommendations that can be done to improve this study. The first recommendation is make comparison for other type of controller for example proportional (P) control, Proportional- Integral (PI) Controlproportional-integral-derivative (PID) controller. The transient respond can be observed for this respond and the best type of controller can be chosen.

The second recommendation is control other type of parameter than flow rate for example, temperature, pressure, and composition. From this study, the transient respond for other parameter can be observed and more data can be collected to make this study more successful.

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Appendix A

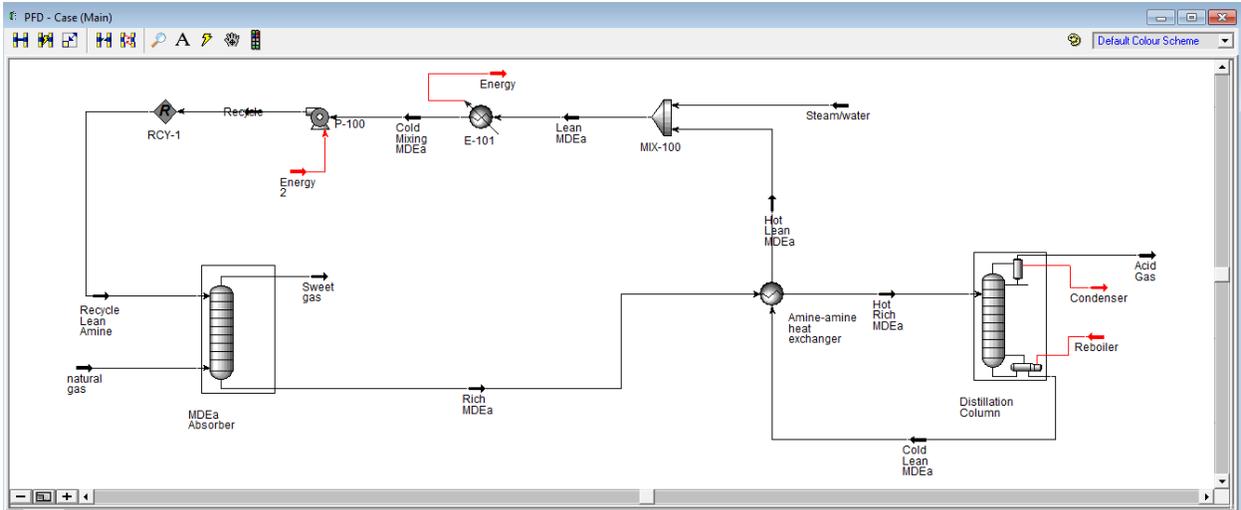


Figure 4.9: Steady-state simulation process flow diagram

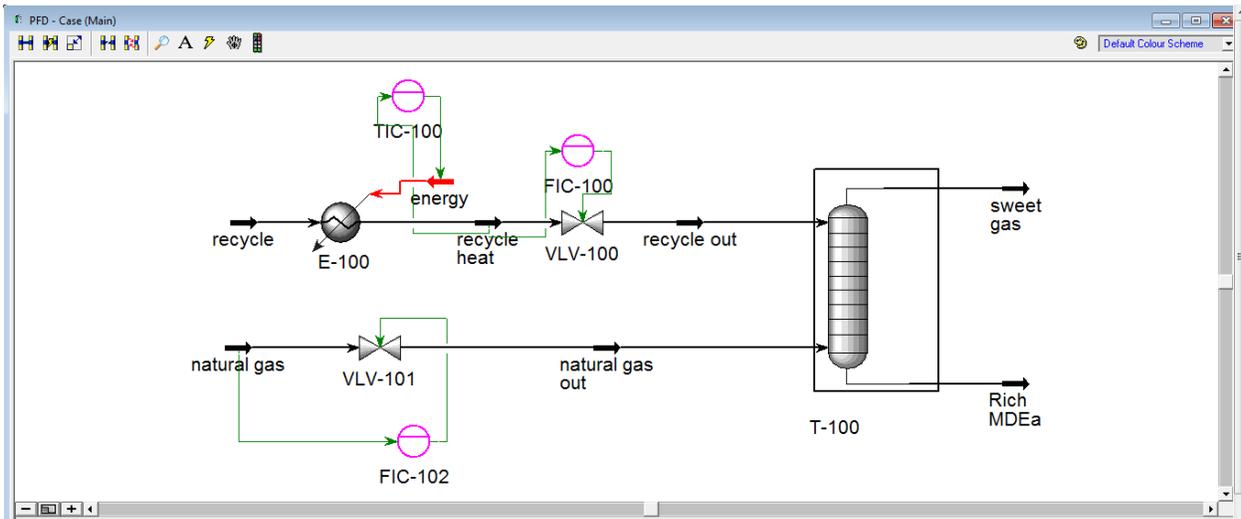


Figure 4.10: Dynamic simulation process flow diagram

Workbook - Case (Main)

Name	recycle	recycle out	natural gas	natural gas out	recycle heat	sweet gas	Rich MDEa	** New **
Vapour Fraction	0.0000	0.0355	0.9979	0.9990	0.0355	1.0000	0.0000	
Temperature [C]	40.00	60.00	46.00	44.41	60.00	74.49	81.15	
Pressure [kPa]	900.0	655.1	800.0	676.7	798.4	655.1	677.0	
Molar Flow [kgmole/h]	5127	5127	5737	5737	5127	5222	5642	
Mass Flow [kg/h]	5.973e+005	5.973e+005	5.893e+004	5.893e+004	5.973e+005	3.854e+004	6.177e+005	
Liquid Volume Flow [m3/h]	576.3	576.3	192.2	192.2	576.3	167.8	600.7	
Heat Flow [kJ/h]	3.477e+008	3.898e+008	5.414e+007	5.414e+007	3.898e+008	5.394e+007	3.900e+008	

Material Streams | Compositions | Energy Streams | Unit Ops

FeederBlock_recycle
E-100

Fluid Pkg: All

Include Sub-Flowsheets
 Show Name Only
Number of Hidden Objects: 0

Horizontal Matrix

Figure 4.11: Initial mass flow rate

Workbook - Case (Main)

Name	recycle	recycle out	natural gas	natural gas out	recycle heat	sweet gas	Rich MDEa	** New **
Vapour Fraction	0.0000	0.0355	0.9979	0.9990	0.0355	1.0000	0.0000	
Temperature [C]	40.00	60.00	46.00	44.42	60.00	73.15	81.28	
Pressure [kPa]	900.0	655.1	800.0	677.2	780.0	655.1	677.0	
Molar Flow [kgmole/h]	5574	5574	5740	5740	5574	5190	6124	
Mass Flow [kg/h]	6.493e+005	6.493e+005	5.896e+004	5.896e+004	6.493e+005	3.703e+004	6.712e+005	
Liquid Volume Flow [m3/h]	626.5	626.5	192.3	192.3	626.5	166.0	652.8	
Heat Flow [kJ/h]	3.780e+008	4.237e+008	5.416e+007	5.416e+007	4.237e+008	5.336e+007	4.245e+008	

Material Streams | Compositions | Energy Streams | Unit Ops

FeederBlock_recycle
E-100

Fluid Pkg: All

Include Sub-Flowsheets
 Show Name Only
Number of Hidden Objects: 0

Horizontal Matrix

Figure 4.12: Recycle flow increase with 10%

Workbook - Case (Main)

Name	recycle	recycle out	natural gas	natural gas out	recycle heat	sweet gas	Rich MDE a	*** New ***
Vapour Fraction	0.0000	0.0355	0.9979	0.9990	0.0355	1.0000	0.0000	
Temperature [C]	40.00	60.00	46.00	44.40	60.00	75.83	80.97	
Pressure [kPa]	900.0	655.1	800.0	676.0	819.0	655.1	677.0	
Molar Flow [kgmole/h]	4579	4579	5740	5740	4579	5268	5051	
Mass Flow [kg/h]	5.334e+005	5.334e+005	5.896e+004	5.896e+004	5.334e+005	4.046e+004	5.519e+005	
Liquid Volume Flow [m3/h]	514.7	514.7	192.3	192.3	514.7	170.2	536.8	
Heat Flow [kJ/h]	3.105e+008	3.481e+008	5.416e+007	5.416e+007	3.481e+008	5.467e+007	3.476e+008	

Material Streams | Compositions | Energy Streams | Unit Ops

FeederBlock_recycle
E-100

Fluid Pkg: All

Include Sub-Flowsheets
 Show Name Only
Number of Hidden Objects: 0

Horizontal Matrix

Figure 4.13: Recycle flow decrease with 10%

Workbook - Case (Main)

Name	recycle	recycle out	natural gas	natural gas out	recycle heat	sweet gas	Rich MDE a	*** New ***
Vapour Fraction	0.0000	0.0355	0.9979	0.9990	0.0355	1.0000	0.0000	
Temperature [C]	40.00	60.00	46.00	44.42	60.00	75.72	81.00	
Pressure [kPa]	900.0	655.1	800.0	677.0	800.0	655.1	677.0	
Molar Flow [kgmole/h]	5088	5088	6311	6311	5088	5788	5611	
Mass Flow [kg/h]	5.927e+005	5.927e+005	6.482e+004	6.482e+004	5.927e+005	4.429e+004	6.132e+005	
Liquid Volume Flow [m3/h]	571.9	571.9	211.4	211.4	571.9	186.9	596.4	
Heat Flow [kJ/h]	3.450e+008	3.868e+008	5.955e+007	5.955e+007	3.868e+008	6.005e+007	3.863e+008	

Material Streams | Compositions | Energy Streams | Unit Ops

FeederBlock_recycle
E-100

Fluid Pkg: All

Include Sub-Flowsheets
 Show Name Only
Number of Hidden Objects: 0

Horizontal Matrix

Figure 4.14: Natural gas flow increase with 10%

Workbook - Case (Main)

Name	recycle	recycle out	natural gas	natural gas out	recycle heat	sweet gas	Rich MDEa	** New **
Vapour Fraction	0.0000	0.0355	0.9979	0.9990	0.0355	1.0000	0.0000	
Temperature [C]	40.00	60.00	46.00	44.41	60.00	72.86	81.30	
Pressure [kPa]	900.0	655.1	800.0	676.4	800.0	655.1	677.0	
Molar Flow [kgmole/h]	5088	5088	5164	5164	5088	4663	5588	
Mass Flow [kg/h]	5.927e+005	5.927e+005	5.304e+004	5.304e+004	5.927e+005	3.307e+004	6.127e+005	
Liquid Volume Flow [m3/h]	571.9	571.9	173.0	173.0	571.9	149.1	595.8	
Heat Flow [kJ/h]	3.450e+008	3.868e+008	4.873e+007	4.873e+007	3.868e+008	4.790e+007	3.876e+008	

Material Streams | Compositions | Energy Streams | Unit Ops

FeederBlock_recycle
E-100

Fluid Pkg: All

Include Sub-Flowsheets
 Show Name Only
Number of Hidden Objects: 0

Horizontal Matrix

Figure 4.15: Natural gas flow decrease with 10%

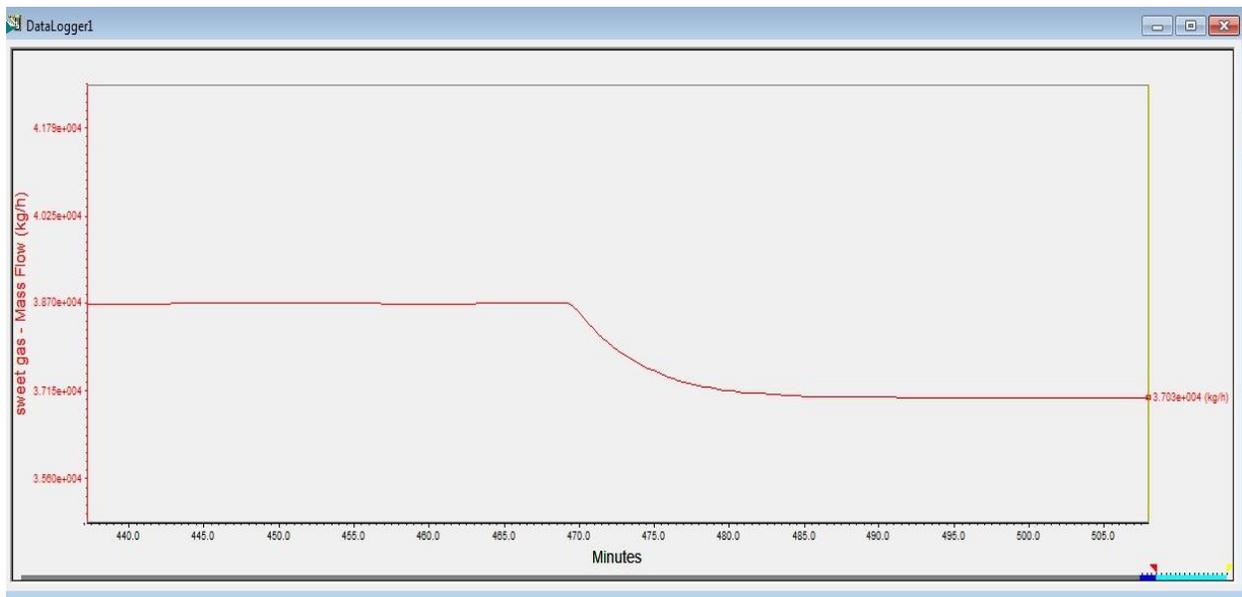


Figure 4.16: Sweet gas characteristic after increased recycle amine flow rate 10%

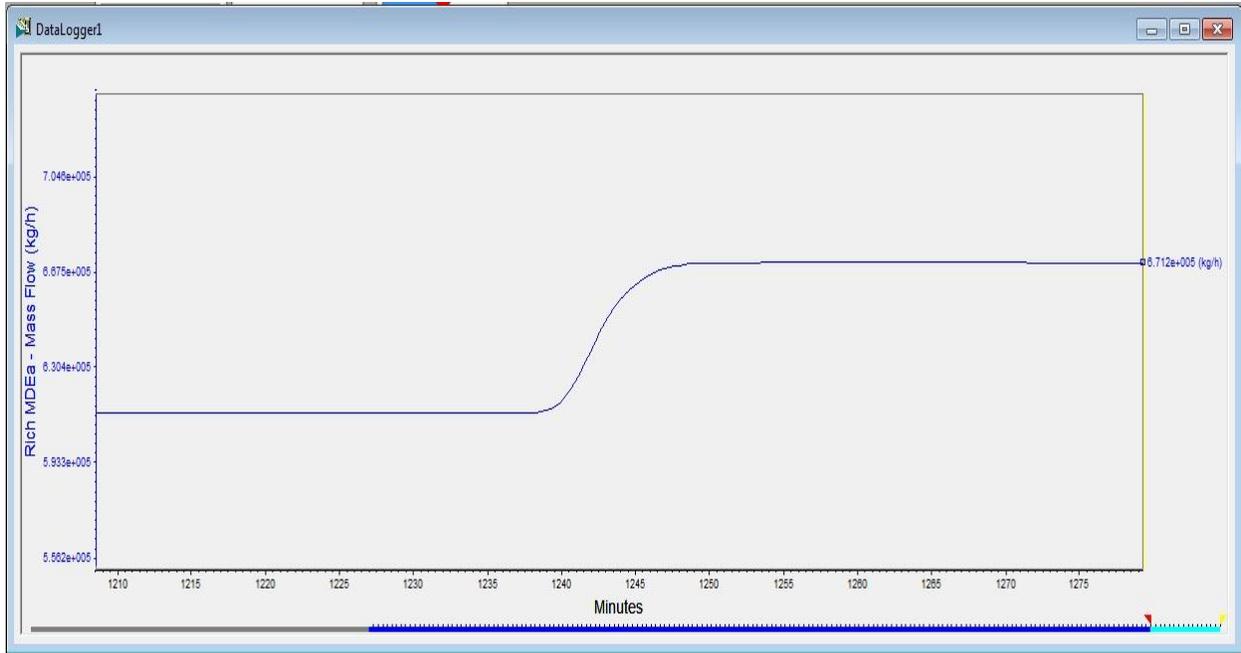


Figure 4.17: Rich amine characteristic after increased recycle amine flow rate 10%

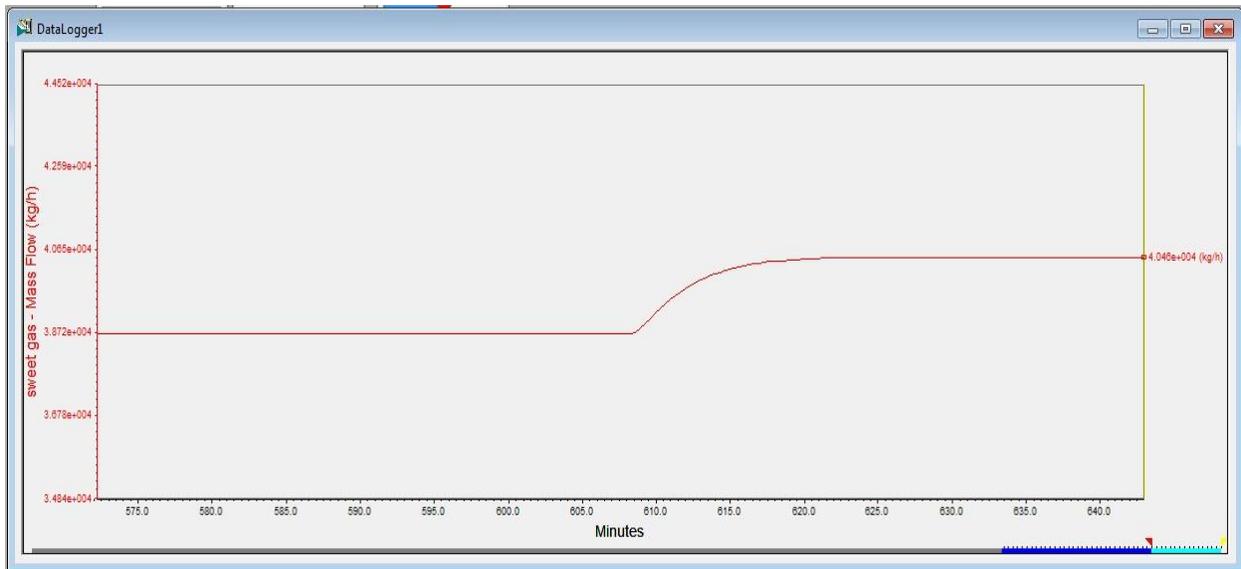


Figure 4.18: Sweet gas characteristic after decreased recycle amine flow rate 10%

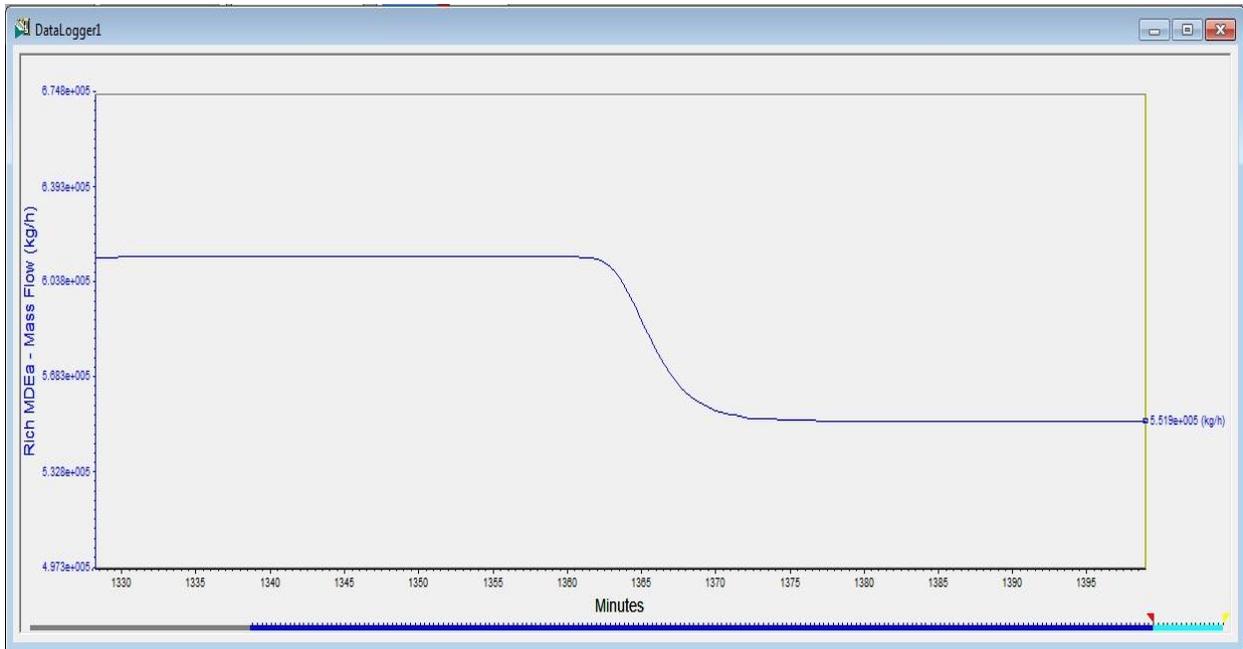


Figure 4.19: Rich amine characteristic after decreased recycle amine flow rate 10%

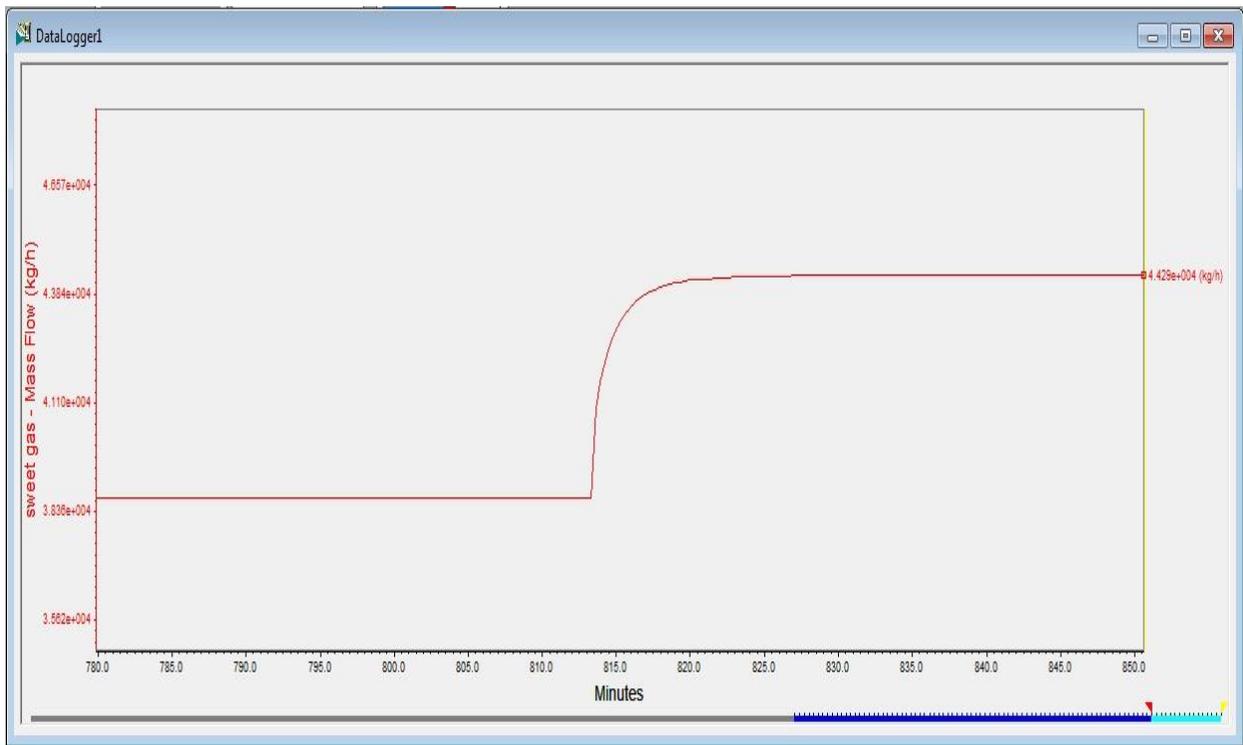


Figure 4.20: Sweet gas characteristic after increased natural gas flow rate 10%

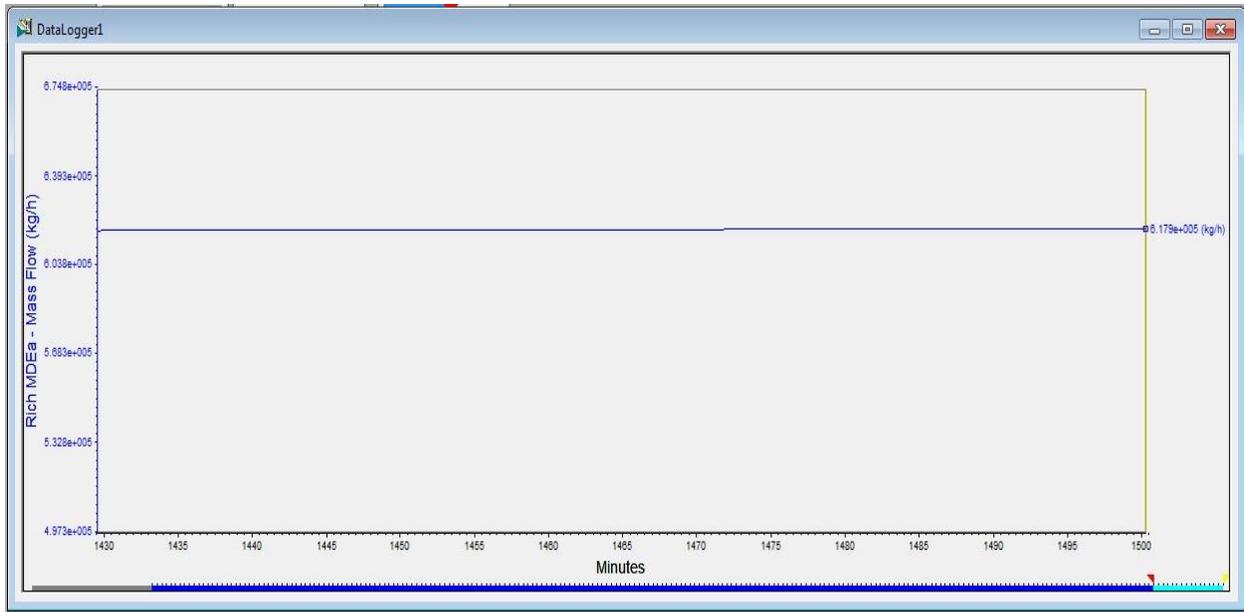


Figure 4.21: Rich amine characteristic after increased natural gas flow rate 10%

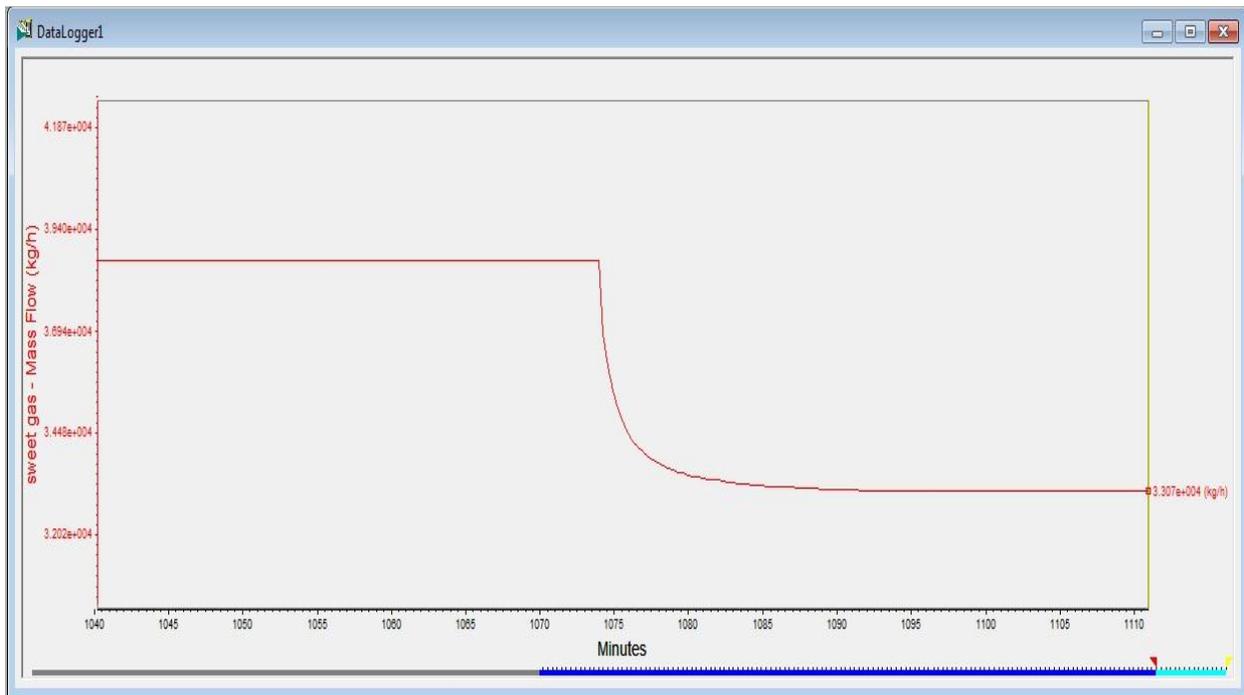


Figure 4.22: Sweet gas characteristic after decreased natural gas flow rate 10%

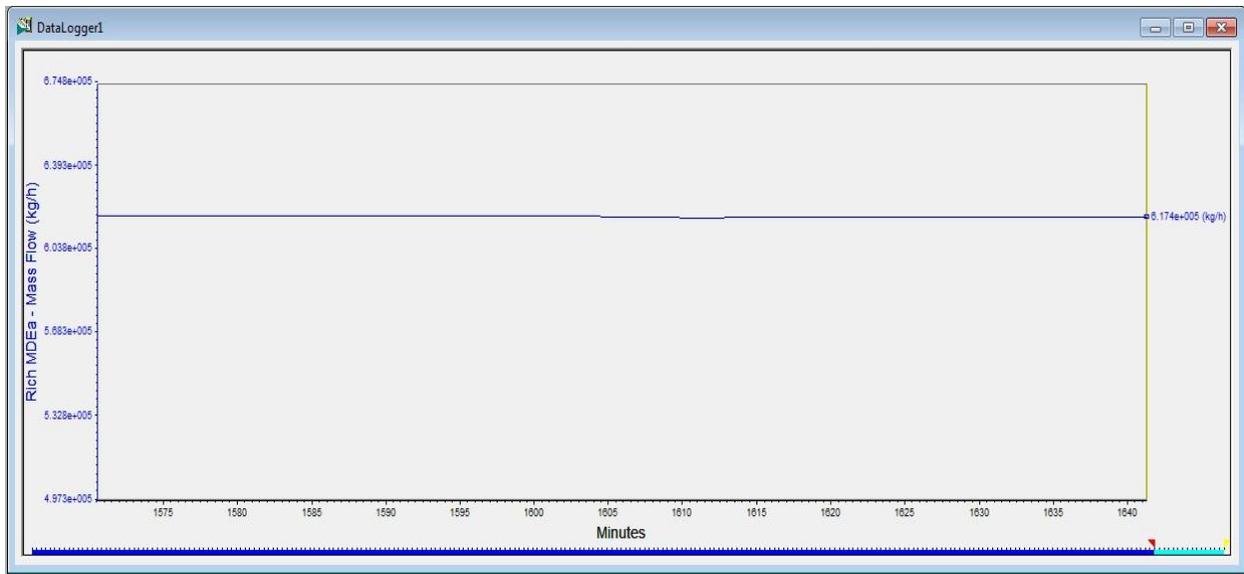


Figure 4.23: Rich amine characteristic after decreased natural gas flow rate 10%

Dynamic Model of CO₂ Removal Using Aspen HYSYS

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ABSTRACT: The objective of this study is to simulate the CO₂ removal process by using Aspen HYSYS. The methodology of this study is divided into two phases. The first phase relates to the model development of steady state and the second phase related to dynamic simulation. In the first phase, the design data are collected from an industry. The simulation results are then compared to the available design data. The second phase basically involves equipment sizing that should be conducted before the dynamic modeling is developed. Validation of dynamic model and real plant data is considered based on normal conditions. The abnormal simulation is then conducted by introducing disturbances and/or faults in the process. As a conclusion, this simulation can be used as training and learning tools for engineers and operators, to understand the dynamic characteristics of the CO₂ removal process and also be able to use the simulation to improve the performance of the CO₂ removal process.

Key words: Aspen HYSYS, carbon dioxide, dynamic simulation.

1. INTRODUCTION

The process of carbon dioxide removal starts from the absorber where lean amine enters the upper stream and the natural gas enters from the lower of the absorber. The reaction occurs and amine absorbs carbon dioxide from natural gas which is called rich amine. Rich amine then transfers to the stripper which releases the carbon dioxide from amine. Then amine is fed back to the absorber, and used all over again. Almost all industries that involve natural gas as a raw material must go through CO₂ removal process before proceeding to further process of natural gas.

The amount of carbon dioxide contents in the natural gas can vary from 4% to 50% depending on the gas source. Before the transportation of natural gas, it must be pre-processed in order to meet the typical pipeline specification of 2–5% carbon dioxide. Aspen Hysys has been used since 2000 to simulate CO₂ removal from gas-based power plants. Aspen Hysys is used in order to calculate permeate and retentate of the system with any number of modules, allowing complex process simulations. The programme has the possibility to use Aspen Hysys capabilities to calculate mass and energy balances and combine in the process model. The important process parameters are flow rates, temperatures, compositions, pressure ratio (between the upstream pressure and downstream pressure over the membrane) and stage cut (ratio of permeate to feed flow rate).

2. METHODOLOGY

Figure 2.1 shows the process flow to make this study successful. The data is taken from the industry to start the simulation in steady-state.

After the whole process is running without any error, then the data from steady-state is taken to make a dynamic simulation at the absorber. Before the dynamic simulation can proceed, sizing and control need to be made. Then the characteristics of the absorption can be observed.

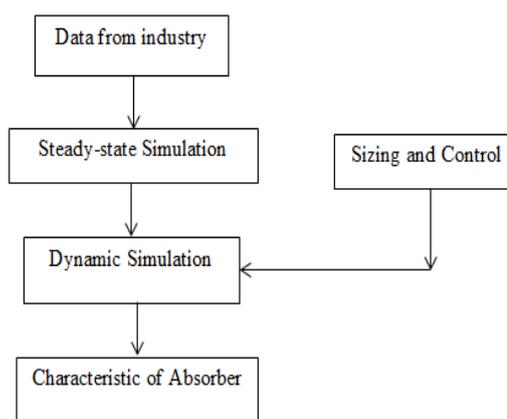


Figure 2.1 Process flow

2. LITERATURE REVIEW

This section will discuss on the process description of the CO₂ and amine as the absorbent in this process.

2.1 Process description

The general process flow diagram of an amine CO₂ removal process is shown in Figure

2.2. The natural gas enters the bottom of the absorber in countercurrent contact with aqueous lean amine solution. Sweet gas leaves the top of the absorber while lean amine that flow downward counter currently to the natural gas and absorbed the CO₂ constituent and become rich solution. The rich solvent from the bottom of the absorber then pass through amine-amine heat exchanger to the stripper where the acid gas absorbed is stripped off at a very high temperature and low pressure. The acid gas then leaves the top of the stripper column. The lean amine from the bottom of the reboiler attached to the stripper flow through amine-amine heat exchanger and through a water air cooler before being introduced back to the top of the absorber.

The amine-amine heat exchanger serves as a heat conservation device. The reminder of the rich solution flows downward through the stripper in countercurrent contact with vapour generated in the reboiler; which strips the acid gas from the rich solution. The stripper overhead products (acid gas and steam) pass through a condenser where the steam is condensed and cooled and returned to the top of the stripper as a reflux, while the acid gas is separated in a separator and sent to the flare or compressed for sequestration process.

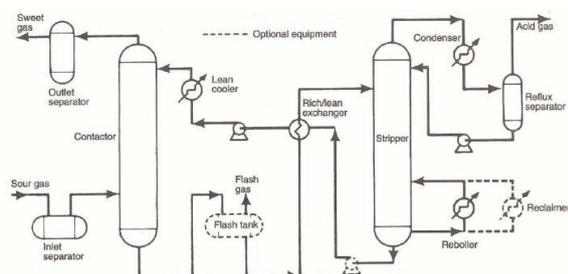
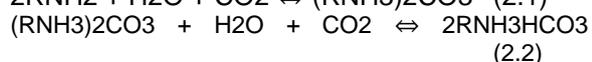
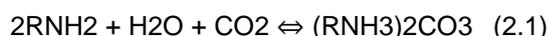


Figure 2.2 Typical Amine Base process Diagram

2.2 Amine Base Process Facilities

The alkanolamines are generally accepted and widely used of the various available solvents for removal of CO₂ from natural gas stream (Bottom, 1930). Monoethanolamine (MDEA) and Diethanolamine (DEA) have made the solvent achieved a pinnacle position in the gas processing industry because of their reactivity and availability at low cost especially. Formation of carbonate bicarbonate:



Formation of carbamate:



The reactions above shown the reaction proceed to the right at low temperature and to

the left at a higher temperature, thus making CO₂ to be absorbed at ambient temperature. The reaction is reversed that is backward reaction is favored at elevated temperature (as obtained in the stripper column) where the carbonate salt formed is decomposed to release the acid gas absorbed, therefore stringent control of stripper column temperature should be adopted to reduce the release of carbonate salt. Reaction (2.1) and (2.2) are slow reaction because carbon dioxide must form carbonic acid with water (slow reaction) before reacting with amine. Elimination of selectivity of hydrogen sulfide is impossible because of reaction (2.3) which predominate when MEA is involved is relatively fast. Methyldiethanolamine (MDEA) and diethanolamine (DEA) are today the most tertiary amines for acid gas removal (Rejoy et.al., 1997).

3 RESULT AND DISCUSSION

3.1 Steady-state Simulation

The table 1 below shows the result from steady-state simulation at the absorber.

Table 1: Component Composition

Name	Sweet gas	Rich MDEA	Acid gas	Recycle MDEA
CH ₄	0.07	0.00	0.00	0.00
H ₂	0.76	0.00	0.00	0.00
N ₂	0.01	0.00	0.00	0.00
CO	0.11	0.00	0.00	0.00
CO ₂	0.02	0.02	0.18	0.00
H ₂ O	0.03	0.90	0.82	0.92
MDEA	0.00	0.08	0.00	0.08

In steady-state simulation, the result for the output stream of absorber and stripper is tabulated. Sweet gas and rich MDEA is output stream of absorber while acid gas and recycle MDEA is output stream for strippers.

3.2 Dynamic Simulation

For the dynamic simulation, an input of flow rate stream is given by increasing and decreasing the flow rate of recycle amine flow rate. The trend or characteristic of CO₂ removal can be observed from the graph in Figure 3.1 and Figure 3.2 below.

The graph in Figure 3.1 shows the flow rate of CO₂ in sweet gas stream after the flow rate of recycle amine at the inlet of the absorber is increased. From the graph, it shows that the flow rate of CO₂ is decreased from 6538.03 kg/hr to 4872.88 kg/hr after an input in applied. From this observation, it can be conclude that, by increasing the recycle amine flow rate, the

amount of CO₂ in the sweet gas is less and the efficiency of CO₂ removal is increase by increasing the amount of amine (MDEA) entering the absorber.

The graph in Figure 3.2 shoes the flow rate of CO₂ in sweet gas stream after the flow rate of recycle amine is decreased. The trend shows the increasing in the amount of CO₂ from 6538.03kg/hr to 8296.91 kg/hr in the sweet gas stream. By observing this trend, it can be conclude that, if the amount of recycle amine entering the absorber is less, the amount of CO₂ in the sweet gas is more.

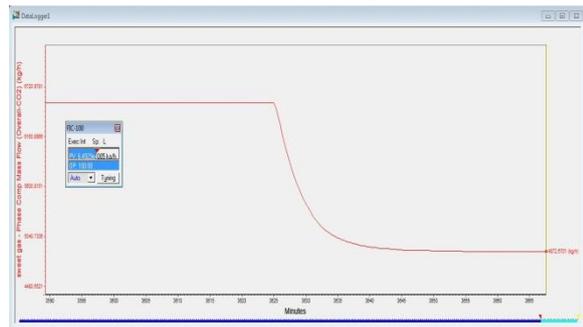


Figure 3.1: Flow rate of CO₂ in sweet gas stream with 10% increase of recycle amine flow rate stream

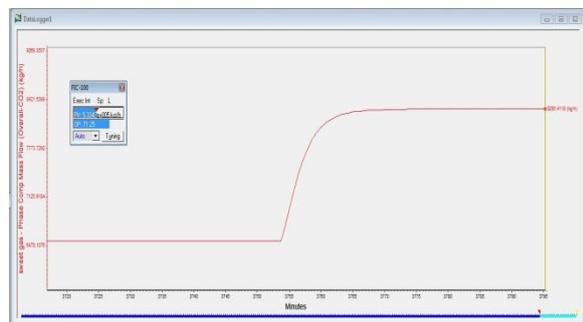


Figure 3.2: Flow rate of CO₂ in sweet gas stream with 10% decrease of recycle amine flow rate stream.

Figure 3.3 shows the flow rate of CO₂ in rich amine after the flow rate of recycle amine is increased. From the observation, it shows that the amount of CO₂ in the rich amine is increased after the flow rate of recycle amine is increased from 26714.76 kg/hr to 29139.58 kg/hr.

In Figure 3.4 shows that the amounts of CO₂ in rich amine steam after the flow rate of recycle amine is decreased. From the observation of Figure 3.4, it shows that the amount of CO₂ in the rich amine stream is less from 26714.76 kg/hr to 24181.56 kg/hr.

An input is given at the natural gas stream is to see if by applied the changes in at the flow rate of natural gas would effects the CO₂ removal. An input that has been applied is by increasing and decreasing the flow rate of natural gas entering the absorber.

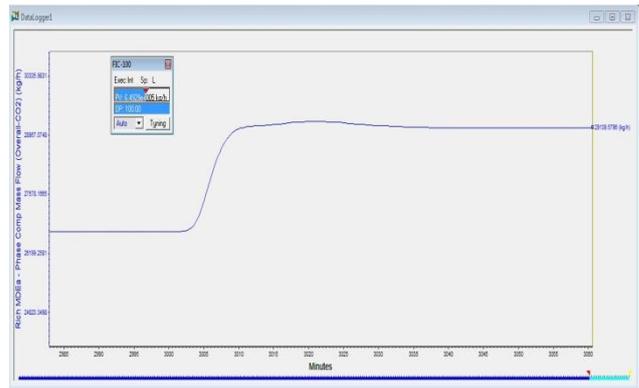


Figure 3.3: Flow rate of CO₂ in rich amine stream with 10% increase of recycle amine flow rate stream.

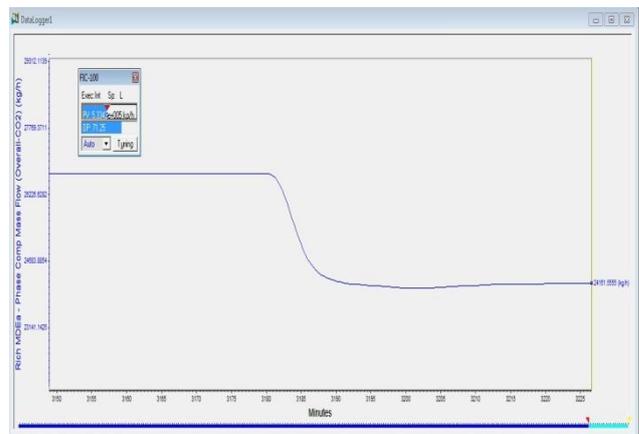


Figure 3.4: Flow rate of CO₂ in rich amine stream with 10% decrease of recycle amine flow rate stream.

Figure 3.5 shows the flow rate of CO₂ in sweet gas stream after the flow rate of natural gas is increased. From the observation of Figure 3.5 below, it shows that the increasing in amount of CO₂ in sweet gas from 6538.03 kg/hr to 8938.25 kg/hr after an input is made.

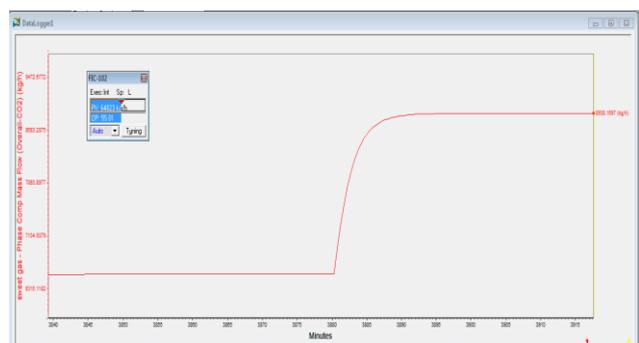


Figure 3.5: Flow rate of CO₂ in sweet gas stream with 10% increase of natural gas flow rate stream.

Figure 3.6 below shows the flow rate of CO₂ in sweet gas after the flow rate of natural gas is decreased. It shows that, the amount of CO₂ in the sweet gas stream is decreased after the flow rate of

natural gas is decreased from 6538.03 kg/hr to 4153.12 kg/hr.

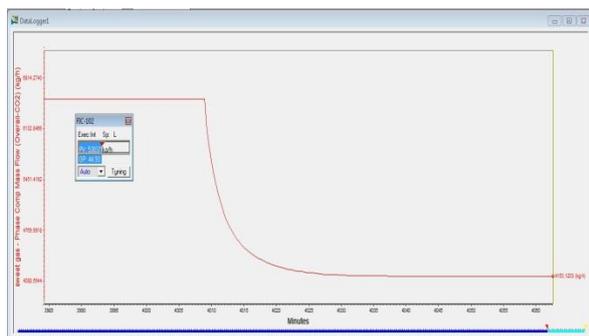


Figure 3.6: Flow rate of CO₂ in sweet gas stream with 10% decrease of natural gas flow rate stream.

Figure 3.7 below is the trend of CO₂ in the rich amine stream after the flow rate of natural gas is increased. The change observed from the Figure 3.7 is the amount of CO₂ in the rich amine stream is slightly increased from 26714.76 kg/hr to 26843.85 kg/hr after an input is made.

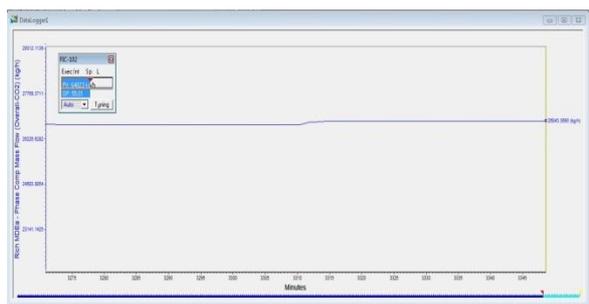


Figure 3.7: Flow rate of CO₂ in rich amine stream with 10% increase of natural gas flow rate stream.

Figure 3.8 shows the flow rate of CO₂ in rich amine stream after the natural gas flow rate is decreased. The CO₂ in the rich amine stream is slightly decreased from 26714.76 kg/hr to 26571.32 kg/hr after the change is made.

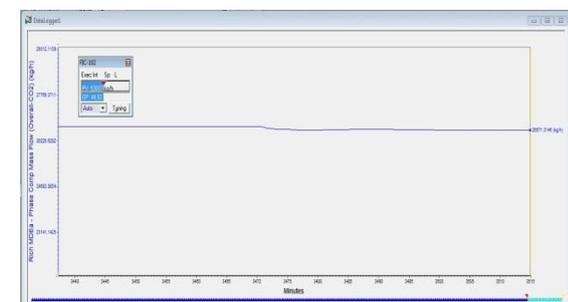


Figure 3.8: Flow rate of CO₂ in rich amine stream with 10% decrease of natural gas flow rate stream.

4. CONCLUSION

Based on the literature reviewed and the results from simulation model the following conclusions can be made:

- The dynamic simulation can be developed using Aspen HYSYS. In this simulation, the component used in real plant is existed and have the same function.
- The characteristics of CO₂ removal can be understand from this simulation.
- The dynamic simulation can be used to control CO₂ removal.
- The performance of CO₂ removal can be improved by using dynamic simulation.

In the future, this simulation can be used widely to obtain the result of the plant process before a real plant can be build. The characteristic of the process can be easily understood by implementing the simulation process and hope that undergraduate student can learn this simulation more in the study.

NOMENCLATURE

percentage	[%]
kilopascal	[kPa]
pounds per square inch pressure	[psi]
degree celcius	[°C]
kilogram	[kg]
volume	[m ³]

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