EFFECT OF DIFFERENT TEMPERATURE USING ENERGY ANALYSIS FOR POWER TO METHANOL PRODUCTION PLANT

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Methanol is one of the valuable chemical that has a high demand all over the world due to its various purposes and usage. Mostly, the large production of methanol are using natural gas as raw material. Lately, the issues of global warming has arising thus it is believed the accumulation of CO2 (carbon dioxide) in the atmosphere is one of the factor that lead to the problem stated. Therefore, one of the way to reduce the CO2 impact to environment is by capturing CO2 from the environment and produce a product which is methanol. As for now, there are no evaluation of energy along with high selectivity and conversion for methanol plant. Usually, the previous researcher only do a research for a higher selectivity but did not including the energy consumption for methanol plant. Therefore, in this paper, the design and simulation of methanol plant also analyzation of the energy consumption using energy analysis is being conducted. There are two objective in this research. First, to design and simulate methanol power to methanol plant using different temperature in the reactor. Second, to analyze the energy consumption of methanol plant using energy analysis by manipulating temperature in the reactor. 3 condition (reactor feed) of methanol plant are simulated using aspen HYSYS V8.8 which are plant 1(442 bar, 280°C), plant 2(76 bar, 280°C) and plant 3 (442 bar, 210°C). The energy is calculated by manual calculation according to standard formula of each equipment and being compared with HYSYS value. From the calculation, it is proven that plant 3 is the least energy required followed by plant 1 and plant 2. For plant 3, the overall energy required is 7,235.992kW that costs RM 256,877.716. Next, plant 2 required 38,655.44kW that costs RM 1,372,623.12 while plant 1 required 10231.1kW that costs RM 363,204.05. Therefore, plant 3 is the least energy and costs required with feed of reactor condition (442 bar, 210°C).

I. INTRODUCTION

The increasing amount of CO_2 being released to the environment has arisen a concern to every community such as industrial community, peoples and government[1]. CO_2 is the main cause of green- house effect thus contribute to global warming. Based on statistic, around one of the third worldwide anthropogenic CO_2 emission comes from industrial activity[2]. This is because, they release a significant amount of CO_2 to the environment without any technology to reduce the emission. With increasing amount of CO_2 at the atmosphere it will contribute to climate change. In order to prevent the accumulation of CO_2 , lot of researchers motivated to study on how to solve the CO_2 problem to environment and how to reduce it. After a lot of research, they found that CO_2 may be captured thus CO_2 should not being released to the environment. There are three method being proposed which are post-combustion capture, pre-combustion capture and oxy-combustion capture. Despite higher cost, this technology is crucial for the preservation of environment.

CO₂ is the contributor to global warming but CO₂ also may be a new material for energy storage[3]. CO2 also may be the key to find the solution for three critical issues facing the world: food ecosystems, the greenhouse issue and energy storage. In order to reduce CO₂ emission to environment, there are three ways. Firstly, use biomass for transportation and heating. Second, non-carbon based electrical energy sources such as wind, solar energy and geothermal energies. Third, use sun power or solar energy for industrial purposes. Carbon capture and storage is one of the way to capture, store and reuse CO₂ as a feedstock in various ways. Carbon capture and storage or abbreviated as CCS aiming to extract CO₂ from flue gasses mostly form power plant, cement plant and many more. This technology aim for 85% CO2 capture and 99.99% purity. In term of sustainability, rather than using energy from carbon source, an improvement of using non-carbon energy source need to be implemented. Sustainability simply mean an avoidance of the depletion natural resources in order to maintain an ecological balance and taking care of social, environment and economic. CO₂ capture is crucial because CO₂ widely known as the material for production of methanol. Methanol is the intermediate product to produce many useable product.CO2 may be transform into methane as said by Paul Sabatier (Nobel laureate of chemistry 1912) who developed the well-known reaction $CO_2 + 4H_2 = CH_4 +$ 2 H₂O.

There are three type of commercialized technology being used for CO_2 capture[2]. It is post-combustion capture, pre-combustion capture and Oxy fuel combustion. All of these technology are set as possible technology to capture CO_2 as the result of brainstorm and literature review by a lot of CO_2 expert researcher. Below is shown the block diagram for the CO_2 capture technology.



Figure I.1: Flow of Post Combustion Capture [2].

For post combustion capture as shown in Figure I.1, the chemical use for absorption is monoethanolamine (MEA) with mass fraction 30%. The flue gas is absorb by absorber and then the CO_2 will go to stripper and DPC (drying, purification cooling & compression) unit. These two unit is installed together to prevent

moisture and unpurified CO_2 to enter the system. Unpurified and wet CO_2 is corrosive to equipment and may corrode the pipeline and pump in plant.



Figure I.2: Flow of Oxyfuel Combustion [2].

Next, Oxyfuel combustion method as in Figure I.2 .Oxyfuel combustion may be distinguished by having air separation unit (ASU) for production of oxygen and CO_2 compressor. In the Oxy-Central configuration, CO_2 gas that at atmospheric pressure is transported to a central location by using blower. DPC takes place at plant level for all oxyfuel combustion to avoid wet flue gas to enter. There are also several adjustment needed in order to convert the furnaces and boiler to oxyfuel mode[2]. In principle, only hydrogen plant is not allowed to follow oxyfuel combustion. MEA and ADIP-X are used to capture CO_2 the same as pre combustion. The result indicate that oxyfuel combustion centralized oxygen production and decentralized CO_2 compression use the most effective and accurate configuration when applying to all industrial plant. This is mainly due to relatively low energy costs compared to post and pre-combustion.

As shown in Figure I.3, methanol can be produced by applying CO_2 capture technology[4]. The hydrogenation of methane to form methanol and hydrogen comes from electrolysis of water. Recycling CO_2 from industrial waste is one of the most efficient and economic also environmental advantage. Methanol is a crucial for replacing gasoline due to its excellent combustion and lower pollution. The majority of large methanol production scale is derived from natural gas. For CO_2 capture, the abatement of CO_2 is highly depend on the waste heat available from the plant to provide thermal energy to capture CO_2 . If the thermal heat is absence, the technology of CO_2 capture may be null. Below is the block diagram for CO_2 capture. The CO_2 is captured from flue gas of coal thermoelectric plant and electrolysis of water producing hydrogen. The process shown is simulated in Aspen Plus. Below is the details of parameter.



Figure I.3: Block Diagram for CO2 Capture [4]

Next is the assessment on energy usage in methanol plant using CHEMCAD. Below is the overall view of methanol Carbon utilisation plant[5]. Therefore, in this section, energy consumption needed in CCU is the main concern. For assessment of energy in Carbon capture utilisation (CCU), it is based on capacity of plant to produce about 440 ktMeOH /year. The energy needed for this plant calculated by considering the studies in pinch analysis, heat exchanger network (HEN) also the financial analysis.



Figure I.4: Block Diagram of CCU Plant[5]

The CCU plant is simulated in CHEMCAD to obtain the parameters needed. As shown, H_2 and CO_2 also utilities being feed to the CCU plant. After reaction occur in the CCU plant, the product will produced which is methanol and by product is water. In CCU plant, the simulation is simulated by CHEMCAD programme. By analysing the CCU plant, its shows that to produce methanol there are many equipment that need energy to work well. The equipment are heat exchanger, boiler, distillation column, furnace, turbine, reactor and many more. All of these equipment's energy need to be fulfilled to ensure they function very well and produce good quality of methanol. Therefore, the analysation and the summary of energy needed in CCU plant is shown below.

Methanol production: 440kt methanol/year Purity: 99.9wt% CO₂ feed: 41,000 std.m3/hr at ambient pressure and temperature. H₂ feed: 123,000 std.m3/hr at 25 bar and ambient temperature. Reactor: Feed condition at 76 bar and 210 °C. Catalyst used: 44,500 kg of Cu/Zn/Al₂O₃.

Energy Consumption on CO₂ Capture Plant Producing 440kt methanol per year:

Electricity for compressor = 16.78MW Electricity for water circulation= 0.58MW Electricity provided by turbines= 8.03MW Heat used to drive the turbines= 37.71MW Heat integrated among process streams= 81.37MW Heating needs= 24.20MW Cooling needs= 47.56MW

II. METHODOLOGY

A. Simulation of plant using HYSYS V8.8

This chapter will focus on the method used to obtain the parameters needed. It also contain the equation and information needed to obtain the result. The first part, the simulation of 3 different methanol plant using Aspen HYSYS V8.8 will be shown including the process flowsheet. Each of the plants have their own condition which are plant 1 is simulated at (442bar, 280°C), plant 2 at (76bar, 280°C) and lastly plant 3 at (442bar, 210°C).

B. Simulation of plant 1 (442 bar, 280°C)



Figure II.1 Process flow diagram of the simulated plant 1 (442 bar, 280°C).

The H₂ fed is 386.1 kg/hr and CO₂ fed is 2831.4 kg/hr. The H₂ fed at 25°C and 30 bar. Then it will be compressed by K-104 to 84.08 bar and 164 °C. CO₂ from the feed at 1 bar and 25 °C will be compressed by K-100,K-101,K-102,K-103 and cool by E-100,E-101,E-102 until it reach 151.6 °C and 84.08 bar before it will mix with H₂. After the mixing, it will mix with recycle stream (26a) and heated again by E-103 before injected to the adiabatic reactor. The adiabatic PFR reactor comes with fixed bed filled with 44,500 kg of Cu/ZnO/Al₂O₃ catalyst. The mixture will fed to the reactor at 280 °C and 442 bar and the reaction occur in the reactor is CO_2 + $3H_2 \leftrightarrow CH_3OH$ (l) + H₂O (g) which is exothermic reaction. The product that come out from reactor will be split to 2 stream which is stream 15 and 18. Stream 15 will be recycle back to E-103 and injected back to the reactor while stream 18 will be sent to E-106. Then. Both of the stream will remix in MIX102 and cooled to 35 °C where methanol and liquid are condensed then separated from the non-reacted gases in knock out drum (KO1). Almost 1% of non-reacted gaseous is purged at 35 °C and 73.4 bar. The liquid stream of KO1 filled by crude methanol which means it consist of methanol, water and residual dissolved gasses. The crude methanol is expanded by 2 series of valve which is VLV101 and VLV102 until the pressure reach at 1.2 bar. Then the compressed crude methanol is fed to flash drum (V-100) to remove all the dissolved gasses present in the crude methanol. The remaining is heated by E-104 until 80 °C and fed to distillation column (T-100) for further separation of methanol and water. The distillation column have 57 stages where 44 stages for rectification and 13 for stripping. The reflux ratio is 1.2. The top product is methanol at 64 °C and 1 bar which is in vapour phase while the bottom product is water at 102 °C and 1.1 bar. The product is methanol with purity 0.9992%.





Figure II.2 Process flow diagram of the simulated plant 1 (76 bar, 280°C).

The H₂ fed is 386.1 kg/hr and CO₂ fed is 2831.4 kg/hr. The H₂ fed at 25 °C and 30 bar. Then it will be compressed by K-104 to 84.08 bar and 164 °C. CO2 from the feed at 1 bar and 25 °C will be compressed by K-100,K-101,K-102,K-103 and cool by E-100,E-101,E-102 until it reach 151.6 °C and 84.08 bar before it will mix with H2. After the mixing, it will mix with recycle stream (26a) and heated again by E-103 before injected to the adiabatic reactor.

The adiabatic PFR reactor comes with fixed bed filled with 44,500 kg of Cu/ZnO/Al2O3 catalyst. The mixture will fed to the reactor at 280 °C and 76 bar by the addition of cooler E-107 to achieve the desired reactor inlet temperature and the reaction occur in the reactor is $CO_2 + 3H_2 \leftrightarrow CH_3OH(l) + H2O(g)$ which is exothermic reaction. The product that come out from reactor will be split to 2 stream which is stream 15 and 18. Stream 15 will be recycle back to E-103 and injected back to the reactor while stream 18 will be sent to E-106. Then. Both of the stream will remix in MIX102 and cooled to 35 °C where methanol and liquid are condensed then separated from the non-reacted gases in knock out drum (KO1). Almost 1% of non-reacted gaseous is purged at 35 °C and 73.4 bar. The liquid stream of KO1 filled by crude methanol which means it consist of methanol, water and residual dissolved gasses. The crude methanol is expanded by 2 series of valve which is VLV101 and VLV102 until the pressure reach at 1.2 bar. Then the compressed crude methanol is fed to flash drum (V-100) to remove all the dissolved gasses present in the crude methanol. The remaining is heated by E-104 until 80 °C and fed to distillation column (T-100) for further separation of methanol and water. The distillation column have 57 stages where 44 stages for rectification and 13 for stripping. The reflux ratio is 1.2. The top product is methanol at 64 °C and 1 bar which is in vapour phase while the bottom product is water at 100.7 °C and 1.1 bar. The product is methanol with purity 0.9943%.

D. Simulation of plant 3 (442 BAR, 210°C)



Figure II.3 Process flow diagram of the simulated plant 1 (442 BAR, 210°C).

The H₂ fed is 386.1 kg/hr and CO₂ fed is 2831.4 kg/hr. The H₂ fed at 25°C and 30 bar. Then it will be compressed by K-104 to 84.08 bar and 164 °C. CO₂ from the feed at 1 bar and 25 °C will be compressed by K-100,K-101,K-102,K-103 and cool by E-100,E-101,E-102 until it reach 151.6 °C and 84.08 bar before it will mix with H2. After the mixing, it will mix with recycle stream (26a) and heated again by E-103 before injected to the adiabatic reactor. The adiabatic PFR reactor comes with fixed bed filled with 44,500 kg of Cu/ZnO/Al₂O₃ catalyst. The mixture will fed to the reactor at 210 $^{\circ}$ C and 442 bar and the reaction occur in the reactor is CO2 + $3H_2 \leftrightarrow CH_3OH(l) + H_2O$ (g) which is exothermic reaction. The product that come out from reactor will be split to 2 stream which is stream 15 and 18. Stream 15 will be recycle back to E-103 and injected back to the reactor while stream 18 will be sent to E-106. Then. Both of the stream will remix in MIX102 and cooled to 35 °C where methanol and liquid are condensed then separated from the non-reacted gases in knock out drum (KO1). Almost 1% of non-reacted gaseous is purged at 35 °C and 73.4 bar.

The liquid stream of KO1 filled by crude methanol which means it consist of methanol, water and residual dissolved gasses. The crude methanol is expanded by 2 series of valve which is VLV101 and VLV102 until the pressure reach at 1.2 bar. Then the compressed crude methanol is fed to flash drum (V-100) to remove all the dissolved gasses present in the crude methanol. The remaining is heated by E-104 until 80 °C and fed to distillation column (T-100) for further separation of methanol and water. The distillation

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column have 57 stages where 44 stages for rectification and 13 for stripping. The reflux ratio is 1.2. The top product is methanol at 64 $^{\circ}$ C and 1 bar which is in vapour phase while the bottom product is water at 102 $^{\circ}$ C and 1.1 bar. The product is methanol with purity 0.9991%.

E. Formula for energy calculation in methanol plant. 1. Equation of heater and cooler duty[7]:

$$Q = \dot{m} \times C_{p,average} \times \Delta T$$

Where:

 \dot{m} =Molar flowrate (Kmol/hr) Cp = Specific heat capacity,(kJ/(Kgmole.°C) Δ T= temperature,°C

2. Equation heat exchanger duty[7]:

$$\Delta T_{\rm im} = \frac{\Delta T2 - \Delta T1}{\ln\left(\frac{T2}{T_1}\right)} \text{ or } \frac{(T_{\rm hi} - T_{\rm CO}) - (T_{\rm ho} - T_{\rm ci})}{\ln((T_{\rm hi} - T_{\rm CO})/(T_{\rm ho} - T_{\rm ci}))}$$

Where:

 $Q(w) = UA\Delta T_{lm}$

U= Film heat transfer coefficient $\left(\frac{W}{m^2 \circ C}\right)$)

A = Total heat transfer area (m²) Δ Tlm = log mean temperature difference (°C)

3. Equation of compressor duty[7]:

Power (KW) = mz_1 RT_1 [
$$\frac{\left(\frac{P_2}{P_1}\right)^{\alpha} - 1}{\alpha}$$
]

m= molar flowrate (mol/s)

z = compressibility

P = pressure (bar)

 T_1 = inlet temperature (K) R = 8.314 J/mol k

 $K = C_P/C_V$

4. Equation of condenser duty[7]:

$$Q_{condenser}(kW) = \dot{m}(H_f - H_v)(\mathbf{I})$$

Where:

 \dot{m} = inlet mass flowrate of condenser (kg/s) H_f = Mass enthalpy aqueous phase (kJ/kg) H_v =Mass enthalpy vapour phase (kJ/kg) T = Reflux ratio

5. Equation of reboiler duty[7]: Qreboiler = (D ×D_H) + (B ×B_H) + Q condenser - (Fi ×F_H)

Where,

 $\begin{array}{l} D= Distillate flow (kg/hr) \\ D_{H} = Distillate mass enthalpy (kJ/kg) \\ B= Bottom mass flow (kg/hr) \\ B_{H} = Bottom enthalpy (kJ/kg) \\ Qcondenser = Condenser duty (kJ/hr) \\ F_{i} = Feed in mass flowrate (kg/hr) \\ F_{i,H} = Feed in mass enthalpy (kJ/kg) \end{array}$

III. RESULTS AND DISCUSSION

Table III.1 Energy analysis of heater and cooler in all 3 plant.					
Plant	Equipment	Q, manual	Q, Hysys	Error (%)	
		calculation	Data (kW)		
		(kW)			

1	E-100	69.58	69.92	0.49
	E-101	91.29	91.38	0.10
	E-102	84.51	84.58	0.08
	E-105	1576.85	1605	1.75
	E-106	1171	1171	0.00
	E-107	352.46	352.40	0.02
	E-108	1039.34	1039	0.03
	Total	4385.03	4413.30	0.64
2	E-100	69.60	69.62	0.03
	E-101	91.30	91.38	0.09
	E-102	84.51	84.58	0.08
	E-105	129.00	129.12	0.09
	E-106	80.66	80.10	0.70
	E-107	189.20	189.24	0.02
	Total	644.27	644.04	0.04
3	E-100	69.58	69.62	0.06
	E-101	91.29	91.38	0.10
	E-102	84.51	84.58	0.08
	E-105	1723	1730	0.40
	E-106	928.00	928.50	0.05
	E-107	326.21	326.20	0.00
	E-108	779.54	779.50	0.01
	Total	4002.13	4009.80	0.20

Table III.2 Energy analysis of compressor in 3 plant.				
Plant	Equipment	Q, manual	Q, Hysys	Error
		((kW)	Data (kW)	(%)
1	K-100	78.76	78.56	0.25
	K-101	91.67	91.38	0.32
	K-102	84.78	84.58	0.24
	K-103	82.26	82.06	0.24
	K-104	211.33	211.40	0.03
	K-105	96.33	96.38	0.05
	K-106	1219	1219	0.00
	K-107	724.40	724.40	0.00
	Total	2588.50	2587.80	0.03
2	K-100	78.76	78.56	0.25
	K-101	91.67	91.38	0.32
	K-102	84.78	84.58	0.24
	K-103	82.26	82.06	0.24
	K-104	211.33	211.40	0.03
	K-105	1949.19	1948	0.06
	TOTAL	2498.00	2496.00	0.08
3	K-100	78.76	78.56	0.25
	K-101	91.67	91.38	0.32
	K-102	84.78	84.58	0.24
	K-103	82.26	82.06	0.24
	K-104	211.33	211.40	0.03
	K-105	64.57	64.60	0.05

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TOTAL	2078 20	2076 70	0.00
K-106	918.59 546.20	917.90 546.20	0.08

Table III.3 Energy analysis of Heat exchanger in all 3 plant.

Plant	Equipmen	Q,	Q,	Error
	t	manual	HYSYS	(%)
		calculation	(kW)	
		(kW)		
1	E-103	1116	1115	0.09
	E-104	344.44	344.44	0
	Total	1460.44	1459.44	0.09
2	E-103	33262.65	33277.78	0.05
	E-104	856.12	851.94	0.49
	Total	34118.770	34129.72	0.03
3	E-103	416.01	416.11	0.02
	E-104	279.22	279.72	0.18
	Total	695.23	695.83	0.10

Table III.4 Energy analysis of condenser.

Plant	Equipment	Q, manual (kW)	Q, HYSYS (kW)	Error, (%)
1	E12	695.832	696.6	0.11025
2	E12	779.45	779.44	0.0007
3	E12	940.62	942.30	0.1780

Table 1	III.5	Energy	analysis	of reboile	:1
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Plant	Equipment	Qr, manual(kW)	Q r, HYSYS(kW)	Error (%)
1	e13	1073.44	1074	0.05
2	e13	652.50	653.6	0.17
3	e13	1392.41	1396	0.26

Table III.6 comparison of total energ	5	1
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Plant	Q(kW)	Costs (RM)
1	10,231.1	363,204.05

2	38,655.44	1,372,623.12
3	7,235.992	256,877.716

The analysed energy analysis of every equipment had an error less than 2%[5] to HYSYS value which indicate that manual calculation is acceptable,

As shown in table above, the comparison on energy needed for the equipment in each plant is calculated. All the energy required by cooler, heater, compressor, reboiler and condenser in each plant is being sum up. For plant 1, the overall energy required is 10203.4kW when it is manually calculated and 10231.1kW from HYSYS value. Referring to TNB, the current industrial tariff is at RM35.50/kW .The total cost for 10231.1kW for industrial plant is RM363, 204.05.

As for plant 2, the total power required calculated manually is 38655.5kW while 38665.44kW is the HYSYS value. The total cost required is RM1, 372,623.12. Plant 3 shows that power required for whole plant is 6913.814kW when calculated manually. HYSYS data shows that plant 3 needs 7235.992kW that costs RM256, 877.716.

IV. CONCLUSION

The simulation of 3 plant has been done in this work which are plant 1, plant 2 and plant 3. The analysis from this work shows that plant 3 has the least cost for power supply followed by plant 1 and the last is plant 2. Plant 3 reactor feed inlet condition is at (442 bar, 210°C) while plant 1 at (442bar, 280°C) and plant 2 at (76 bar, 280°C). The analysis of energy had been conducted in every methanol plant. The results shows that the large difference of power requirement of each plant mainly because of the high difference of heat exchanger power requirement to meet the condition of reactor R-101 feed. For plant 3, E-13 require duty at 416.11kW, plant 1 require 1115kW while for plant 2 it require 332277.78kW. The difference E-103 duty makes a huge different to power supply needed for every plant. The temperature parameter before entering the reactor also playing a significant role. This can be proven, as the higher the temperature upon entering the reactor, the higher the energy needed to operate the plant. In this case, high energy needed by the heat exchanger specifically. It also shows that plant 3 has the least energy and costs required followed by plant 1 and plant 2. For plant 3, the overall energy required is 7,235.992kW that costs RM 256,877.716. Next, plant 2 required 38,655.44kW that costs RM 1,372,623.12 while plant 1 required 10231.1kW that costs RM 363,204.05. As for future work, some modification need to be done to increase the accuracy of the result. First is, consider or use more suitable fluid package in aspen HYSYS V8.8. In this work, NRTL is being used. Second is, try a different parameter entering the reactor feed such as low temperature but still suitable for reaction. This may because the energy needed is reduced because temperature is directly proportional to power. Third is, a proper equipment used for simulation in aspen HYSYS V8.8 such as higher efficiency of compressor because there is so many compressor in plant 1, plant 2 and plant 3.

ACKNOWLEDGMENT

Thank you to my supervisor and Universiti Teknologi Mara.

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