

**PROCESS DESIGN AND INTEGRATION OF SHALE GAS TO  
METHANOL**

An Undergraduate Research Scholars Thesis

by

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## **ABSTRACT**

Process Design and Integration of Shale Gas to Methanol. (May 2013)

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Recent breakthroughs in horizontal drilling and hydraulic fracturing technology have made huge reservoirs of previously untapped shale gas and shale oil formations available for use. These new resources have already made a significant impact on the United States chemical industry and present many opportunities for new capital investments and industry growth. As in conventional natural gas, shale gas contains primarily methane, but some formations contain significant amounts of higher molecular weight hydrocarbons and inorganic gases such as nitrogen and carbon dioxide. These differences present several technical challenges to incorporating shale gas with current infrastructure designed to be used with natural gas. However, each shale presents opportunities to develop novel chemical processes that optimize its composition in order to more efficiently and profitably produce valuable chemical products.

This paper is aimed at process synthesis, analysis, and integration of different processing pathways for the production of methanol from shale gas. The composition of the shale gas feedstock is assumed to come from the Barnett Shale Play located near Fort Worth, Texas, which is currently the most active shale gas play in the US. Process simulation and published data were used to construct a base-case scenario in Aspen Plus. The impact of different processing

pathways was analyzed. Key performance indicators were assessed. These include overall process targets for mass and energy, economic performance, and environmental impact. Finally, the impact of several factors (e.g., feedstock composition, design and operating variables) is studied through a sensitivity analysis.

The results show a profitable process above a methanol selling price of approximately \$1.50/gal. The sensitivity analysis shows that the ROI depends much more heavily on the selling price of methanol than on the operating costs. Energy integration leads to a savings of \$30.1 million per year, or an increase in ROI of 2% points. This also helps offset some of the cost required for the oxygen necessary for syngas generation through partial oxidation. For a sample shale gas composition with high levels of impurities, preprocessing costs require a price differential of \$0.73/MMBtu from natural gas. The process is also environmentally desirable because shale gas does not lead to higher GHG emissions than conventional natural gas. More water is required for hydraulic fracturing, but some of these concerns can be abated through conservation techniques and regulation.

## **DEDICATION**

To my family and friends,

For encouraging me to pursue undergraduate research and supporting me through the entire process.

## **ACKNOWLEDGEMENTS**

Thanks to Dr. Mahmoud El-Halwagi for assistance with the process analysis, energy integration, and cost estimation, Kerron Gabriel for assistance with process design and simulation set up, and Mohamed Nouredin for assistance with process design.

## NOMENCLATURE

C2 – ethane

C3 – propane

DEA – diethanolamine

GHG – greenhouse gas

kWh – kilowatt hour

LPG – liquefied petroleum gas

MDEA – methyldiethanolamine

MEA – monoethanolamine

MeOH – methanol

MMscf – million standard cubic feet

MMBtu – million Btu (British thermal unit)

NGL – natural gas liquids

ROI – return on investment

WGS – water-gas shift

# CHAPTER I

## INTRODUCTION

In order to meet the energy demands of the twenty-first century, engineers and scientists are working to develop new methods of discovering, extracting, and refining fossil fuels including oil, coal, and natural gas. While the development of alternative energy technologies continues and the use of renewable energy sources increases, fossil fuels still fulfill the majority of the United States' energy needs: approximately 85%, with natural gas supplying about 22% of the total [1].

Natural gas is an odorless, colorless mixture of light hydrocarbons and other gases. The primary component is methane, with the remaining fraction consisting of a mixture of heavier hydrocarbons including ethane and propane. Crude natural gas may also contain other light gases such as nitrogen, helium, and water in small concentrations. Table 1 shows the variability of natural gas concentration and composition due to variations from individual wells.

In light of concerns about environmental pollution and greenhouse gas emissions, consumption of natural gas as a fuel source has grown due to its clean burning nature and high energy content. The main byproducts of combustion of natural gas are carbon dioxide and water, according to the chemical reaction below.





Additional byproducts include carbon monoxide, sulfur dioxide, nitrogen oxides, and hydrocarbons; however, these chemicals are present in much lower concentrations in natural gas than in other fossil fuels.

Table 1. Chemical Composition of Conventional Natural Gas [2]

<b>Components</b>	<b>Formula</b>	<b>Typical (mol %)</b>	<b>Extreme (mol %)</b>
Methane	CH <sub>4</sub>	80-95	50-95
Ethane	C <sub>2</sub> H <sub>6</sub>	2-5	2-20
Propane	C <sub>3</sub> H <sub>8</sub>	1-3	1-12
Butane	C <sub>4</sub> H <sub>10</sub>	0-1	0-4
C5 Alkanes and higher hydrocarbons	C <sub>5</sub> +	0-1	0-1
Carbon Dioxide	CO <sub>2</sub>	1-5	0-99
Nitrogen	N <sub>2</sub>	1-5	0-70
Hydrogen Sulfide	H <sub>2</sub> S	0-2	0-6
Oxygen	O <sub>2</sub>	0	0-0.2
Helium	He	0-0.1	0-1
Other inert gases	traces		

Natural gas has an additional advantage over other fossil fuels due to its large domestic availability, which addresses political and economic concerns over dependence on foreign oil supplies. In the United States, 84% of the natural gas consumed is produced in the country and 97% is produced in North America [1]. As energy needs continue to rise, natural gas will remain an important resource in the American economy. Natural gas is a key resource for many diverse sectors of the economy, including industrial chemicals and fuels, power generation, transportation fuels, and residential heating.

### **The emerging shale gas industry in the United States**

As the demand for natural gas continues to rise, new sources and techniques for extracting natural gas are being developed. Unconventional production, which includes but is not limited to

shale gas production, now accounts for 46% of the total U.S. production of natural gas [1]. Shale gas production in the United States has been growing consistently over the past decade and Figure 6 shows that shale gas is projected to increase over the next twenty-five years to become the primary source of natural gas produced in the United States. Shale gas includes natural gas sources from low-permeability shale, a sedimentary rock that consists primarily of consolidated clay-sized particles [1]. The low natural permeability of shale has been the limiting factor to the production of shale gas resources because only small volumes of gas flow naturally to a wellbore [1]. However, breakthroughs in modern drilling technology have made it possible to increase gas flow from the shale formation and make development of shale reservoirs economical.

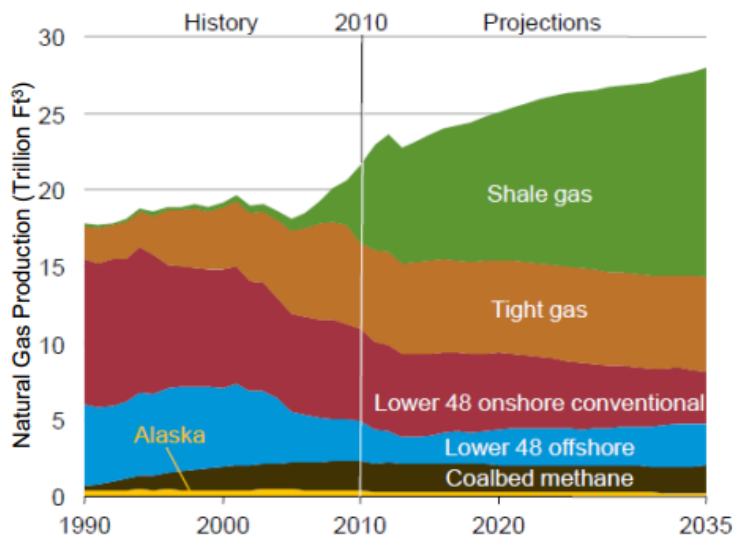


Figure 1. Projections of U.S. Shale Gas Production [3]

The primary difference between modern shale gas development and conventional natural gas development is the extensive use of modern drilling techniques such as horizontal wells and hydraulic fracturing. Drilling of shale gas wells includes both traditional vertical wells as well as horizontal wells. Horizontal well drilling has been an increasingly utilized technique because

it provides exposure to greater volume of a formation: a single well pad with horizontal wells can access the same reservoir volume as sixteen vertical wells [1]. As a result, fewer drill pads are necessary which also reduces the infrastructure necessary to develop a well. While helping to optimize product recovery and profit, these techniques can also help to reduce the overall environmental impact of gas recovery and production. The hydraulic fracturing technique is also used to increase the well's exposure to natural gas in a rock formation. This is achieved by injection of a fluid under high pressure into the formation, which relieves the internal stresses and causes cracks to form in the rock. Fracturing fluids are typically composed of a mixture of water and sand with chemical additives.

Like in conventional natural gas, the largest fraction of shale gas consists of methane. However, some shale gas formations contain significant amounts of higher molecular weight hydrocarbons, including ethane and propane, as well as other inorganic gases such as nitrogen and carbon dioxide. Compounds in shale gas may not be present in natural gas or may be present only in negligible amounts. These differences present several technical challenges to incorporating the use of shale gas with current infrastructure designed to be used with conventional natural gas. However, each shale gas basin presents many opportunities to develop novel chemical processes that optimize its composition in order to more efficiently and profitably produce valuable chemical products.

### **Natural gas processing**

Once the crude natural gas has been extracted from underground reservoirs, it must be processed to remove impurities resulting from the drilling process or from the well itself before the gas can

be used in an industrial or commercial application. Although no national standards exist, each pipeline has strict specifications for heat content, removal of particulate matter, and maximum concentrations of contaminants such as nitrogen, carbon dioxide, and hydrogen sulfide, and natural gas liquids. Some of the most common impurities found in natural gas are listed below in Table 2.

Table 2. Common Impurities In Natural Gas [4]

<b>Name/Description</b>	<b>Formula</b>
Hydrogen Sulfide	H <sub>2</sub> S
Carbon Dioxide	CO <sub>2</sub>
Water Vapor	H <sub>2</sub> O
Sulfur Dioxide	SO <sub>2</sub>
Nitrogen Oxides	NO, NO <sub>2</sub>
Volatile Organic Compounds (VOCs)	
Volatile Chlorine Compounds	HCl, Cl <sub>2</sub>
Volatile Fluorine Compounds	HF, SiF <sub>4</sub>
Basic Nitrogen Compounds	
Carbon Monoxide	CO
Carbonyl Sulfide	COS
Carbon Disulfide	CS <sub>2</sub>
Organic Sulfur Compounds	
Hydrogen Cyanide	HCN

Processing of natural gas involves three main steps: removal of impurities, dehydration, and separation into light and heavy fractions. In order to prepare the crude gas for processing, acid-forming components such as carbon dioxide and hydrogen sulfide must be removed. Next, dehydration is central to the purification process in order to prevent condensation inside pipelines during transport. Similarly, some pipeline standards do not allow for high nitrogen content, so nitrogen is typically removed via a cryogenic separation process and discharged to the atmosphere. Additionally, drilling process water must be treated due to soluble contaminants

from the gas and particulate matter (i.e. dirt and sand) which infiltrate the water during the drilling process. Figure 2 summarizes the major steps in processing crude natural gas.

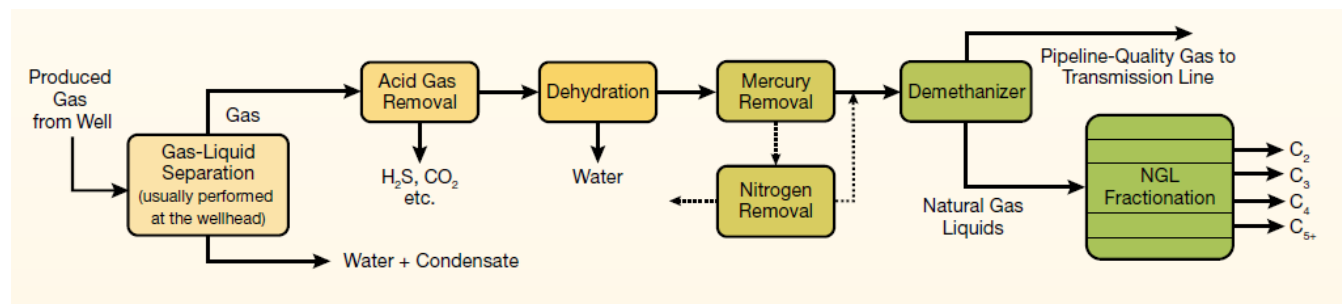


Figure 2. Natural Gas Purification Process [5]

The primary acid forming components in natural gas are carbon dioxide (CO<sub>2</sub>) and hydrogen sulfide (H<sub>2</sub>S). Many techniques have been developed to remove these components either together or with selectivity for one component. One technique that serves to remove both components is absorption with an alkanolamine, such as monoethanolamine (MEA), diethanolamine (DEA), or methyldiethanolamine (MDEA).

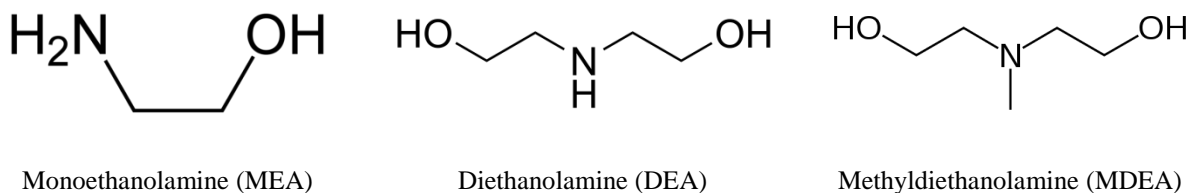


Figure 3. Alkanolamines for Acid-Gas Removal

In the alkanolamine molecules, the hydroxyl group serves to reduce vapor pressure and increase water solubility while the amino group reacts with the acidic gases. Additionally, acid-gas components can be removed from natural gas with physical solvents, catalytic reactions, or other absorbents including ammonium salts and water.

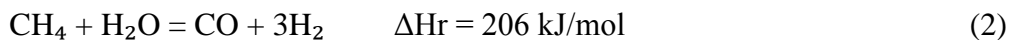
Water vapor can be removed through adsorption in glycol solution or adsorption on solid desiccants such as silica and alumina. Water can also be used as an absorbent to remove other impurities including major contaminants like ammonia, hydrogen cyanide, sulfur dioxide, and carbon dioxide.

Once impurities are removed from natural gas feedstocks, the hydrocarbons are separated into light and heavy fractions through cooling and partial condensation in a heat exchanger. Modern plants use cryogenic separation to separate propane and butane, also known as liquefied petroleum gas (LPG). In this process, crude gas is cooled and partially condensed under high pressure in a heat exchanger, then expanded, heated and sent to a separation column where the bottoms products consist of the C3 plus products. The light hydrocarbons (ethane and methane) are recycled from the top of the column. Ethane is separated in a similar manner as the LPG process, but with a lower temperature profile.

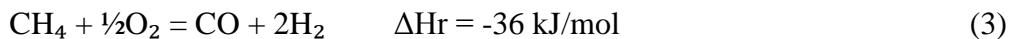
### **Synthesis gas generation**

Natural gas serves as an important raw material for the production of many industrial chemicals. One of the most important derivatives of natural gas is synthesis gas, a mixture of carbon monoxide, hydrogen, and nitrogen gases. Synthesis gas is the primary feedstock for the manufacture of several essential commodity chemicals including methanol and ammonia. Purification of crude natural gas is necessary for the production of synthesis gas because components such as sulfur and chlorides poison the nickel catalyst used to generate synthesis gas. Common methods for the generation of synthesis gas include steam reforming, partial

oxidation, and autothermal reforming. In steam reforming, the primary component of natural gas, methane, reacts with water according to the following endothermic reaction:



For partial oxidation, methane is reacted with oxygen from air according to the following exothermic reaction:



Oxygen present in excess or insufficient amounts will result in the formation of byproducts carbon dioxide and coke (solid carbon). Autothermal reforming combines the previous two techniques by using the energy generated from partial oxidation of hydrocarbons to drive the endothermic reaction in steam reforming.

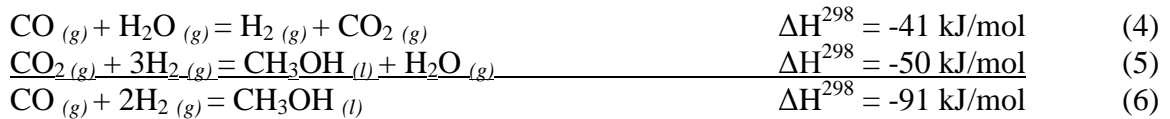
### **Methanol production**

Methanol, also known as methyl alcohol or wood alcohol, is a clear, colorless, flammable liquid with the chemical formula  $\text{CH}_3\text{OH}$ . Methanol is among one of the ten most important organic chemicals because it plays a crucial role as a reactant in the manufacture of many other basic chemical compounds. Approximately forty percent of methanol produced goes into formaldehyde production, which occurs by oxidizing methanol in the presence of a copper catalyst resulting in dehydrogenation. Acetic acid can also be produced by reacting methanol with carbon monoxide.

Methanol is typically produced on an industrial scale using a catalytic reaction of synthesis gas at high pressure. In order to produce methanol, first syngas must be generated from the primary feed source using one of the methods discussed in the previous section. Typically, synthesis gas

is generated from natural gas but current research is developing syngas generation methods utilizing gasification of biomass and gasification of coal. The product stream includes hydrogen and carbon monoxide gas as well as a small amount of unreacted methane, nitrogen, and carbon dioxide.

Equilibrium for methanol formation is favored by low temperatures and high pressures, so the reactor feed conditions are typically 50-100 atm and 230-260 °C [6]. The reaction takes place over a CuO/ZnO/Al<sub>2</sub>O<sub>3</sub> catalyst. Methanol synthesis actually occurs as a combination of two reactions in the syngas mixture: the first involving carbon dioxide and hydrogen and the second involving carbon monoxide and water generated in the system. The overall reaction shows a net exothermal conversion of carbon monoxide and hydrogen gases, the primary components of syngas, to liquid methanol.



During this process, some side reactions occur which form impurities including dimethyl ether, methyl formate, and butanol, which must be removed during the final purification of the process.



## CHAPTER II

### METHODS

Differences in shale gas composition present both challenges and opportunities for innovation in the chemical industry. In this text, the production of methanol from synthesis gas will serve as a sample industrial process to explore some of these possibilities.

Process simulation using ASPEN Plus and published data were used to simulate at 5,000 ton per day methanol plant as the base case. The complete process flow diagrams can be found in Appendix A. The front end of the process, which includes synthesis gas generation through partial oxidation, was modeled using data from Buping, et al. (2010) [7]. For this analysis, the partial oxidation process was selected for the simulation of syngas generation because the reaction is exothermic and does not yield excess hydrogen. The maximum yield for synthesis gas generation occurs when the components are present in a stoichiometric ratio, 2:1. Partial oxidation leads to a CO/H<sub>2</sub> ratio very close to the optimum, about 1.8. However, cost optimization among the three syngas generation processes requires a much more complex analysis which is beyond the scope of this text. The reader may refer to Nouredin et al. (2012) for more information on these design considerations [8]. The methanol reactor was modeled using temperature and pressure conditions cited above and primary chemical reactions and side reactions using the RGIBBS thermodynamic equilibrium model of ASPEN Plus simulation.

In order to perform the analysis, information was gathered from various sources in order to estimate capital cost and operating costs. Cost of utilities, raw materials, and labor were extracted from literature coupled with simulation results [9-11].

Shale gas preprocessing cost and profit from NGL separation was estimated from literature values and flow rates from the simulator. The preprocessing cost was then used to determine a price differential between natural gas and shale gas. The chemical composition of shale gas represented using values from gas produced from the Barnett Shale play, located in northeast Texas near the Fort Worth area [1]. The area was first developed in the 1980's and was nicknamed the "Grandfather Shale," because it served as the development ground for the modern techniques that made shale gas production economical in the United States. It continues to be the most active shale gas play in the United States, which is why this location was selected as the feed for this study [1]. Values for composition of various wells from the Barnett Shale are shown in Table 3.

Table 3. Barnett Shale Gas Composition [12]

Well	C1	C2	C3	CO <sub>2</sub>	N <sub>2</sub>
1	80.3	8.1	2.3	1.4	7.9
2	81.2	11.8	5.2	0.3	1.5
3	91.8	4.4	0.4	2.3	1.1
4	93.7	2.6	0.0	2.7	1.0
Avg	86.8	6.7	2.0	1.7	2.9

These data show the wide variability of possible chemical compositions of shale gas formations. While some areas of the Barnett Shale Play are fairly consistent with conventional natural gas sources, others contain much higher concentrations of hydrocarbons, carbon dioxide and

nitrogen. Data from Well 1 was used in the simulation in order to analyze the scenario with the highest deviation from conventional natural gas composition.

## CHAPTER III

### RESULTS

#### Economic

Detailed stream data from the process simulation can be found in Appendix B. A basis of 7,920 operating hours per year is used. Stream data along with cost estimations were used to generate the following cost and sales estimations.

Table 4. Cost and Sales Estimation

				<b>MM \$</b>	
<b>Fixed Capital Investment</b>				1,300.00 [13]	
<b>Operating Costs</b>	<b>Flow Rate</b>		<b>Unit Cost (\$)</b>		<b>Cost (MM\$/y)</b>
<b>Raw</b>					
<b>Materials</b>	Natural Gas	155.8 MMscf/d	3.50 /Mscf [14]		179.95
	Oxygen	361394 lb/hr	0.05 /lb [15]		143.11
<b>Utilities</b>	Heating	179.95 MMBtu/hr	4.00 /MMBtu		1.43
	Cooling	1829.78 MMBtu/hr	1.50 /MMBtu		21.74
	Power	14746 kWh	0.05 kWh		0.24
	Waste Treatment	94963 lb/hr	0.53 /tonne		0.18
<b>Labor</b>					3.80
<b>Sales</b>	<b>Flow Rate</b>		<b>Unit Price (\$)</b>		<b>Annual Sales (\$MM/y)</b>
			2.00 /gal or		1000.00
<b>Methanol</b>	5000 TPD		0.30 /lb		

A sensitivity analysis was performed to evaluate the ability of the process to withstand changes in feedstock and product values. Figure 4 shows the ROI against methanol price ranging from \$1.00 - \$4.00 per gallon and natural gas price ranging from \$2.00 to \$6.00 per MMBtu.

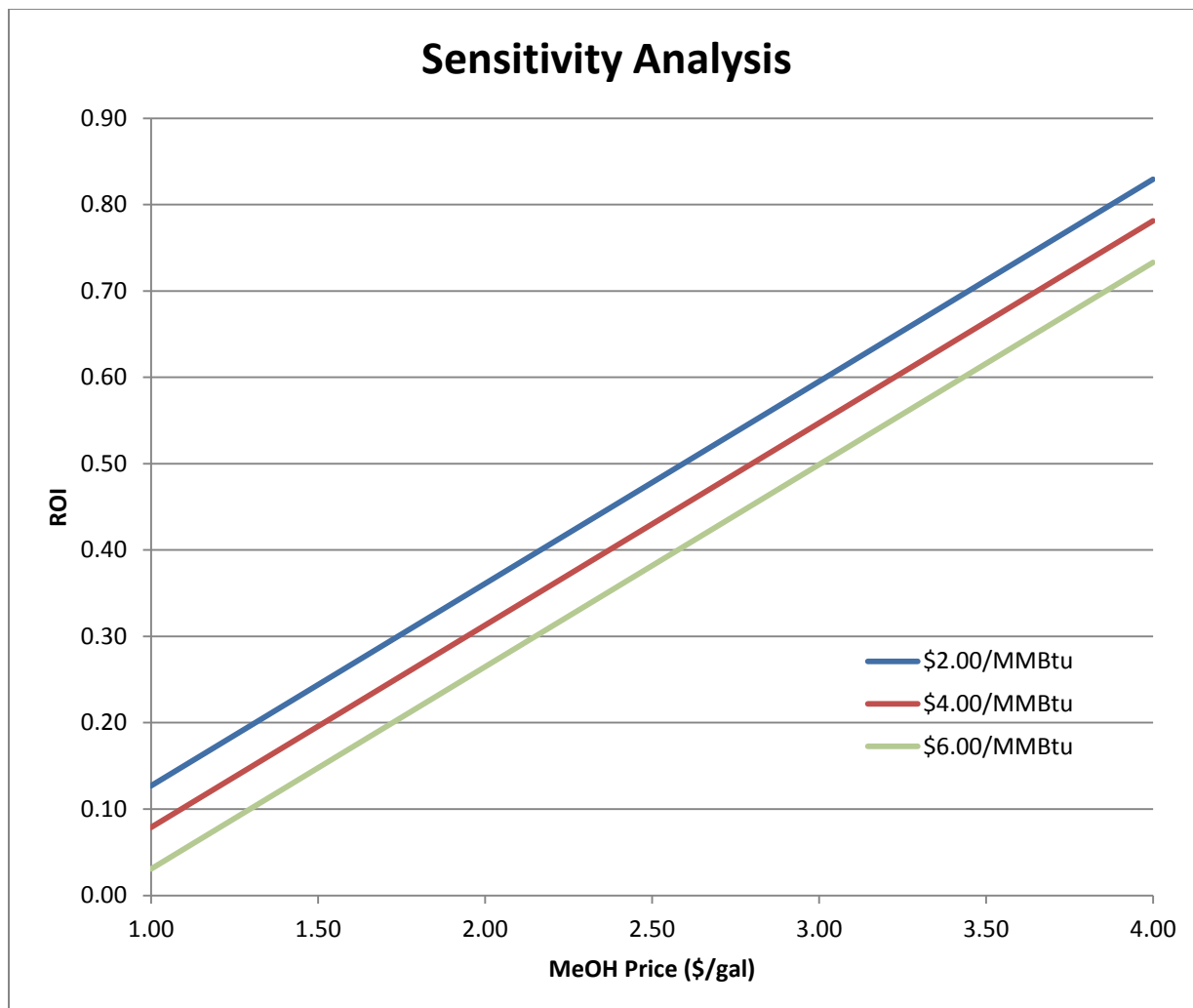


Figure 4. Sensitivity Analysis

Analysis of the inlet gas stream was used to estimate the preprocessing cost for shale gas. For each calculation, 100% removal was assumed. The primary cost factors included were acid gas removal and nitrogen gas removal. Additionally, some of the total cost is offset through separation of the natural gas liquids (NGLs): ethane and propane. The final cost was then used to determine a price differential between shale gas from the wellhead in comparison with pipeline quality natural gas. Results are shown in Table 5 and Table 6.

Table 5. Preprocessing Cost Estimation

	<b>Flow Rate</b>		<b>Unit Cost (\$)</b>		<b>\$ 10<sup>6</sup> Annual</b>
Acid Gas Removal	23148	lbmol/hr	0.37	/Mscf feed [16]	25.95
N2 Removal	23148	lbmol/hr	1.30	/Mscf feed [17]	90.45
C2 Credit	1874.988	lbmol/hr	0.22	/gal [18]	35.85
C3 Credit	532.404	lbmol/hr	0.97	/gal [19]	42.92
<b>Total</b>					<b>37.63</b>

Table 6. Shale Gas Price Differential

	<b>Unit Cost (\$/kscf)</b>	<b>Total Cost (MM\$/y)</b>
Natural Gas	3.50	179.95
Shale Gas	2.77	142.32
$\delta$	0.73	37.63

### Energy Integration

The operating cost can be reduced through the use of heat integration and cogeneration. The data for the hot and cold streams are given in Table 7.

Table 7. Heat Exchanger Data

<b>Heat exchanger</b>	<b>Supply Temperature (°F)</b>	<b>Target Temperature (°F)</b>	<b>Heat Duty (MMBtu/hr)</b>
O2-Heat	79	392	25.98
WGS-Heat	104	572	153.98
Heat-Rec	2319	104	966.30
Cool	614	104	174.04
MeOH Cool	464	302	144.63
Recycle Cool 1	296	140	113.42
Recycle Cool 2	140	113	13.14

The O2-Heat exchanger takes the inlet flow of oxygen gas and heats it to 200°C before entering the POX reactor. The Heat-Rec exchanger cools the syngas mixture from the POX reactor down to 40°C and compresses the mixture to 39.5 bar. Condensed liquids are separated from the gas

stream in the flash column and then the gas stream is heated again in the WGS-Heat exchanger to 300°C before entering the WGS reactor. The products from this reactor are then sent to the Cool exchanger where they are again cooled to 40°C. Unit MeOH Cool takes the products from the methanol reactor and cools them down to 150°C and expands them to 81 bar. Units Recycle Cool 1 and Recycle Cool 2 continue to step down the temperature and pressure to 60°C and 77.3 bar, then 45°C and 75.6 bar before the crude methanol product is separated from the recycle stream in a final flash column.

By carrying out heat integration through thermal pinch analysis, the targets for minimum heating and cooling utilities are reduced to 0 and 1,649.83 MM Btu/hr. The cooling utility can be further reduced and electric power can be produced using cogeneration. Excess heat is extracted from the hot streams to produce steam which is let down through turbines. Using combined heat and power targeting, the cooling utility is reduced to 620 MMBtu/hr and the cogenerated electric power is 90.54 MW [20]. Since the total power demand of the process is 14.55 MW, then the net power generation of the process is 75.99 MW. This corresponds to an annual value of \$30.1 MM/yr. The following sensitivity analysis shown in Figure 5, which accounts for the savings due to energy integration, shows a corresponding increase in ROI of approximately 2.0 percentage points. Detailed Calculations for the Energy Integration Analysis can be found in Appendix D.

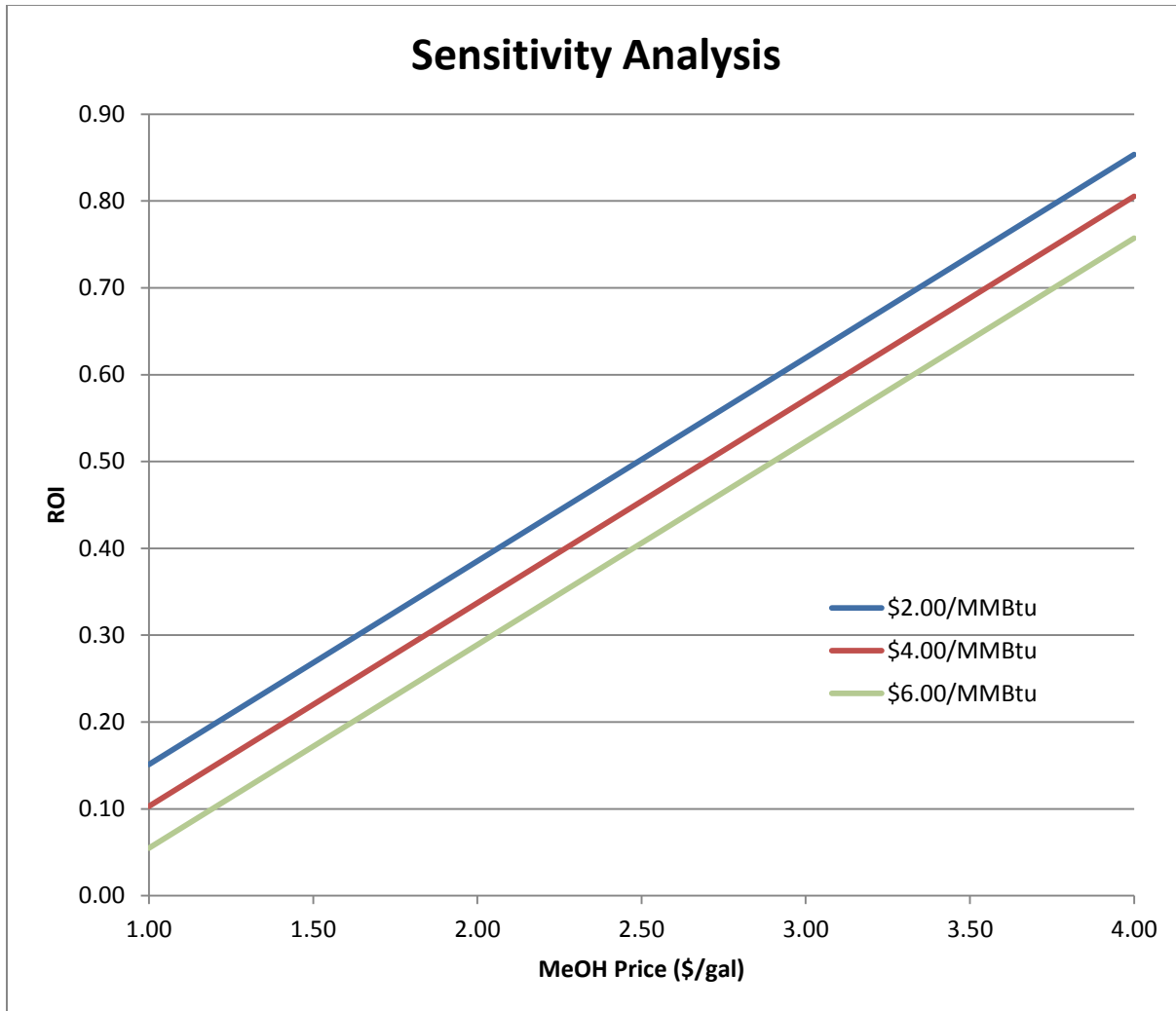


Figure 5. Sensitivity Analysis after Energy Integration

### Environmental

Water is an important resource in multiple aspects of shale gas production, including drilling mud and hydraulic fracturing fluid. Approximately 2-4 million gallons of water are required per well for hydraulic fracturing [21]. This water is typically acquired from sources such as groundwater, surface water, flowback/produced water reuses, treated municipal wastewater, and



acid mine drainage, with groundwater being the most typical as it is generally available close to production wells [3].

As hydraulic fracturing technology has developed over the previous decade, the demand for water resources in shale gas production has increased. Consequently, water conservation efforts have also increased due competing interests of energy production with agricultural and health needs. Although water use for shale gas production is relatively minor (<1%) when compared to irrigation (56%) and municipal (26%) water use in Texas, it presents a greater strain in small areas with limited water resources [22]. Additionally, municipal water use is projected to stay relatively constant while shale gas water is projected to increase greatly over the next 30-40 years [22]. Some limits are already in place due to over abstraction of groundwater in the past for irrigation limits, and many other water conservation methods are being developed for shale gas production [22]. For instance, water from drilling mud, flowback, and produced water can be reused using purification techniques such as filtration, chemical precipitation, reverse osmosis, and evaporation/distillation. Additional benefits of recycling include reducing costs of water acquisition and flowback treatment and disposal. However, the benefits of this approach are limited as recycling and reuse depend on the amount of injected water, and the amount that returns to the surface is only a fraction of the initial amount, about 30%-70% [21]. Current researchers are exploring the possibility of replacing fracturing fluid with gases such as propane, nitrogen or carbon dioxide. Additionally, some operators have started exploring brackish groundwater, however this option involves risk of contamination during transport and increased potential of well corrosion [22].

Although natural gas burns much cleaner than other fossil fuels, it has been debated whether methane emissions during natural gas production and transportation amount to greater total greenhouse gas emissions. Upstream sources of fugitive emissions are relatively small (2.8%) compared to emissions from the power station, pipeline, and common elements [21]. In one study performed by Burnham and Han, results show that shale gas life cycle emissions statistically indistinguishable from conventional natural gas, 23% lower than gasoline, and 33% lower than coal [23]. Another study performed by Stephenson, Valle, and Riera-Palou found that unconventional gas emissions are about 1.8-2.4% higher than conventional gas base case, agreeing with the results from Burnham and Han [21].

## **CHAPTER IV**

### **CONCLUSIONS**

The results of the simulation and cost estimation demonstrate that production of methanol from shale gas would be profitable and a desirable business investment above a methanol selling price of approximately \$1.50/gal. This corresponds with an ROI of at least 20% or a payback period shorter than five years. The sensitivity analysis shows that the process operating cost depend primarily on the raw natural gas feedstock. However, the ROI depends much more heavily on the selling price of methanol than on the operating costs. Energy Integration accounts for a cost savings of \$30.1 million per year and corresponds to an increase in ROI of approximately 2% points. The choice of partial oxidation for synthesis gas generation adds an addition cost for oxygen as a raw material, but some of this cost can be offset through energy integration.

Further analysis led to a cost estimation for the preprocessing of shale gas required to reach pipeline standards, which is necessary for delivery of the raw material to the proposed plant site. Because shale gas can have a chemical composition much different than natural gas, these preprocessing costs may lead to a price differential between shale gas and conventional gas. In the scenario analyzed, the preprocessing costs were dominated by nitrogen removal, with some of the costs being offset from the sale of natural gas liquids (C2 and C3). However, these preprocessing costs require that the shale gas from the wellhead be sold at a lower price than pipeline-quality natural gas. This case shows a clear price differential at \$0.73/MMBtu, but other sources of shale gas with fewer impurities would have a narrower price differential.

For an environmental perspective, the greenhouse gas emissions for shale gas preprocessing are statistically indistinguishable from those for conventional natural gas. In comparison to other sources of fossil fuels such as petroleum and coal, natural gas has much lower emissions; therefore, shale gas as a raw feedstock provides the same benefit of helping to reduce carbon emissions. Additionally, drilling for shale gas requires water intensive techniques including hydraulic fracturing. This water usage presents some concerns in domestic and semi-arid regions where availability of fresh water is more restricted. Water conservation techniques can be used to reduce water usage and environmental regulation may set limits on water usage in the future, as has been done with water for irrigation.

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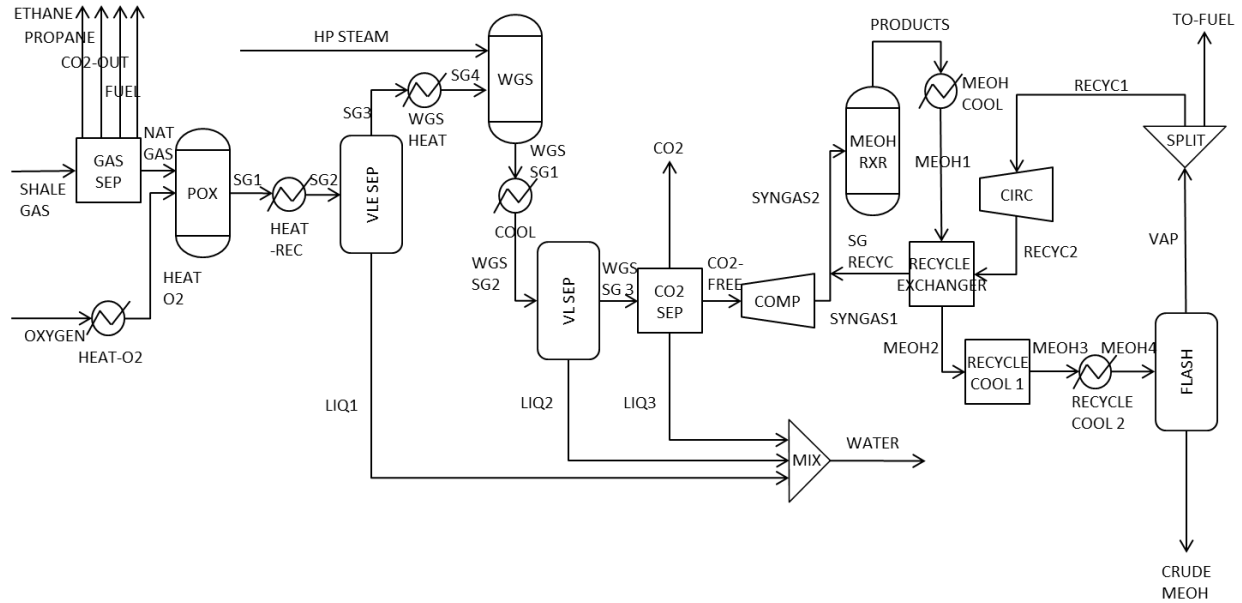
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# APPENDIX A

## PROCESS FLOW DIAGRAMS

### Overall Process



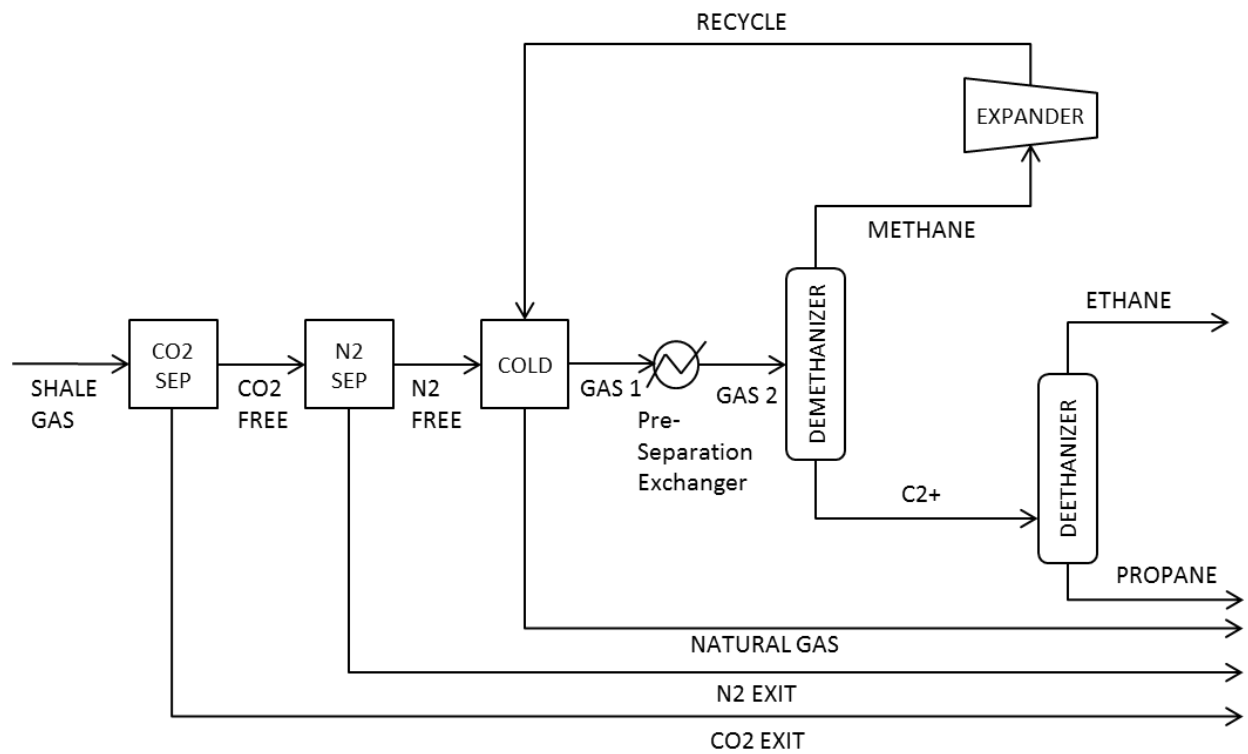
First oxygen gas is heated to 200°C. The heated oxygen and natural gas are fed to the POX reactor where the raw materials react at 20 bar in order to form hydrogen gas and carbon monoxide in approximately a 1.8:1 ratio. In the HEAT-REC exchanger the products are cooled to 40°C and pressurized to 39.5 bar. In order to adjust the ratio to the stoichiometric value of 2.0, the gas mixture is sent through a flash column and then to the WGS reactor at 300°C where a water-gas shift reaction occurs.



Next, the products from the WGS reactor are cooled back down to 40°C and sent to a flash column where the liquid water separates from the syngas. The next unit removes carbon dioxide

from the water-gas shift reaction. Next, the gas is compressed to 75 atm and sent to the MEOHRXR where it reacts at 240°C to form methanol vapor. The products from this reaction are then sent through a recycle loop with heat exchangers and compressors in order to maximize conversion of the feedstock. The crude methanol product is separated from the recycle stream in a flash column. The recycle ratio is set at 0.5.

### Gas Separation

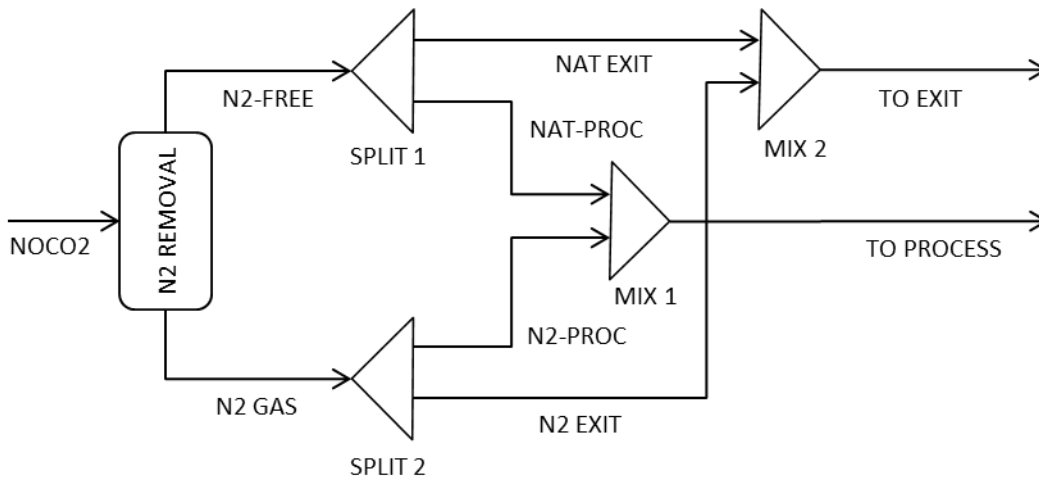


Before the shale gas feedstock can be sent via pipeline to the methanol plant, it must first undergo several preprocessing steps in order to remove contaminants that are limited by pipeline standards. The process diagram above shows that the gas is first sent through a carbon dioxide removal unit and then through a nitrogen gas separation unit (details show in following diagram). Next the gas is sent through a heat exchanger and a series of distillation columns in order to remove the NGLs. The first cryogenic column has 15 stages and removes methane from the



higher boiling hydrocarbons. In the second cryogenic column, ethane and propane are separated through 23 stages and purified in order to be sold for a profit. Both columns have a molar reflux ratio of 1.5.

### Nitrogen Separation



The process diagram above shows the natural gas inlet stream entering at the left into a separation unit. The gas is then split into a nitrogen-rich and nitrogen-free stream. Each stream goes through another separation step and the nitrogen gas is released to the atmosphere while the process gas is sent to a heat exchanger before it enters the demethanizer and deethanizer columns.

## APPENDIX B

### SIMULATION STREAM DATA

	CO2	CO2-FREE	CO2-OUT	CRUDEMEOH	ETHANE	FUEL
Mole Flow lbmol/hr						
H2	0	30105.04	0	3.14E-03	0	0
WATER	0	94.74258	0	2.695566	0	0
CH4	0	50.14277	0	30.59069	0.078948	1597.942
N2	0	15.34547	0	2.113667	6.11E-09	1813.256
C2H6	0	3.65E-04	0	2.74E-04	1694.966	161.1872
C3H8	0	6.51E-09	0	5.77E-09	7.596043	45.7692
CO	0	15052.9	0	404.0464	0	0
METHANOL	0	0	0	12523.65	0	0
BUTANOL	0	0	0	1.762827	0	0
C2H6O-01	0	0	0	0.367579	0	0
ACETONE	0	0	0	0.6523228	0	0
O2	0	5.91E-10	0	1.73E-10	0	0
CO2	226.8504	2.680371	1737.82	55.11302	2.836543	8.357854
Total Flow lbmol/hr	226.8504	45320.86	1737.82	13020.99	1705.478	3626.513
Total Flow lb/hr	9983.641	4.85E+05	76481.11	4.16E+05	51428.08	83663.95
Total Flow cuft/hr	2270.854	4.87E+05	14864.06	8820.684	15651.81	41956.35
Temperature F	100	104	104	113	40.79148	98.31344
Pressure psia	500	572.8991	572.8991	1096.485	389.6959	500
Vapor Frac	1	1	1	0	1	1
Liquid Frac	0	0	0	1	0	0
Solid Frac	0	0	0	0	0	0
Enthalpy Btu/lbmol	-1.70E+05	-15865.61	-1.70E+05	-1.00E+05	-37764.75	-16671.43
Enthalpy Btu/lb	-3852.03	-1481.387	-3853.185	-3137.149	-1252.369	-722.643
Enthalpy Btu/hr	-3.85E+07	-7.19E+08	-2.95E+08	-1.30E+09	-6.44E+07	-6.05E+07
Entropy Btu/lbmol-R	-6.617316	1.373276	-6.929996	-53.67263	-50.37662	-16.24108
Entropy Btu/lb-R	-0.1503601	0.128224	-0.1574648	-1.680739	-1.670609	-0.7039888
Density lbmol/cuft	0.0998965	0.09308	0.1169142	1.476188	0.1089636	0.0864353
Density lb/cuft	4.396426	0.9968849	5.14537	47.14053	3.28576	1.994071
Average MW	44.0098	10.70997	44.0098	31.93395	30.15465	23.07008
Liq Vol 60F cuft/hr	194.6181	38827.49	1490.9	8518.03	2313.088	3216.297

	HEAT O2	HP-STEAM	LIQ1	LIQ2	LIQ3
Mole Flow lbmol/hr					
H2	0	0	5.00E-04	5.49E-06	3.41E-06
WATER	0	983.1172	4658.411	50.12463	22.50542
CH4	0	0	2.758614	0.0293126	0.017671
N2	0	0	0.0892899	9.50E-04	5.79E-04
C2H6	0	0	4.28E-05	4.54E-07	2.65E-07
C3H8	0	0	1.98E-09	2.10E-11	1.25E-11
CO	0	0	120.4079	1.205964	0.732065
METHANOL	0	0	0	0	0
BUTANOL	0	0	0	0	0
C2H6O-01	0	0	0	0	0
ACETONE	0	0	0	0	0
O2	11294	0	8.87E-12	9.43E-14	0
CO2	0	0	139.0785	3.107723	2.98E-03
Total Flow lbmol/hr	11294	983.1172	4920.746	54.46859	23.25872
Total Flow lb/hr	3.61E+05	17711.13	93462.82	1074.056	426.3779
Total Flow cuft/hr	2.74E+05	15196.14	1537.793	17.45731	7.135988
Temperature F	392	481.4268	104	104	104
Pressure psia	377.0981	572.8991	572.8991	572.8991	794.6365
Vapor Frac	1	1	0	0	0
Liquid Frac	0	0	1	1	1
Solid Frac	0	0	0	0	0
Enthalpy Btu/lbmol	2225.072	-1.01E+05	-1.23E+05	-1.25E+05	-1.20E+05
Enthalpy Btu/lb	69.53609	-5621.948	-6456.023	-6331.834	-6548.123
Enthalpy Btu/hr	2.51E+07	-9.96E+07	-6.03E+08	-6.80E+06	-2.79E+06
Entropy Btu/lbmol-R	-3.181569	-13.71614	-36.97206	-37.24206	-36.49904
	-	-			
Entropy Btu/lb-R	0.0994277	0.7613615	-1.94655	-1.888656	-1.991006
Density lbmol/cuft	0.0411957	0.0646951	3.199875	3.120103	3.259356
Density lb/cuft	1.318213	1.165502	60.77723	61.52473	59.75038
Average MW	31.9988	18.01528	18.99363	19.71881	18.33196
Liq Vol 60F cuft/hr	9689.274	284.2519	1571.962	18.21944	7.153334

	MEOH1	MEOH2	MEOH3	MEOH4	NAT-GAS	OXYGEN
Mole Flow lbmol/hr						
H2	10010.28	10010.28	10010.28	10010.28	0	0
WATER	2.703435	2.703435	2.703435	2.703435	0	0
CH4	69.65949	69.65949	69.65949	69.65949	16989.82	0
N2	28.57612	28.57612	28.57612	28.57612	15.43571	0
C2H6	4.55E-04	4.55E-04	4.55E-04	4.55E-04	17.13801	0
C3H8	7.23E-09	7.23E-09	7.23E-09	7.23E-09	2.03E-03	0
CO	4369.74	4369.74	4369.74	4369.74	0	0
METHANOL	12633.69	12633.69	12633.69	12633.69	0	0
BUTANOL	1.764569	1.764569	1.764569	1.764569	0	0
C2H6O-01	0.5142695	0.5142695	0.5142695	0.5142695	0	0
ACETONE	0.6704506	0.6704506	0.6704506	0.6704506	0	0
O2	1.01E-09	1.01E-09	1.01E-09	1.01E-09	0	11294
CO2	103.4267	103.4267	103.4267	103.4267	86.0272	0
Total Flow lbmol/hr	27221.03	27221.03	27221.03	27221.03	17108.43	11294
Total Flow lb/hr	5.54E+05	5.54E+05	5.54E+05	5.54E+05	2.77E+05	3.61E+05
Total Flow cuft/hr	1.35E+05	1.33E+05	94392.71	91257.57	2.51E+05	1.70E+05
Temperature F	302	296.3073	140	113	78.8	78.8
Pressure psia	1174.806	1174.806	1121.142	1096.485	377.0981	377.0981
Vapor Frac	0.6806229	0.6665614	0.5286863	0.5216568	1	1
Liquid Frac	0.3193771	0.3334386	0.4713137	0.4783432	0	0
Solid Frac	0	0	0	0	0	0
Enthalpy Btu/lbmol	-50513.42	-50762.57	-54929.36	-55412.01	-32873.68	-74.94573
Enthalpy Btu/lb	-2481.549	-2493.789	-2698.489	-2722.199	-2028.208	-2.342142
Enthalpy Btu/hr	-1.38E+09	-1.38E+09	-1.50E+09	-1.51E+09	-5.62E+08	-8.46E+05
Entropy Btu/lbmol-R	-19.30193	-19.62616	-25.50496	-26.27779	-25.73844	-6.546079
	-	-				-
Entropy Btu/lb-R	0.9482367	0.9641652	-1.25297	-1.290936	-1.587985	0.2045726
Density lbmol/cuft	0.2011598	0.2054419	0.2883806	0.2982879	0.0681314	0.0664557
Density lb/cuft	4.094728	4.181893	5.87016	6.071829	1.10429	2.126505
Average MW	20.3556	20.3556	20.3556	20.3556	16.20824	31.9988
Liq Vol 60F cuft/hr	20677.17	20677.17	20677.17	20677.17	14686.11	9689.274

	PRODUCTS	PROPANE	RECYC1	RECYC2	SGRECYC	SHALEGAS
Mole Flow lbmol/hr						
H2	10010.28	0	5005.139	5005.159	5005.159	0
WATER	2.703435	0	3.93E-03	3.93E-03	3.93E-03	0
CH4	69.65949	2.17E-11	19.5344	19.53438	19.53438	18587.84
N2	28.57612	8.79E-23	13.23123	13.23123	13.23123	1828.692
C2H6	4.55E-04	1.696676	9.03E-05	9.03E-05	9.03E-05	1874.988
C3H8	7.23E-09	479.0367	7.32E-10	7.33E-10	7.33E-10	532.404
CO	4369.74	0	1982.847	1982.753	1982.753	0
METHANOL	12633.69	0	55.02155	55.02163	55.02163	0
BUTANOL	1.764569	0	8.71E-04	8.71E-04	8.71E-04	0
C2H6O-01	0.5142695	0	0.0733452	0.073345	0.073345	0
ACETONE	0.6704506	0	9.06E-03	9.06E-03	9.06E-03	0
O2	1.01E-09	0	4.17E-10	4.16E-10	4.16E-10	0
CO2	103.4267	6.64E-07	24.15683	24.15685	24.15685	324.072
Total Flow lbmol/hr	27221.03	480.7334	7100.017	7099.943	7099.943	23148
Total Flow lb/hr	5.54E+05	21174.87	69144.32	69141.72	69141.72	4.44E+05
Total Flow cuft/hr	2.32E+05	847.739	41218.44	41096.4	50591.79	2.60E+05
Temperature F	464	160.2282	113	114.1885	248	100
Pressure psia	1102.196	391.8959	1096.485	1102.196	1102.196	500
Vapor Frac	1	0	1	1	1	1
Liquid Frac	0	1	0	0	0	0
Solid Frac	0	0	0	0	0	0
Enthalpy Btu/lbmol	-45200.09	-49024.06	-14359.7	-14349.84	-13394.6	-32102.44
Enthalpy Btu/lb	-2220.523	-1112.994	-1474.512	-1473.539	-1375.45	-1675.37
Enthalpy Btu/hr	-1.23E+09	-2.36E+07	-1.02E+08	-1.02E+08	-9.51E+07	-7.43E+08
Entropy Btu/lbmol-R	-12.66708	-76.45461	-1.157561	-1.153378	0.343989	-25.81403
	-					
Entropy Btu/lb-R	0.6222896	-1.73575	-0.118863	0.1184367	0.035323	-1.347189
Density lbmol/cuft	0.1173209	0.5670772	0.1722534	0.1727631	0.140338	0.0889486
Density lb/cuft	2.388137	24.97806	1.677509	1.682428	1.366659	1.704381
Average MW	20.3556	44.04701	9.738614	9.738349	9.738349	19.1614
Liq Vol 60F cuft/hr	20677.17	670.9974	6079.568	6079.505	6079.505	21081.11

	SG1	SG2	SG3	SG4	SYNGAS1	SYNGAS2
Mole Flow lbmol/hr						
H2	29171.35	29171.35	29171.35	29171.35	35110.2	30105.04
WATER	4753.854	4753.854	95.44336	95.44336	72.24109	72.23716
CH4	52.9307	52.9307	50.17209	50.17209	69.65949	50.1251
N2	15.43571	15.43571	15.34642	15.34642	28.57612	15.34489
C2H6	4.08E-04	4.08E-04	3.65E-04	3.65E-04	4.55E-04	3.65E-04
C3H8	8.51E-09	8.51E-09	6.53E-09	6.53E-09	7.23E-09	6.50E-09
CO	16108.21	16108.21	15987.8	15987.8	17034.92	15052.17
METHANOL	0	0	0	0	55.02163	0
BUTANOL	0	0	0	0	8.71E-04	0
C2H6O-01	0	0	0	0	0.073345	0
ACETONE	0	0	0	0	9.06E-03	0
O2	6.00E-10	6.00E-10	5.91E-10	5.91E-10	1.01E-09	5.91E-10
CO2	948.9932	948.9932	809.9148	809.9148	26.83424	2.677387
Total Flow lbmol/hr	51050.77	51050.77	46130.03	46130.03	52397.54	45297.6
Total Flow lb/hr	6.39E+05	6.39E+05	5.45E+05	5.45E+05	5.54E+05	4.85E+05
Total Flow cuft/hr	4.21E+06	4.96E+05	4.95E+05	9.04E+05	3.08E+05	2.57E+05
Temperature F	2319.394	104	104	572	122.7678	104
Pressure psia	362.5943	572.8991	572.8991	572.8991	1102.196	1102.196
Vapor Frac	1	0.9036108	1	1	1	0.9996128
Liquid Frac	0	0.0963892	0	0	0	3.87E-04
Solid Frac	0	0	0	0	0	0
Enthalpy Btu/lbmol	-10524.56	-29452.83	-19514.23	-16176.22	-15499.86	-15829.84
Enthalpy Btu/lb	-841.2304	-2354.171	-1651.034	-1368.616	-1465.717	-1478.588
Enthalpy Btu/hr	-5.37E+08	-1.50E+09	-9.00E+08	-7.46E+08	-8.12E+08	-7.17E+08
Entropy Btu/lbmol-R	13.72227	-1.877333	1.866263	6.174613	0.1023631	0.0285566
Entropy Btu/lb-R	1.096824	0.1500556	0.1578983	0.5224136	9.68E-03	2.67E-03
Density lbmol/cuft	0.012112	0.1028673	0.0932409	0.0510302	0.1702405	0.175956
Density lb/cuft	0.1515331	1.286964	1.102052	0.6031468	1.800281	1.883795
Average MW	12.51091	12.51091	11.8194	11.8194	10.57493	10.70606
Liq Vol 60F cuft/hr	41093.26	41093.26	39521.29	39521.29	44899.85	38820.34

	TO-FUEL	WGS SG3	WGS SG1	WGS SG2	WATER	VAP
Mole Flow lbmol/hr						
H2	5005.139	30105.04	30105.04	30105.04	5.09E-04	10010.28
WATER	3.93E-03	94.74258	144.8672	144.8672	4731.041	7.87E-03
CH4	19.5344	50.14277	50.17209	50.17209	2.805598	39.06879
N2	13.23123	15.34547	15.34642	15.34642	0.0908186	26.46245
C2H6	9.03E-05	3.65E-04	3.65E-04	3.65E-04	4.36E-05	1.81E-04
C3H8	7.32E-10	6.51E-09	6.53E-09	6.53E-09	2.02E-09	1.46E-09
CO	1982.847	15052.9	15054.11	15054.11	122.3459	3965.694
METHANOL	55.02155	0	0	0	0	110.0431
BUTANOL	8.71E-04	0	0	0	0	1.74E-03
C2H6O-01	0.0733452	0	0	0	0	0.1466906
ACETONE	9.06E-03	0	0	0	0	0.0181278
O2	4.17E-10	5.91E-10	5.91E-10	5.91E-10	8.96E-12	8.34E-10
CO2	24.15683	1740.5	1743.608	1743.608	142.1892	48.31366
Total Flow lbmol/hr	7100.017	47058.68	47113.14	47113.14	4998.473	14200.03
Total Flow lb/hr	69144.32	5.62E+05	5.63E+05	5.63E+05	94963.26	1.38E+05
Total Flow cuft/hr	41218.44	5.04E+05	9.60E+05	5.04E+05	1562.399	82436.88
Temperature F	113	104	613.8253	104	104.0196	113
Pressure psia	1096.485	572.8991	572.8991	572.8991	572.8991	1096.485
Vapor Frac	1	1	1	0.9988439	0	1
Liquid Frac	0	0	0	1.16E-03	1	0
Solid Frac	0	0	0	0	0	0
Enthalpy Btu/lbmol	-14359.7	-21526.84	-17952.2	-21646.3	-1.23E+05	-14359.7
Enthalpy Btu/lb	-1474.512	-1802.965	-1502.441	-1811.605	-6455.032	-1474.512
Enthalpy Btu/hr	-1.02E+08	-1.01E+09	-8.46E+08	-1.02E+09	-6.13E+08	-2.04E+08
Entropy Btu/lbmol-R	-1.157561	1.397678	6.026266	1.353006	-36.97216	-1.157561
Entropy Btu/lb-R	-0.118863	0.1170615	0.5043455	0.1132347	-1.946062	-0.118863
Density lbmol/cuft	0.1722534	0.0933167	0.0490685	0.0934214	3.199229	0.1722534
Density lb/cuft	1.677509	1.114173	0.5863047	1.116264	60.7804	1.677509
Average MW	9.738614	11.93969	11.94869	11.94869	18.99845	9.738614
Liq Vol 60F cuft/hr	6079.568	40318.39	40336.61	40336.61	1597.335	12159.14

## APPENDIX C

### CALCULATIONS

Abbreviations:

FCI = Fixed Capital Investment

WCI = Working Capital Investment

TCI = Total Capital Investment

AOC = Annual Operating Cost

AATP = Annual After-Tax Profit

AFC = Annualized Fixed Cost

ROI = Return on Investment

**Capital Cost:** \$1.3 Billion

**Operating Costs:**

Raw Materials

$$\text{Natural Gas: } C_{NG} = 155.8 \frac{\text{MMscf}}{\text{day}} * 1000 \frac{\text{kscf}}{\text{MMscf}} * \$3.50 \frac{1}{\text{kscf}} * 330 \frac{\text{day}}{\text{year}}$$

$$\text{Oxygen: } C_{O_2} = 361394 \frac{\text{lb}}{\text{hr}} * \$0.05 \frac{1}{\text{lb}} * 24 \frac{\text{hr}}{\text{day}} * 330 \frac{\text{day}}{\text{year}} \quad [24]$$

Utilities

$$\text{Heating: } C_{Heat} = 1.800 * 10^8 \frac{\text{Btu}}{\text{hr}} * \frac{\text{MMBtu}}{10^6 \text{Btu}} * \$4.00 \frac{1}{\text{MMBtu}} * 24 \frac{\text{hr}}{\text{day}} * 330 \frac{\text{day}}{\text{year}}$$

$$\text{Cooling: } C_{Cool} = 1.830 * 10^8 \frac{\text{Btu}}{\text{hr}} * \frac{\text{MMBtu}}{10^6 \text{Btu}} * \$1.50 \frac{1}{\text{MMBtu}} * 24 \frac{\text{hr}}{\text{day}} * 330 \frac{\text{day}}{\text{year}}$$

$$\text{Compressor Power: } C_{Pr} = 14781 \frac{\text{kW}}{\text{day}} * 1 \text{ day} * 24 \frac{\text{hr}}{\text{day}} * \$0.05 \frac{1}{\text{kWh}} * 330 \frac{\text{day}}{\text{year}}$$

Waste Water Treatment:

$$C_{WWT} = 94963 \frac{\text{lb}}{\text{hr}} * \frac{\text{kg}}{2.2 \text{ lb}} * \frac{\text{tonne}}{1000 \text{ kg}} * \$0.53 \frac{1}{\text{tonne}} * 24 \frac{\text{hr}}{\text{day}} * 330 \frac{\text{day}}{\text{year}}$$

$$\text{Labor: } C_{labor} = 30 \text{ employees} * \frac{\$60,000}{\text{employee}} + 20 \text{ employees} * \frac{\$100,000}{\text{employee}}$$

$$\text{Sales: } S = 5000 \frac{\text{ton}}{\text{day}} * 2000 \frac{\text{lb}}{\text{ton}} * \frac{\text{gal}}{6.6 \text{ lb}} * \$2.00 \frac{1}{\text{gal}} * 330 \frac{\text{day}}{\text{year}}$$



### Process Analysis:

$$\text{FCI} = \$1.3 \text{ billion}$$

$$\text{WCI} = 0.15 * \text{FCI}$$

$$\text{TCI} = \text{FCI} + \text{WCI}$$

$$\text{AFC} = (\text{FCI} - \text{Salvage value}) / \text{Recovery Period}$$

$$\text{Salvage Value} = 0.10 * \text{FCI}$$

$$\text{Recovery Period} = 10 \text{ years}$$

$$\text{AATP} = (\text{Sales} - \text{AFC} - \text{AOC}) * (1 - \text{Tax Rate}) + \text{AFC}$$

$$\text{Tax Rate} = 30\%$$

$$\text{ROI} = \text{AATP} / \text{TCI}$$

### Preprocessing Costs:

Acid Gas Removal:

$$C_{AGR} = 23148 \frac{\text{lbmol feed}}{\text{hr}} * 379.5 \frac{\text{scf}}{\text{lbmol feed}} * \frac{\text{kscf}}{1000 \text{ scf}} * \$0.37 \frac{1}{\text{kscf}} * 24 \frac{\text{hr}}{\text{day}} * 330$$

Nitrogen Removal:

$$C_{N_2} = 23148 \frac{\text{lbmol feed}}{\text{hr}} * 379.5 \frac{\text{scf}}{\text{lbmol feed}} * \frac{\text{kscf}}{1000 \text{ scf}} * \$1.30 \frac{1}{\text{kscf}} * 24 \frac{\text{hr}}{\text{day}} * 330 \frac{\text{day}}{\text{year}}$$

$$\text{C2 Credit: } S_{C2} = 1875 \frac{\text{lbmol}}{\text{hr}} * 30.07 \frac{\text{lb}}{\text{lbmol}} * \frac{\text{gal}}{2.74 \text{ lb}} * \$0.22 \frac{1}{\text{gal}} * 24 \frac{\text{hr}}{\text{day}} * 330 \frac{\text{day}}{\text{year}}$$

$$\text{C3 Credit: } S_{C3} = 532 \frac{\text{lbmol}}{\text{hr}} * 44.10 \frac{\text{lb}}{\text{lbmol}} * \frac{\text{gal}}{4.22 \text{ lb}} * \$0.97 \frac{1}{\text{gal}} * 24 \frac{\text{hr}}{\text{day}} * 330 \frac{\text{day}}{\text{year}}$$

$$\text{Total Preprocessing Cost: } C_P = C_{AGR} + C_{N_2} - S_{C2} - S_{C3}$$

**Cost Differential:**

$$\delta = \$3.50 \frac{1}{kscf \text{ NG}} - \frac{C_{NG} - C_P}{155.8 \frac{MMscf}{day} * 1000 \frac{kscf}{MMscf} * 330 \frac{day}{year}}$$

## APPENDIX D

### DETAILED CALCULATIONS FOR THE COMBINED HEAT AND POWER INTEGRATION

#### Heat Exchanger Network Data

Heat exchanger	FC <sub>p</sub> (Btu/°F)	In (°F)	Out (°F)	Duty (Btu/hr)
O <sub>2</sub> -Heat	82992	79	392	25976388
WGS-Heat	329023	104	572	153982535
Heat-Rec	436254	2319	104	966302898
Cool	341257	614	104	174041053
MeOH Cool	892803	464	302	144634153
Recycle Cool 1		296	140	113424228
Recycle Cool 2		140	113	13138160

The first hot stream Heat-Rec can heat the two cold streams completely (it has enough Btu/hr and its temperature is higher than both cold streams).

Target for minimum heating utility = 0

Target for minimum cooling utility = 1829.78 – 179.95 = 1,649.83 MM Btu/hr.

The cooling utility can be further reduced using cogeneration. Heat-Rec, Cool, and E1 can be used to generate steam which can be used in steam turbines to produce power.

After heat integration, remaining duty of Heat-Rec = 966 – 180 = 786 MM Btu/hr

This heat can be used until a temperature of 212 °F.

Therefore, extractable heat from 2319 to 212 =  $786 \cdot (2319 - 212) / (2319 - 104)$

$$= 748 \text{ MM Btu/hr}$$

Similarly, extractable heat from Cool =  $174 \cdot (614 - 212) / (614 - 104) = 137$  MM Btu/hr.

For E1, all of its heat is extractable because its outlet temperature is high enough (302 °F).

Therefore, total extractable heat to be used in generating steam =  $748 + 137 + 145 = 1,030$  MM Btu/hr.

$$\begin{aligned} \text{Target for minimum cooling after steam generation/cogeneration} &= 1,650 - 1,030 \\ &= 620 \text{ MM Btu/hr} \end{aligned}$$

$$1 \text{ MM Btu} = 1.055 \cdot 10^6 \text{ kJ} = 1.055 \cdot 10^6 \text{ kW}_s = 1.055 \cdot 10^6 / 3600 = 293 \text{ kWh}$$

Assuming that 30% of steam enthalpy will be converted to electric power:

$$\text{Produced power} = 0.3 \cdot 1,030 = 309 \text{ MM Btu/hr} = 309 \cdot 293 = 90,537 \text{ kWh/hr} = 90,537$$

$$\text{kW} = 90,537 \cdot 7920 \text{ hr/yr} = 717 \text{ MM kWh/yr}$$

Assuming a value of \$0.05/kWh:

$$\text{Annual value of electric energy} = 717 \cdot 10^6 \cdot 0.05 = \$35.9 \text{ MM/yr}$$

Produced power = 90,537 KW

#### Compressor details

Compressor	Power requirement
COMP	14528.7
CIRC	17.7

Total power demand =  $14,529 + 18 = 14,547$  kW

$$\text{Net power generation} = 90,537 - 14,547 = 75,990 \text{ kW}$$

$$\begin{aligned} \text{Annual value of net power generation} &= 75,990 \text{ kW} \cdot 7920 \text{ hr/yr} \cdot \$0.05/\text{kWh} \\ &= \$30.1 \text{ MM/y} \end{aligned}$$