

Production of Ethylene from Natural Gas

Team #5

The Lindgren Group, LLC, a subsidiary of MichiChem Corp.

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Using Thermal Cracking and Cryogenic Distillation to Create and
Separate Natural Gas Components

Final Report

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Executive Summary

Ethylene is a product in constant demand for its use in the production of polyethylene, a material with a multitude of applications. Ethylene itself is produced by thermally cracking ethane, a component of natural gas. The Lindgren Group has designed a process capable of producing 500 million pounds of ethylene per year from raw natural gas. Additional products such as interstate pipeline quality (IPQ) natural gas, propylene, and hydrogen are also produced to be sold. The process consists of 5 stages: impurity removal, phase separation, light component separation, heavy component separation, and reactions.

Stage 1 is the impurity removal process where carbon dioxide and hydrogen sulfide impurities are removed from the natural gas stream. This process is an amine sweetening processes and consists of an absorber and a stripper that uses diglycolamine (DGA) as the absorbing fluid. In the absorber, the DGA is contacted with all of the inlet gas and removes the impurities. The purified or “sweet” gas is sent to the second stage.

In the second stage, water and heavy (C5+) hydrocarbons are removed. By pressurizing and cooling the stream, the process condenses these heavy components into the liquid phase so that they can be decanted from a series of two three-phase separators. What remain are hydrogen, nitrogen, and light (C1-C5) hydrocarbons, which are sent to the third stage.

In the third stage, the stream is cooled to cryogenic temperatures by the refrigeration stage in stage 2. The stream enters the demethanizer which cryogenically removes methane, nitrogen, and hydrogen from the inlet stream. The methane is sent to the IPQ natural gas line and the hydrogen and nitrogen are separated using a membrane separator. The heavier components are sent to the fourth stage.

The fourth stage cryogenically separates saleable components from the components that need to be processed further. Saleable components include ethylene, propylene, and butanes. The remainder, mainly ethane and propane, is sent to the fifth stage.

The fifth stage consists of two operations: the hydrogenator and cracker. The hydrogenator saturates the recycled alkynes into alkanes. The resulting stream then enters the cracker where the alkanes are cracked into ethylene and propylene. Some alkynes and long-chain hydrocarbons are also produced. This ethylene-rich stream is then sent back to stage two where the phase separators and subsequent stages separate out ethylene, propylene, and other saleable products.

Safety of workers and the environment is our highest priority. Toxic hydrogen sulfide, carbon dioxide, and flammable hydrocarbons are produced from the raw natural gas. Additionally, extreme temperatures ranging from -149°C to 850°C and pressures up to 30 atmospheres are present in our process. Proper precautions and safety nets will be designed and implemented for the safety of plant workers, the environment, and the surrounding community.

Finally, we report that our process has a net present value of \$87.7 million after 10 years of production at a minimum acceptable rate of return of 11%. Depreciation is calculated based on the 7-year MACRS schedule.

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NOMENCLATURE TABLE

Symbol	Meaning	Symbol	Meaning
t_1	arbitrary time	R	reflux ratio
t_2	breakthrough time	R_{min}	minimum reflux ratio
t_s	stoichiometric time	N	number of stage
X_e	bead loading in equilibrium with feed gas	N_{min}	minimum number of stages
X_f	residual bed loading prior to adsorption step	X	conversion
L_{e1}	length of bed in equilibrium with feed gas at t_1	W	catalyst weight
L_{s1}	length of bed to stoichiometric front at t_1	k_i	rate constant
L_{b1}	length of bed to breakthrough gas concentration at t_1	R	gas constant
L_e	length of bed in equilibrium with feed gas at t_b	$-r'_i$	reaction rate
L_{s1}	length of bed to stoichiometric front at t_b (=LES)	T	temperature
L_b	total length of bed	ϵ	volumetric expansion per mol reacted
v_g	superficial gas velocity	d	diameter
K	constant	API°	API gravity
ρ_{amine}	amine density	SG	specific gravity
ρ_{gas}	gas density	τ	residence time
T	space time (i.e. residence time)	V	volume
V	volume	\dot{V}	volumetric flowrate
V_o	volumetric flowrate	η	efficiency
ρ	density	v_g	velocity of gas
m_{ra}	mass flow rate of rich amine solution	Q	Volumetric flowrate
Q	duty	A	Cross-sectional area
U	overall heat transfer coefficient	n_p	molar flow rate of permeate stream
ΔT_{LM}	logmean temperature difference	$y_{p_{H_2}}$	mole fraction of I in permeate stream
ΔT_2	difference between outlet temperatures	n_F	molar flow rate of feed stream
ΔT_1	difference between inlet temperatures	$x_{F_{H_2}}$	mole fraction of I in feed stream
Cp	heat capacity	$x_{R_{H_2}}$	mole fraction of I in retentate stream
m	mass	P_{H_2}	permeability of I thorough membrane
T_{in}	temperature in	l_m	membrane thickness
T_{out}	temperature out	P_p	pressure of permeate stream
A	area	P_F	pressure of feed stream
P	pressure	A_m	membrane area
N	number of stages	α_{H_2,N_2}^*	separation factor
K	Souders-Brown constant	θ	minimum reject concentration (i.e. cut)
P2	pipe outlet pressure	r_a'	rate of reaction
P1	pipe inlet pressure	F_{a0}	molar flow rate
Δp	pressure drop	P_i	partial pressure of component i
L	length	C_a	concentration of species a
l	length	Y	pressure drop factor
f_t	friction factor	μ	dynamic viscosity
C_t	pressure drop coefficient	\emptyset	void fraction
G	superficial mass velocity	B_0	Packed bed constant
D_p	effective particle diameter		

LIST OF ABBREVIATIONS

Abbreviation	Full Term	Abbreviation	Full Term
IPQ	interstate pipeline quality	BCC	body-centered-cubic
LNG	liquefied natural gas	HCP	hexagonal-close-packed
FFDs	process flow diagrams	HC	hydrocarbon
MEA	monoethanolamine	DI	deionized
DEA	diethanolamine	SCR	selective catalytic reduction
DGA	diglycolamine	FRC	flame-retardant clothing
MDEA	Methyldiethanolamine	PPE	personal protective equipment
ITM	ion transport membrane	SCBA	self-contained breathing apparatus
MTZ	mass transfer zone	API	American Petroleum Institute
LUB	length of unused bed	PSA	pressure swing adsorption
LES	length of equilibrium section	FUG	Fenske-Underwood-Gilliland method
Nox	Nitrogen Oxide's	scf	standard cubic feet
TCI	total capital investment	MM	million
TPC	total production cost	MMSCFD	million standard cubic feet per day
NPV	net present value	psi	pounds per square inch
FCI	fixed capital investment	ID	inner diameter
ISBL	inside boundary limit	atm	atmospheres
OSBL	outside boundary limit	Kgal	thousands of gallons
R-grade	refinery grade	Alkanes	saturated hydrocarbons
DCFRoR	discounted cash flow rate of return	Olefins	double bonds
MARR	Minimal acceptable rate of return	Alkynes	triple bonds
FCC	face-centered-cubic		

1 INTRODUCTION

The following sections introduce the design challenge our team was given and describe what we have done to fulfill this requirement.

1.1 Problem Statement

MichiChem has acquired the rights to natural gas wells that produce raw gas. MichiChem has assigned us the task of designing a process that will use the raw gas to produce 500 million pounds of ethylene per year as well as interstate pipeline quality (IPQ) natural gas. As of today, the 22nd of April 2013, we have accomplished our goal of providing MichiChem with a solution that is both technically sound and economically feasible.

1.2 Purpose

The purpose of this report is to present our completed design process in full detail. The process has been divided into five stages. Stream compositions and flow rates have been determined, and a full economic analysis has been performed on the system as a whole. Environmental health and safety concerns have been reviewed and are incorporated into the design and plant layout. This report contains an informational background section, a detailed design section, information about safety hazards to the environment and employees, and an economic evaluation. More detail for each section is provided in the list of sections.

1.3 List of Sections

- Background – The background addresses current industrial practices for impurity removal, separation, and reaction. Each alternative is discussed.
- Process Design – The process design describes our proposed commercial process in detail, using individual stage diagrams as visual aids.
- Economic Potential Analysis – This section shows the net present value of this process. Equipment capital and operating costs are evaluated, and the effects of raw materials and the sale of finished products are shown.
- Environmental Health and Safety – As safety is MichiChem's top priority, this section describes ways to minimize the dangers to the plant workers and the environment.

1.4 Decision Criteria

While designing this process, a variety of criteria were considered. Decisions affecting technical and economic feasibility and environmental impact were evaluated as an active part of the design process so that all considerations were accounted for.

From a technical standpoint, the design must be accurate and feasible. This involved ensuring that all mass and energy balances were correct and that the equipment chosen would perform as required by the design. This was the first priority; a design that does not work does not satisfy the problem statement.

The second most important decision criteria were the environmental and safety effects. As the design developed, considerations about emissions and worker safety were brought up and solutions were incorporated into the original design. The most apparent risk to the environment was the removal of hydrogen sulfide from the raw gas. To solve this problem, the distillation

column that separates the hydrogen sulfide from the carbon dioxide was designed so that the carbon dioxide which is released into the atmosphere has only trace amounts of hydrogen sulfide.

The decision criteria with the lowest priority were the economic considerations. These concerns were addressed after the design was fully functional because preliminary economic analyses showed that our process was profitable. Most changes made to the design for economic reasons involved heat integration. For example, condenser and reboiler streams of adjacent distillation columns were crossed to minimize the electricity required by the system.

2 BACKGROUND

This section provides background information that presents research that supports the design decisions made in this project.

2.1 Conceptual Process Design

In industry, production of ethylene consists of three distinct steps – impurity removal, separation, and reaction. Impurity removal eliminates compounds which are either harmful to the environment or process or will not be used later. Separation divides the stream by component so that the different fractions are sent to the proper location. The reaction step converts the alkane inputs into alkene products. Figure 1 shows this in the form of a block diagram. Several process method alternatives exist for each of these steps and are discussed below.

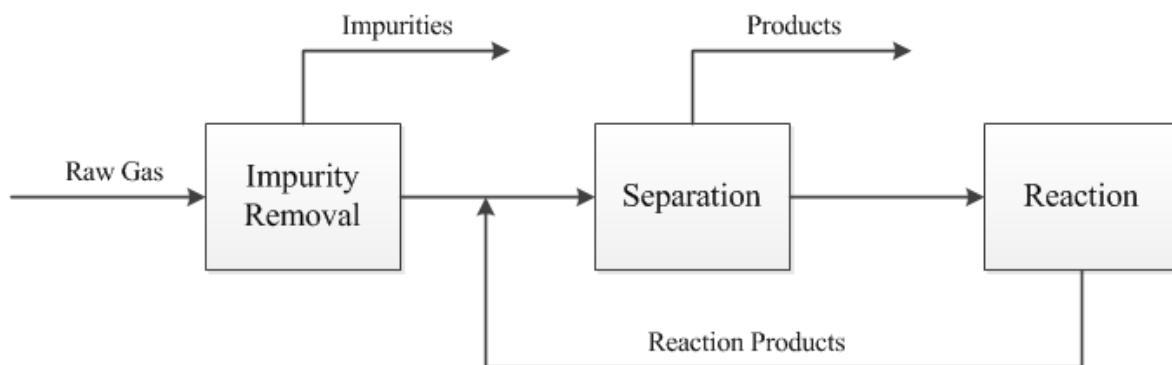


Figure 1: Conceptual block diagram showing major chemical processes in our design

2.2 Impurity Removal

Beside hydrocarbons, natural gas wells contain several impurities that must be removed. Impurities in natural gas wells include hydrogen sulfide (H_2S) and carbon dioxide (CO_2) [1]. H_2S causes multiple problems from a safety and environmental perspective. Prior to treatment, H_2S -rich natural gas, also known as “sour gas,” can be extremely corrosive and reduce the

expected lifetime of equipment and pipelines if not effectively removed [2]. CO₂ in appreciable quantities can make transportation more costly, lower the combustion quality of the gas, and is corrosive in certain environments [1]. Due to these effects, it is common industrial practice to remove CO₂. Three alternative methods exist to remove impurities in the raw gas – absorption, membrane separation, and liquid oxidation. More information pertaining to the specifications of each process can be found in Appendix A.

2.2.1 *Absorption*

The absorption process with amines is the most common industrial practice for large-scale natural gas sweetening [3]. Keeping the temperature between 30°C and 60°C and the pressure between 5 and 120 bar(a) promotes absorption [4]. Different amine solutions are used for different processes. Four of the most common amines are monoethanolamine (MEA), diethanolamine (DEA), diglycolamine (DGA), and methyldiethanolamine (MDEA) [5]. Their characteristics are summarized below.

- MEA is the most reactive of the amines and can reduce hydrogen sulfide down to 1 ppm. Due to its extensive corrosive properties, the amine concentration generally ranges from 10% to 15%.
- DEA is popular for high pressure gas impurity removal systems and is weaker than MEA, so concentrations up to 35% can exist without posing a threat to the system. DEA is an improvement on MEA in that it can be regenerated without losses.
- DGA removes more acid per volume than MEA. It is the preferred amine in cold climates because of its low freezing point.
- MDEA is the most selective absorbent for hydrogen sulfide in carbon dioxide is MDEA. The concentration can be up to 60%. MDEA is also the most expensive and its effectiveness must be weighed with its financial drawbacks. [5]

Unfortunately, absorption processes cause the exiting natural gas stream to be saturated with water. This necessitates the use of dehydration equipment to remove the water prior to distillation. One such process, known as glycol dehydration, uses triethylene glycol as an absorbent due to its high absorption capacity for water. The glycol particle absorbs water and falls to the bottom of the contactor to be removed. An advantage of this process is its ability to reuse triethylene glycol by heating the hydrate until the glycol releases the water as a gas. [2]

2.2.2 *Membrane Separation*

The second method, the gas permeation process, can be used for both impurities (CO₂, and H₂S). Porous polymer films separate the gas mixture by using partial pressure as the driving force [6]. For very sour gas, membranes can be used in conjunction with an amine process to lower amine costs. Adsorption through the films can separate the impurities with high selectivity and can improve with higher pressures and flow rates. [1] The overall operating costs are lower for membrane processes than for absorption processes with high impurity concentrations. However, the concentration of impurities in our stream is low, reducing the driving force and making membrane processes less effective.

2.2.3 *Liquid Oxidation*

The third alternative for H₂S removal requires cooling the stream before the reaction. Liquid oxidation uses a liquid solution to selectively remove hydrogen sulfide from the stream and then oxidizes it, forming elemental sulfur. This process can reduce hydrogen sulfide concentrations in the gas stream to below 1 ppm. An additional step is necessary to filter unwanted sulfur

byproducts from the pure sulfur so that it can be sold [1]. This alternative for H₂S removal has high costs due to solvent losses and uses several environmentally hazardous chemicals that must be treated with extreme care [1]. Because of this, liquid oxidation should only be used as a last resort.

2.2.4 Waste Disposal

For any of the above processes, once the H₂S has been removed it can be sold to an offsite facility and reduced to elemental sulfur [1]. One of the most common processes for this reaction is the Claus process [2].

2.2.5 Unit Operation Selection

Due to the high flow rates in the system and the low temperatures present in Michigan, absorption using DGA is the most reasonable choice.

2.3 Separation

The objective of separating our natural gas feed is to extract saleable IPQ natural gas, ethylene, hydrogen, and propylene from the reactions stage and impurity removal stage. This section discusses background research on the separations desired, process alternatives, and current industrial practices.

2.3.1 Separations Background

Separation occurs when differences in components (solubility, volatility, boiling point, molecular geometry, molecular size, and a variety of other properties) are exploited. Larger differences in component properties signify easier separation, whereas smaller differences signify more difficult separation.

2.3.2 Process Alternatives

A variety of technologies are available for separation of our natural gas feed, shown in Table 1. These gas-separation technologies are adsorption, absorption, cryogenic, membrane and ion transport membrane (ITM). Characteristics of each process technology are presented. Status is the degree to which the process technology has been utilized in industry. Economic range is the typical production range where the process technology is feasible. Purity limit is the maximum purity limit that can be produced economically. Start-up time is the time required to restart the process and reach purity after a shutdown.

Table 1: Comparison of gas-separation technologies used in industry. [2] [7]

Process Technology	Status	Economic Range (lb/year)	Purity limit (vol. %)	Start-up time
Adsorption	Semi-mature	< 102 million	95	Minutes
Absorption	Developing	Undetermined	99+	Hours
Cryogenic	Mature	>13 million	99+	Hours
Membrane	Semi-mature	< 13 million	> 97	Minutes
Ion Transport Membrane	Developing	Undetermined	99+	Hours

2.3.3 Current Industrial Practices

As shown in Table 1, industry has utilized cryogenic technologies the most for LNG separations followed by adsorption, absorption, and membrane processes. This is due to the fact that the majority of feed streams that industry processes are very large, making it more economical to select cryogenic technologies over other alternatives.

2.3.4 Requirements and Constraints

There are three major types of constraints for our separation train: products, purities, flow rates.

2.3.4.1 Products

As a requirement, MichiChem desires to produce ethylene at 500 MM lb/year and Interstate Pipeline Quality (IPQ) natural gas. In addition, as soft requirements, we aim to produce hydrogen, propylene for the market. Byproduct naphtha (C5+) will be used as fuel in providing heat duty for our cracker.

2.3.4.2 Purities

The only requirement for purity is the criteria for IPQ natural gas, as shown in Table 2. The purity of our other products is classified by grade, which signifies its purity level, and thus its worth. Since the grade of hydrogen, ethylene and propylene is not specified, factors such as separation costs and pricing will affect our final specifications.

Table 2: Specifications for interstate pipeline quality natural gas

Composition (Mol%)	Minimum	Maximum
Methane	75	100
Ethane	0	10
Propane	0	5
Butanes	0	2
Pentanes Plus	0	0.5
Nitrogen and other inert	0	4
Carbon dioxide	0	4

Maximum level of trace components:

Hydrogen sulfide 1g/100scf
Water vapor 20g/100scf

2.3.4.3 Flow rates

The separation train must be able to process the 6500 lb/min hydrocarbon stream from the phase-separation stage to produce 500 MM lb/year of ethylene.

2.3.5 Unit Operation Selection

Due to the large amount of ethylene required, cryogenic separation is the only method available that can economically separate our desired products. After subsequent separations, flow rates will be lowered to ranges where separation can be economically feasible by alternative methods, but when this threshold occurs, most streams have already been separated to their desired byproducts.

2.3.6 Molecular Sieve Dehydration

Cryogenic distillation is extremely sensitive to water; therefore, any streams fed to the cryogenic distillation train must have almost all water removed so that water does not freeze in the columns. Flash separation can be used to remove most of the water by condensing it to a liquid; however, the last of the water needs to be removed by a more powerful method, such as adsorption by molecular sieves.

Adsorption removes impurities by passing a stream through an *adsorbent* bed. Impurities (adsorbate) will adhere (adsorb) onto the molecular sieve adsorbent. The adsorbent at the start of the bed is the first to be filled to its equilibrium concentration of impurity (water); then, the “front” of “used up” adsorbent moves down the bed. Once the front reaches the end of the bed, the process switches over to a second bed. The first bed is then heated to approximately 350°C to release the water, thereby regenerating the bed and allowing the cycle to continue. [8] An illustration of adsorbent bed loading is shown in Figure 2, below.

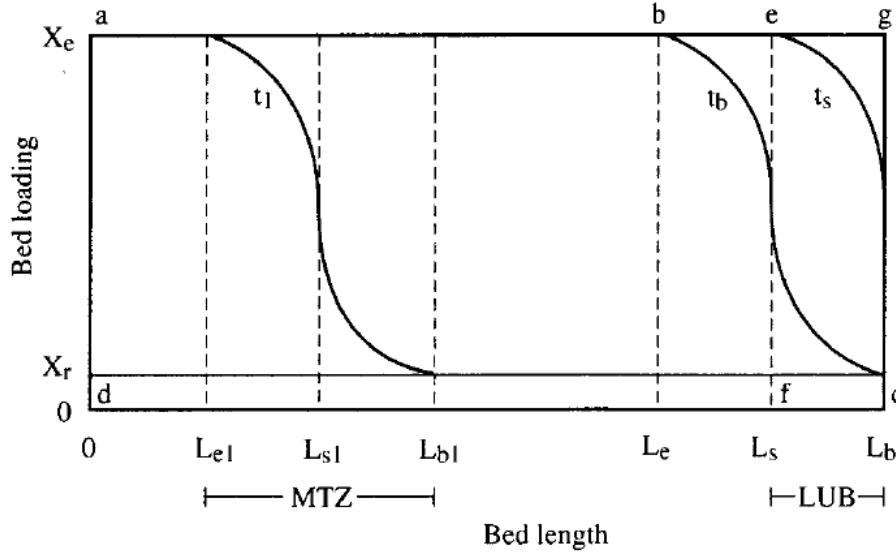


Figure 2: The concentration profiles of water the adsorbent bed at arbitrary time t_1 , breakthrough time t_b , and stoichiometric time t_s . [8]

The mass transfer zone (MTZ) is the region of the bed in which the adsorbate is actively being adsorbed. The MTZ is approximately constant throughout a bed's loading cycle and can be estimated from correlations. Once the leading edge of the MTZ reaches the end of the bed, *breakthrough* occurs, and the concentration of impurity in the gas leaving the bed would begin to rise. As such, there is a region at the end of the bed, known as the *length of unused bed* (LUB), which does not get loaded to capacity. The remaining volume of the bed that does get loaded is referred to as the *length of equilibrium section* (LES). [8]

Critical design considerations for adsorption processes include the sorbent material, bed diameter, cycle length, and mass transfer zone width. The primary consideration in sorbent material is the degree to which the stream needs to be purified. Given the low tolerance for water (the dew point of the effluent gas should be below -100°C), molecular sieve adsorbent is the best option. The bed diameter is the primary factor that determines the pressure drop through the packing. Wider beds will allow for lower superficial velocity, decreasing frictional losses and tightening the MTZ. Pressure drop is calculated via a modified version of the Ergun equation. The bed length is a function of the cycle duration (how long a bed will last before needing regeneration) and the length of the MTZ.

The desiccant is regenerated by heating, as the desiccant has a lower affinity for the impurity at higher temperature. As the bed is heated, a regeneration gas is flowed through to flush out the impurity, decreasing the impurity partial pressure in the gas, thereby driving the regeneration. Regeneration is energy-intensive because the impurity must be vaporized and the desiccant and regeneration gas must be heated up to 400°C. The regeneration gas flow rate depends on the time available for regeneration, which is based on the cycle time. [8]

2.4 Reaction

Our process utilizes two different reactions—thermal cracking and hydrogenation—to convert feeds and undesired side products into the desired products.

2.4.1 Thermal Cracking

The raw natural gas fed to the process is a mixture of light alkanes (saturated hydrocarbons). Saturated hydrocarbons contain the maximum possible amount of hydrogen per molecule, meaning they only contain single bonds. The desired product, ethylene (C_2H_4), is an alkene (commonly referred to as an olefin), meaning that it has a double bond and two fewer hydrogen atoms than ethane. If two additional hydrogen atoms are removed, resulting in a triple bond, the alkyne acetylene (C_2H_2) is formed.

Thermal (steam) cracking was specified by MichiChem as the preferred method for converting the alkane feed into ethylene. Steam cracking is a form of pyrolysis, which is the thermal decomposition of hydrocarbons without combustion. Cracking induces free radical reactions that cause the ethane and propane components of the natural gas to be converted to ethylene and propylene, though dozens of minor products are also formed. [9] Some of the possible reaction products from a cracker are illustrated in Figure 3.

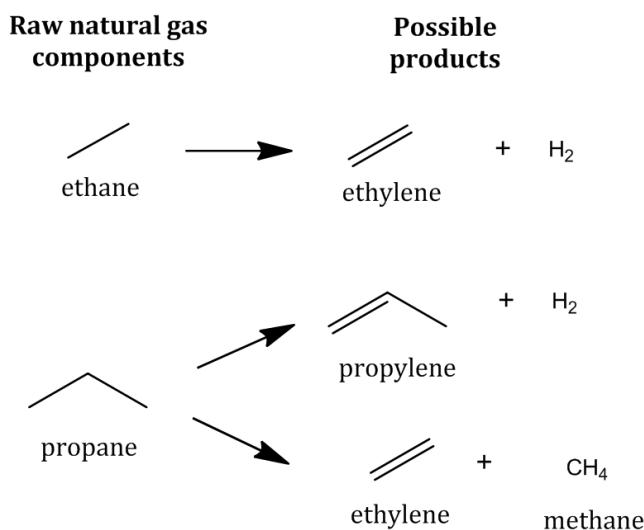


Figure 3: A sample of some of the cracking reactions that can occur with natural gas

2.4.1.1 Reaction Selectivity

As mentioned previously, the cracking reactions occur via the formation and reaction of free radicals—carbon atoms with unpaired valence electrons—when the feedstock is heated above approximately $650^{\circ}C$. These highly reactive radicals will readily strip other molecules of hydrogen atoms, in turn creating more radicals that will react with each other to form a very large number of possible products, including ethylene. Cracking reactions must be performed with very short residence times (0.1-0.5s) in order to ensure high yields of ethylene. The longer that radical reactions proceed, the more undesired heavy olefin and diolefin (molecules with two double bonds) products will form. [9]

In order to increase the selectivity of cracking towards ethylene, steam is usually mixed with the hydrocarbon feeds. The addition of steam decreases the partial pressure of hydrocarbons in the reactor, thus making the undesired secondary reactions (which decrease the total number of

moles of gas) less thermodynamically favorable. [9] Steam can be removed from the reactor products using flash tanks and desiccant beds.

The final consideration in reaction selectivity is temperature. Radicals will begin to form above approximately 650°C, so the reactor feed is typically heated to this temperature. The radical reactions occur in the reactor “coil” around 775-875°C, with higher temperatures yielding more ethylene. Cracking reactions are highly endothermic, so as more heat is supplied to the reactor coil, the conversion of the feed will improve. [9]

While there are several complex models to predict the composition of cracker gas products, Zimmermann and Wazl provide some approximations for the selectivities that can be expected under normal industrial conditions. [9]

2.4.2 Hydrogenation

A small amount of alkynes are produced in the cracking process. They are not useful or saleable, so a hydrogenation process is necessary. In this process particularly, the hydrogenator performs two reactions. It converts acetylene into ethylene and propyne into propylene. While these alkenes are formed in this process, they are not hydrogenated further into alkanes. It has been generally accepted that the adsorption of acetylene on the palladium catalyst is much stronger than that of ethylene [10]. This results in the selective hydrogenation of alkynes. The reactions occurring in the hydrogenator are shown in Figure 4.

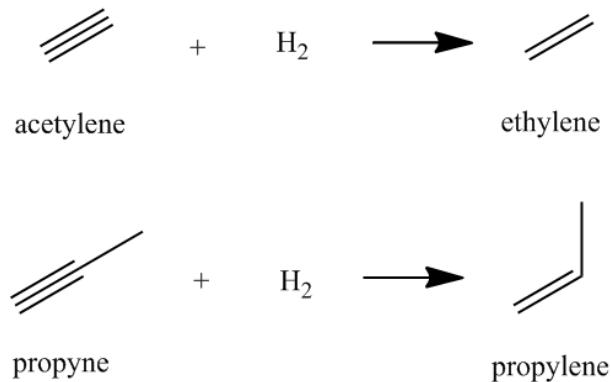


Figure 4: Hydrogenation reactions of alkynes to alkenes

Each of these reactions requires one molecule of hydrogen. Research shows that a 2:1 molar ratio of hydrogen to alkyne improves the conversion in this process resulting in over a 90% yield [10].

The most selective catalyst for this reaction is palladium on an alumina support. The typical lifetime of a Pd/Al₂O₃ catalyst is five to ten years, but by choosing a reaction temperature lower than 0.3 times the melting point of the palladium (1,555°C), the rate of metal sintering can be greatly minimized, lengthening the lifetime of the catalyst. The recommended operating pressure is 25 atm. [11]

Hydrogenation is a strongly exothermic reaction, and according to the Le Chatelier principle, the equilibrium of this reaction shifts towards the alkene products at decreasing temperatures. Because of this, it is typically preferable to separate the hydrogenator into multiple packed beds with inter-stage cooling. [12] However, after calculating the heat produced in our process, we found cooling to be unnecessary. This is described further in the process design section.

3 PROCESS DESIGN

The following sections describe the process that has been developed. The description starts at a high level, and then the individual stages are discussed in detail. Fully detailed process flow diagrams (PFDs) are available in Appendix N.

3.1 Overall Process

The gas that enters the plant from the wellhead is a mixture of hydrocarbons, inert, and impurities. The following stages process the raw gas into saleable products:

- Stage 1 sweetens the gas to remove the impurities, namely CO₂ and H₂S. These are removed for environmental reasons which will be discussed later. The sweetened gas is then sent to Stage 2.
- In Stage 2, water and pentanes and heavier hydrocarbons are removed by pressurizing and cooling the stream. This causes these components to condense, and then they are decanted. The naphtha, or heavy hydrocarbons, is sold for further refining. What remain are light hydrocarbons and a small amount of nitrogen which are further separated in Stage 3.
- Stage 3 first cools the light hydrocarbon stream to cryogenic temperatures before sending it into the separation train. This stage begins with a demethanizer. The tops product includes methane, nitrogen, and hydrogen. The methane is separated from the lighter components and sent to the IPQ natural gas line for sale. The nitrogen and hydrogen are further separated using a membrane. Some of this hydrogen is sent to Stage 5 and the remainder is sold. The bottoms product of the demethanizer is sent to Stage 4.
- Stage 4 is the second half of the cryogenic distillation train and removes the butanes for local fuel. Ethylene and propylene are removed and sold, and the ethane and propane enter Stage 5.
- In the first part of Stage 5, the alkynes, having now passed through the system twice, are hydrogenated into alkenes. The stream is then sent to the second half of the stage, the reactor. The reactor uses steam cracking to form the alkenes ethylene and propylene and also some alkynes and heavy hydrocarbons. The reactor effluent is sent back to Stage 2 where the heavy cracking components are removed and what remains goes to the separation train where the products are removed.

Figure 5 shows the overall block diagram. The flow rates and components of each stream are identified.

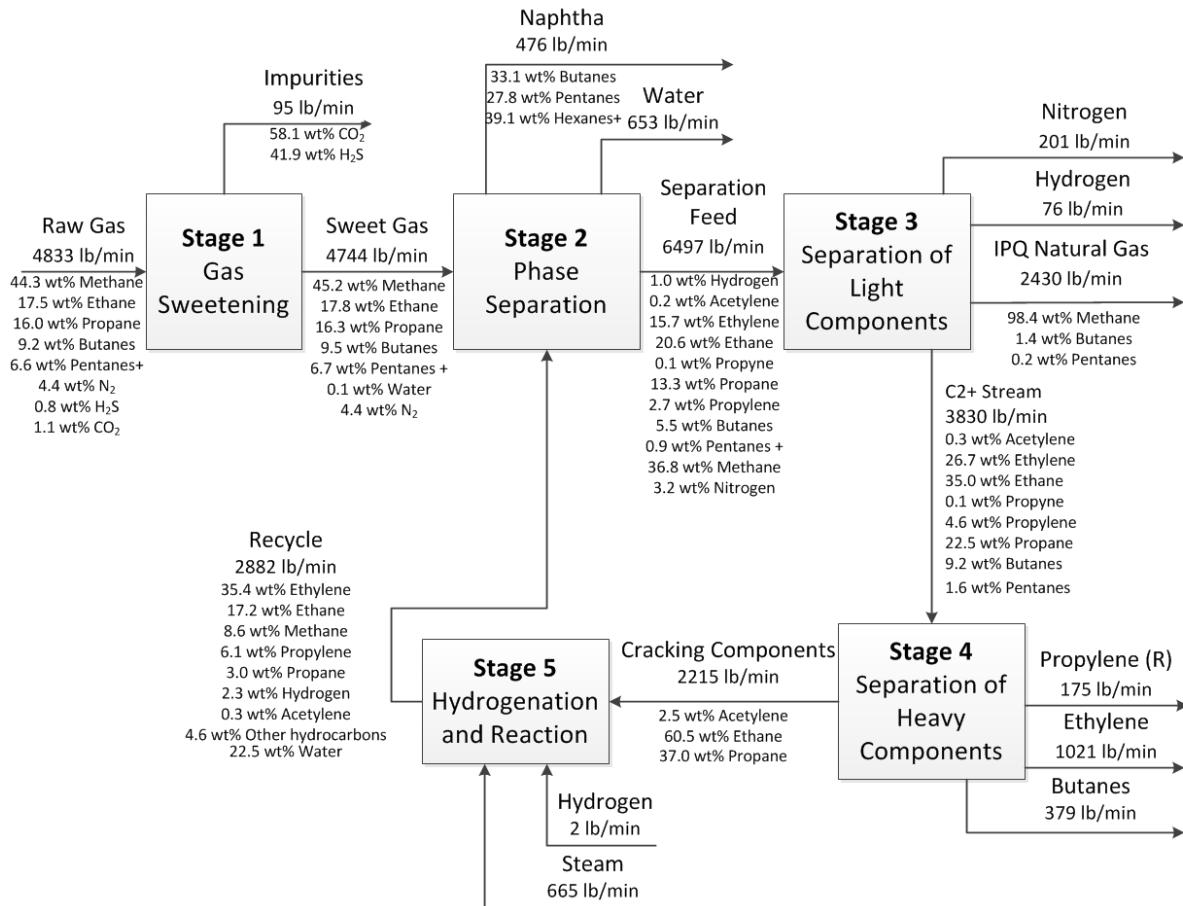


Figure 5: Overall block diagram

3.2 Stage 1: Impurity Removal

The process known as amine gas sweetening is used very heavily in industry due to its proven success at being both affordable and effective. The overall objective of this stage is to remove CO₂ and H₂S because they can cause severe corrosion, side reactions, and decreased performance in columns, piping, and reactors. The natural gas without CO₂ and H₂S, also known as sweet gas, is sent to Stage 2. The CO₂ and H₂S are stripped from the amine solution and then separated by a distillation column. The purified H₂S is sold at a discounted price to a refinery, turning it from a costly waste to a byproduct. The amine process for the MichiChem plant can be seen below in Figure 6.

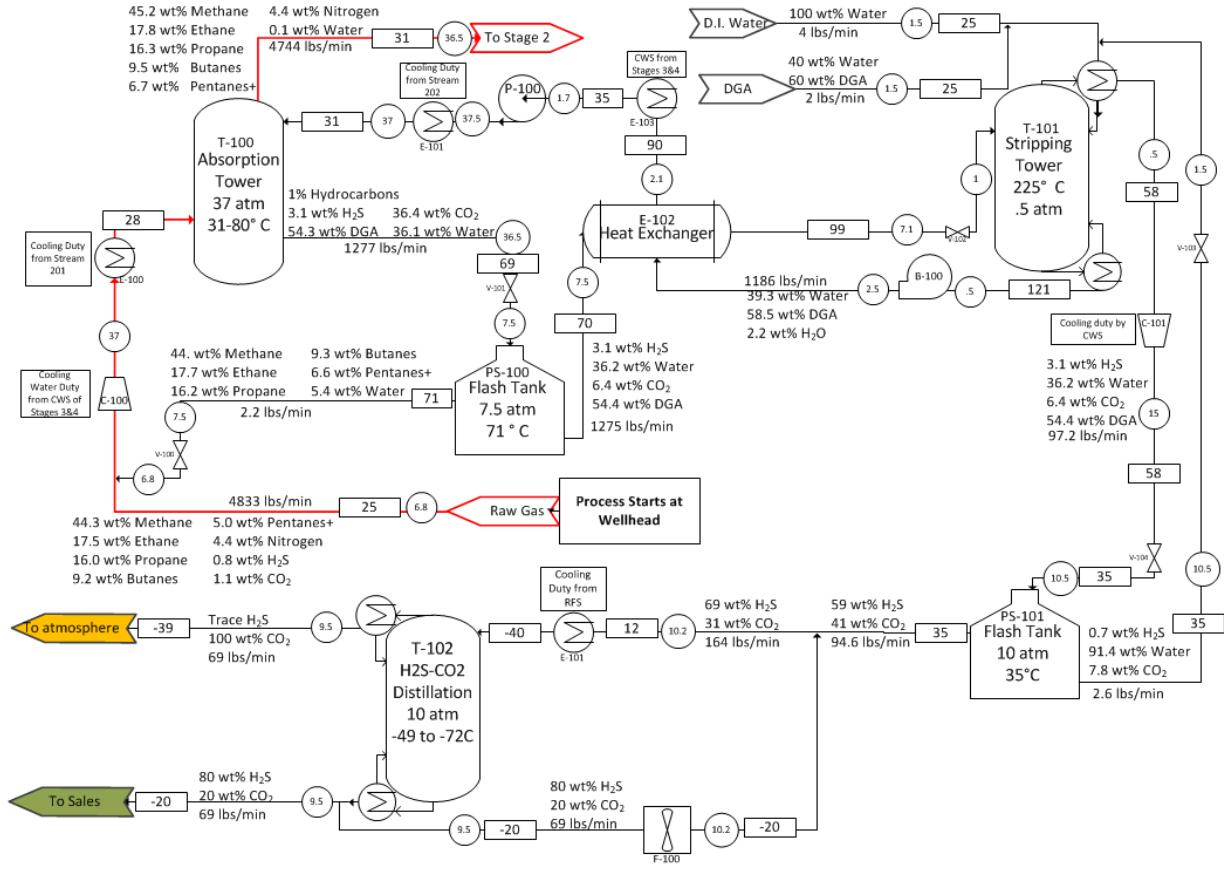


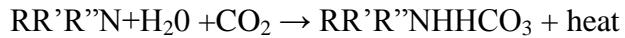
Figure 6: Stage 1 diagram, impurity removal

3.2.1 Objective

The objective of Stage 1 is to remove CO₂ and H₂S from the raw gas feed with an amine solution, strip the amine feed, and achieve greater than 80% purity of H₂S to be sold off at discount pricing. This will be achieved primarily through the use of an absorption tower, a stripping tower, and a distillation column. The equipment specification in terms of flow rate temperature and pressure can be seen in Figure 6.

3.2.2 Background

Amines preferentially react with CO₂ and H₂S, removing them from the gaseous phase and into the liquid phase. If the CO₂ and H₂S are not removed prior to distillation, thermal cracking, or distribution of IPQ gas, severe corrosion can occur as well as drastically decreased reaction selectivity [8]. The reaction mechanism for H₂S and CO₂ are shown below [13]:



Amine solutions can load a certain mole amount of acid gas per mole amine seen in Figure 7 below. As can be seen, the different amines constitute different levels of loading of acid gas.

Process	MEA	DEA	DGA	DIPA	MDEA	Mixed Solution	Selexol	K ₂ CO ₃
Amine Type	Primary	Secondary	Primary	Secondary	Tertiary	Tertiary	—	—
Reactivity	High	Moderate	Moderate	Moderate	Moderate	Moderate	Good	Excellent
Stability	Fair	Good	Fair	Good	Good	Good	High	None
HC Absorptivity	Low	Moderate	High	Moderate	High	High	Yes	No
Vaporization Losses	High	Moderate	High	Moderate	Low	Low	Low	None
H ₂ S Selective Organic S Removal	No	No	No	No	Yes	Yes	Yes	No
Corrosivity	High	Moderate	Moderate	Low	Low	High	High	Low
Tendency to Foam	Low	Low	Low	Moderate	High	High	Low	Low
Cost	Low	Low	Moderate	Low	Moderate	High	High	Low
Degradability, H ₂ S	None	None	None	None	None	None	None	None
CO ₂	Some	Low	Some	Some	Low	None	None	None
COS	Yes	Minor	Some	Severe	Minor	None	None	None
Solvent Conc., wt %	15–20	20–35	45–65	30–40	40–55	50–80	100	25–35
AG mol/mol	0.3–0.4	0.5–0.6	0.3–0.4	0.3–0.4	0.3–0.45	0.3–0.4	3–6	4–6
Loading scf/gal Circulation, gal/mol AG	100–165	60–125	50–75		65–110	65–110		
Steam Rate, lb/gal	1.0–1.2	0.9–1.1	1.1–1.3		0.9–1.1	0.8–1.1	None	0.6–0.8
Reboiler Temp, °F	240	245	260	255	250	250	80	
Freezing Pt., °F	15	20	–40	16	–25	–20		
Heat of Reaction								
Btu/lb AG, H ₂ S	620	550	675		500	500		
CO ₂	660	630	850		600	600		

Note: AG is "acid gas."

Figure 7: Overview of different amines physical and chemical characteristics [13].

Diglycolamine, DGA, was chosen for the MichiChem plant for several reasons. First it is non-selective, removing both CO₂ and H₂S at the same time to optimize the gas sweetening process. Second, DGA can operate at the lowest temperature compared to other amines, and due to MichiChem's location, extreme climate must be prepared for. Third, DGA has low tendency to foam, a detrimental process that can occur in absorption and stripping towers and causes sub-optimal performance.

Amine sweetening is a process that has been in use for decades. Many plants run at similar well gas compositions to our own. By modeling their amine process specifications, the natural gas purity criteria can be met.

Michisite's natural gas contains 1.2 mol% acid gas composed of nearly equal parts of hydrogen sulfide (0.57%) and carbon dioxide (0.63%). MichiChem's wellhead produces 5000 lb/min or 112.77 MMSCFD, containing 98 pounds of acid gas. Similarly plant B-1 data, shown in Figure 8, feeds 121 MMSCFD containing 104 pounds of acid gas at the lower bounds. By modeling our impurity removal stage with the plant data given in Figure 1, we expect the acid gas remaining in

the stream to our separations process will contain less than 0.25 grams per 100 scf of H₂S and lower than 0.01 volume percent CO₂.

Plant	A	B-1	B-2
Gas Feed Rate, MMscfd	6	121	83
Solution Flow rate, gpm	172	556	426
Solution Concentration, wt% DGA	50	60	56.5
Feed Gas Analysis			
H ₂ S vol%	5.48	0.5–1.25	0.74
CO ₂ vol%	6.52	1.5–3.75	3.46
Outlet Gas Analysis			
H ₂ S gr/100 scf	0.205	<0.25	0.01–0.05
CO ₂ vol%	—	<0.01	0.0093
Lean Solution Loading			
H ₂ S, gr/gallon	2		~21
CO ₂ mole/mole amine	0.04		0.09
Rich Solution Loading			
H ₂ S mole/mole amine	0.09		0.06
CO ₂ mole/mole amine	0.18		0.33
Absorber			
No. of trays	25		20
Pressure, psig	140		550
Lean Solution Temp., °F	120		88
Rich Solution Temp., °F	156		171
Stripper			
No. of trays, stripping	21		16
No. of rays, reflux	4		4
Pressure, psig	13		7.25
Reboiler temperature, °F	255		250
Sources: Plant A data from Harbison and Dingman (1972). Plant B-1 data from Holder (1966). Plant B-2 data courtesy Fluor Daniel (1995)			

Figure 8: Operating Data for aqueous DGA plants treating natural gas [8].

3.2.3 Process Description

Raw gas enters the plant at a rate of 4833 pounds per minute, or 112.77 MMSCFD, at 100 psi and 25° C. The gas must first be compressed before entering the absorption tower to drive the amine reaction forward and increase acid gas loading. The gas is compressed by one 9-stage compressor, sized by the method in Appendix J, increasing the pressure of the natural gas to 37.5 atmospheres. Cooling water from E-401 cools the compressor at 10,265 lb/min. The gas is then cooled to 28 °C with cooling water from stream 201 before entering the absorber.

The absorption tower is sized at 20 trays with a height of 34 feet and an inner diameter of 97". Due to the absorption tower having no heat exchange with the surroundings due to insulation, the temperature profile can be expected to be similar to that in Figure 9. This profile curve supports the assumption that the vapor gas leaving the tower is equal in temperature to the entering lean amine solution. The bubble in the temperature profile between stages one and eight is due to the amine reaction generating 73,647 btu/min. The sweet gas leaves the top of the absorption tower with less than 0.25 gr/scf of H₂S and below 0.01 volume percent CO₂, at 4,744 lb/min, below the recommended guidelines for IPQ gas, and is sent to Stage 2 to remove water and naphtha.

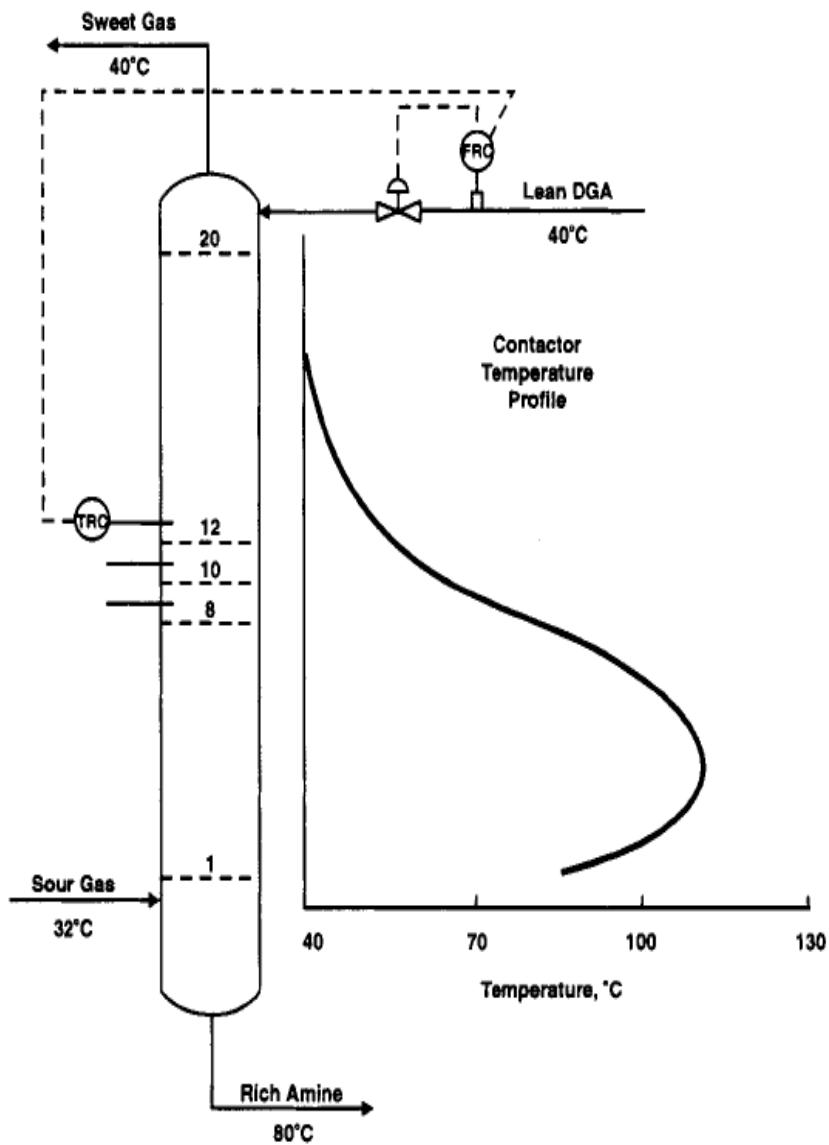


Figure 9: Sample Absorber Temperature Profile [8].

The bottoms product of the absorption tower is known as the rich amine solution because the acid gas has chemically bonded to the amine. However, an average of 2 SCF of natural gas per gallon of amine is entrained with the liquid leaving the bottoms. Due to the problems hydrocarbons cause during the regeneration cycle and the increase in efficiency by recycling the hydrocarbons to the stream, a phase separator tank is installed directly downstream of the amine absorber at the end of stream 102. The phase separator has been sized for a residence time of 15 minutes at a capacity of 3000 gallons [13]. For the calculations of the phase separator, see Appendix B. The pressure drop from V-100 forces virtually all the hydrocarbons to leave through the vapor exit stream.

The lean/rich heat exchanger, E-102, is important for keeping heating costs down. The pressure drop is estimated to be 0.4 atmospheres and the approach temperature to be 40 °F. The approach temperature is a standard for the lean/rich amine heat exchanger which this heat exchanger

adheres to [8]. It is currently sized to a heat exchange rate of 66,400 btu/min with a cross-sectional area of 250 m². For sample heat exchanger calculations, please see Appendix I.

The rich amine solution is sent to the stripping tower, T-101, at 1275 lb/min at 99 °C. The amine solution for plant B has a reboiler temperature of 121 °C. The stripper is held at low pressure, 7.25 psi, and high temperature to force the equilibrium of the amine-acid gas reaction backwards. The stripping tower requires condenser and reboiler duties of 571,200 and 203,900 btu/min respectively. The condenser is cooled by 38,000 lb/min of cooling water. The reboiler is heated by 227 lb/min of low pressure steam. The tower is 46 feet tall, with a 79" inner diameter. Like Plant B, the stripping tower has 20 trays with a tray spacing of 24" [8]. The amine solution, having been regenerated, is sent to the lean/rich heat exchanger. Stream 105, the bottoms stream of the stripping tower, has a small amount of CO₂ in it as the solution cannot be completely regenerated [13]. The amine solution does lose some water to the absorption top stream, stream 101, and is replaced at a rate of 2 pounds/min from stream 116 [13]. Trace amounts of DGA will be lost through T-100, T-101, and normal mechanical loss, and is accounted for by the addition of 4 lb/min of DGA from stream 115. For a calculation of the energy balance, and the sizing of the tower itself, see Appendix A. The distillate of the tower is almost pure acid gas. This is to be expected as once the acid gas breaks free of DGA, the boiling point difference between the acid gas and the DGA/water mix is well over 100° C.

A small amount of water does leave with the distillate of T-101, requiring it to be removed prior to the H₂S/CO₂ distillation column. H₂S is corrosive in the presence of water, and the phase separation tank, PS-101, removes this water. Prior to the flash tank, the stream is compressed to 15 atmospheres and flashed back to 10.5 atmospheres and 35 °C. This flash tank is sized at 100 gallons, calculated in the same manner as D-100. The pressure drop is 4.5 atm and removes virtually all of the water from the distillate stream before being sent back to the reflux of T-101 to increase efficiency.

The distillation column operates with a feed temperature of -37 °C, so refrigeration must be used to cool it, requiring a refrigeration duty of 19,500 btu/min. Although some other streams in this process could also cool this stream, the H₂S- and CO₂- rich streams would contaminate the sweet gas streams if any of the heat exchanger tubes failed. Due to this concern, the refrigeration fluid chosen is Freon-22 which is used nowhere else in the process. This duty requires 190 pounds per minutes at -60 °C to cool the stream effectively. Stream 110 enters the distillation column at the 18th tray of 30. The reboiler duty is 14,930 btu/min with a condenser duty of 24,060 btu/min. The reboiler is heated by cooling water at 1035 lb/min while the condenser is cooled by Freon-22 at a rate of 3200 pounds per minute. The purities in the two outlet streams include trace amounts of H₂S in the distillate and 80% by weight in the bottoms stream. MichiChem can sell the low-grade bottoms for 30% retail cost according to supervisor recommendations. The distillate, with only trace amounts of H₂S, can be released to the atmosphere.

3.3 Stage 2A: Water and Naphtha Removal

Stage 2A is responsible for the removal of heavy hydrocarbons and water from the combined stream of fresh sweet gas and recycled cracker products. The fresh sweet gas from Stage 1 contains some water and a fair amount of heavy hydrocarbon. The water must be removed because it would freeze in the cryogenic towers, and the heavier hydrocarbons are removed

because they are more valuable as a naphtha side product than as a cracker feed. Stage 2 is depicted in Figure 10 below.

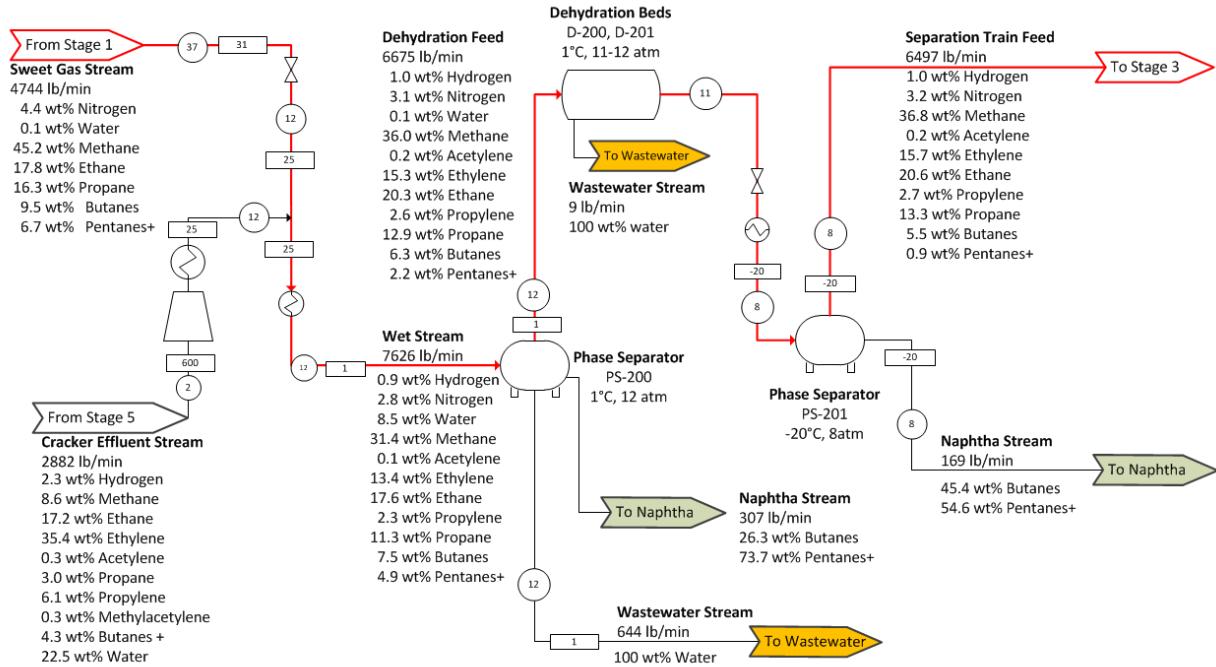


Figure 10: Stage 2A diagram, naphtha and water removal

The streams from Stages 1 and 5 are combined at 12 psi. (The stream from Stage 5 needs to be cooled and compressed; the stream from Stage 1 needs to be throttled.) At this higher pressure, the combined stream can be refrigerated to 1 °C without concern of the water freezing. At the elevated pressure and cooler temperature, over 98% of the water will liquefy. Much of the heaviest hydrocarbons will also liquefy. Our process takes advantage of the immiscibility of hydrocarbons in water to separate the two liquid phases in a liquid/liquid/vapor separator.

There was a careful balance to strike in considering the operating conditions of the first separator. A higher pressure would have allowed more water to condense out in the separator; however, some of the valuable gaseous products (ethylene and propylene in particular) would also start to condense and would end up in the naphtha sales stream where they would sell at a lower value.

The first phase separator is able to remove a large amount of the water without incurring expensive equipment costs; however, there is still a considerable amount of water that must be removed before moving to cryogenic distillation. Two common methods for effectively removing almost all water from a gas stream are adsorption and glycol dehydration. Glycol dehydration is typically used for removal of larger water concentrations from larger flow systems due to its complexity and cost; however, adsorption can be scaled down very well to meet the smaller dehydration needs of our process [8].

The adsorption process requires two adsorbent beds operating on an alternating 8-hour schedule. When a bed is active, it accepts the gas feed saturated with water. Upon exiting the 1/16" sphere molecular-sieve adsorbent packing, the gas has a dew point of less than -100°C, meaning that any trace water would not liquefy unless the process temperature falls below the dew point [8]. Each bed is 5 feet long and 16 feet in diameter. The pressure drop through the bed is 15.5 psi, so the dry gas exits at 11 atm. Calculations for the dehydrator are shown in Appendix C.

After the gas is dehydrated, the temperature can be lowered in order to condense out more of the heavy hydrocarbons into the valuable naphtha product. Again, there is a balance in selecting a temperature low enough to condense most of the C6 and C7 molecules but high enough to prevent the ethylene and propylene from condensing into the naphtha and resulting in a loss of product. The pressure of the second phase separator was chosen at 8 atm so that the pressure matches up with the beginning of the separation train. Since there is no water in the second separator, only a two-phase separator is needed.

Supporting calculations for the water and naphtha removal stage are shown in Appendix B.

3.4 Stage 2B: Cryogenic Refrigeration

Stage 2B is responsible for cooling the dehydrated hydrocarbon stream leaving Stage 2A and entering Stage 3 to a temperature that allows cryogenic distillation to be feasible. In this system, a 3-step cascade process using phase separators, throttle valves, and coil-wound heat exchangers (CHWEX). A compressor-expander system, also known as a turboexpander, was also implemented to create the high pressures required to reach cryogenic temperatures. A refrigerant composed of 20 wt% nitrogen, 35 wt% methane, and 40 wt% propane was used since its cooling curve more closely matches the cooling curve our hydrocarbon streams as compared to other single-component refrigerants.

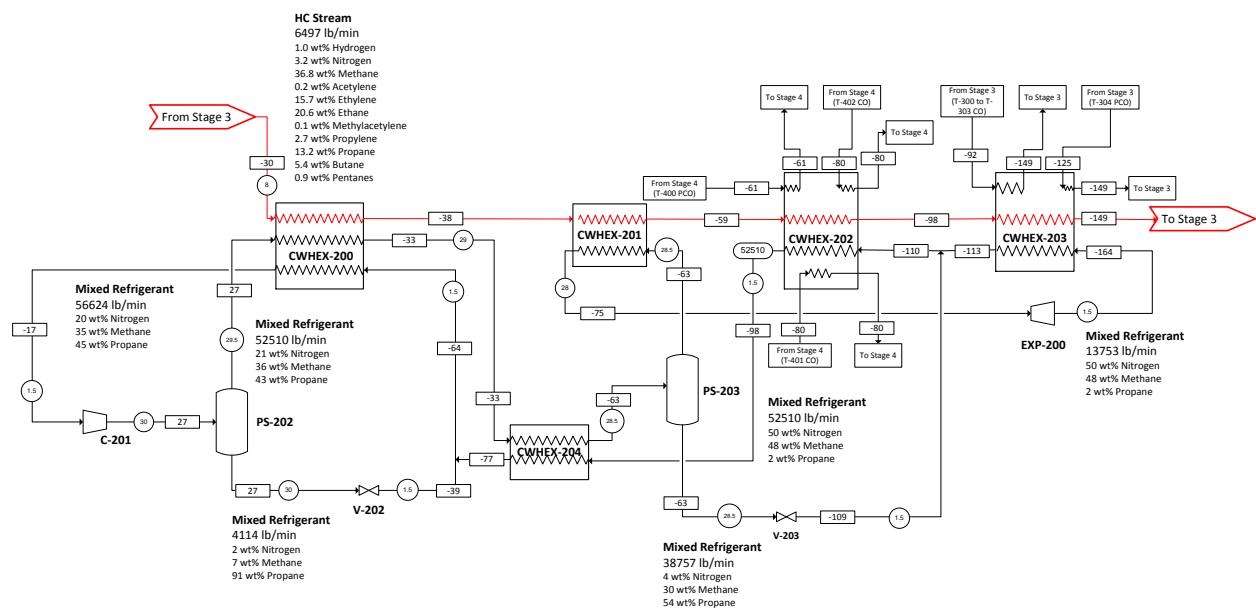


Figure 11: Stage 2B diagram, cryogenic refrigeration

As shown in Figure 11, refrigerant at a temperature of -17°C is compressed to 30 atm by C-201. The refrigerant is then sent to PS-202 where gaseous refrigerant is separated from the liquid refrigerant. The liquid refrigerant is throttled to a temperature of -39°C where it mixes with a cold stream from CHWEX-204. This stream then enters CHWEX-200 to provide cooling duty. The gaseous refrigerant from PS-202 enters CHWEX-200 and CHWEX-204 where it is cooled even further until it reaches PS-203. The gaseous refrigerant from PS-203 provides cooling duty at -75°C to CHWEX-201 then expanded to a temperature of -164°C to provide cooling duty to CWHEX-203. The liquids stream from PS-203 is throttled to a temperature of -109°C and mixed with the refrigerant stream leaving CHWEX-203. This stream, at a temperature of -110°C provides cooling duty to CHWEX-202 and CHWEX-204.

Stage 2B, due to cryogenic temperatures, will be constructed using stainless steel. More information regarding the size of phase separators, heat exchangers, piping, and utility can be found in Appendices B, I, K, and L, respectively. In addition, Appendix D contains more information about the development of our cryogenic refrigeration system.

3.5 Stage 3: Separation of Light Components

Separation of the hydrocarbon feed from Stage 2 is achieved by exploiting the differences in physical properties of its individual components. The overall objective of this stage is to separate out the light components of our natural gas feed: hydrogen, nitrogen, and methane. Methane is sent to the market as Interstate Pipeline Quality (IPQ) natural gas. As shown in Figure 12, the C2+ stream will be sent to Stage 3 for further processing. This section presents the objective of the stage, step through how the stage works, introduce the equipment required, and then goes over sizing and operation specifics.

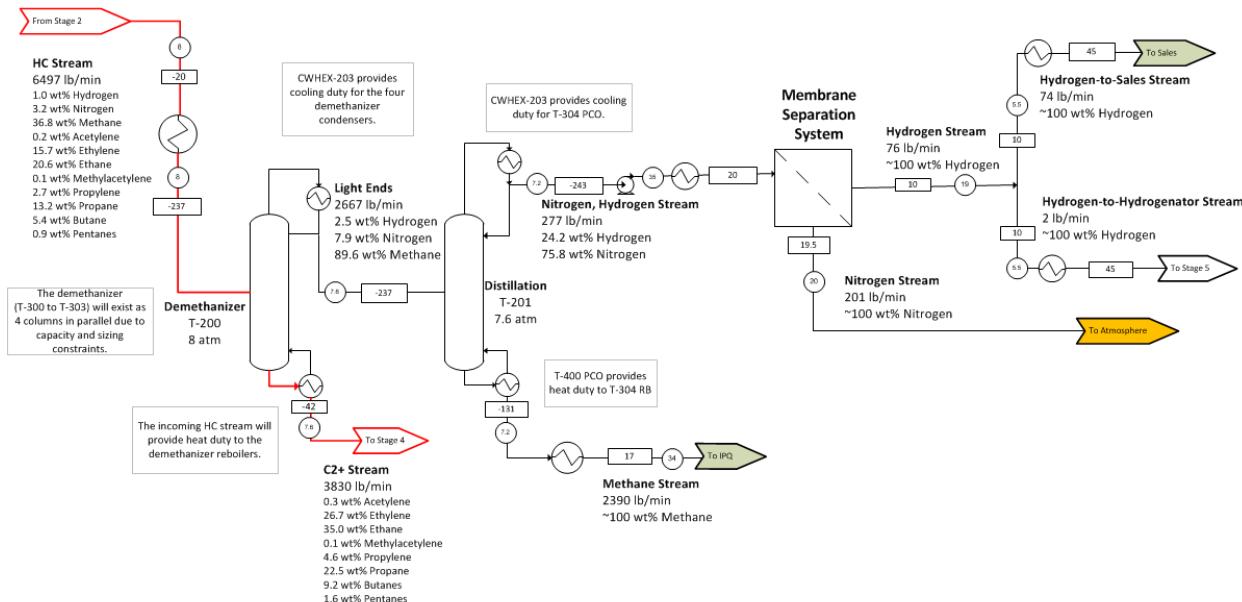


Figure 12: Stage 3 diagram, light component separation

The objective of Stage 3 is to produce high purity natural gas, which is primarily methane, by separating out light components consisting of primarily methane, hydrogen and nitrogen. The IPQ natural gas must be within the specifications shown in Table 3.

Table 3: Criteria IPQ natural gas

Composition (Mol %)	Minimum	Maximum
Methane	75	100
Ethane	0	10
Propane	0	5
Butanes	0	2
Pentanes Plus	0	0.5
Nitrogen and other		
Inerts	0	4
Carbon dioxide	0	4
Hydrogen sulfide	0	1g/100scf
Water vapor	0	20g/100scf

To economically achieve this objective our process design must: (1) cool our hydrocarbon feed from Stage 2 to a liquid, (2) separate out desired components for the market, further processing, or as fuel, and (3) improve the energy performance of our distillation system through the use of thermal couplings. The separation system will be stepped through in this section. Justification for selection of major steps, operating performances, sizing, utility requirements, and sizing will be discussed.

Cryogenic distillation is used in industry to separate components that liquefy below -50°C. The gaseous HC Stream, which enters at a pressure of 8 atm, is liquefied from a temperature of 28°C to -30°C by first using cold duty from cryogenic product streams (hydrogen/nitrogen mixture, methane, propane, and ethane) and finally down to -150°C before it is fed into the distillation column at a pressure of 8 atm. Hydrogen, nitrogen, and methane was separated from the rest of the feed in the C2+ Splitter (T-300, T-301, T-302, T-303), which is configured with 4 distillation towers in parallel. This was done to keep column diameters lower than 15 feet to allow for shipping of the column via highways.

The light ends distillate product from the C2+ Splitter consists of primarily hydrogen, nitrogen, and methane. This mixture then enters the demethanizer (T-304) where a pure methane stream leaves from the bottoms at a temperature of -131°C at a pressure of 6.8 atm. A bit of byproduct butanes from Stage 4 is added to the methane stream. The methane stream also provides some cooling duty to the HC Stream. Before the methane stream vaporizes, it is pressurized to 35 atm using a pump, and then heated to 17°C to be sent out as IPQ natural gas. The nitrogen, hydrogen stream exits the demethanizer at a temperature of -149°C at a pressure of 7.6 atm. This stream is heated up to 17°C using heating duty from T-400 and T-402 condensers. The hydrogen-nitrogen stream is then separated using a system of three membrane separators to produce a stream of 99.2 mol% purity hydrogen both for sales and for the hydrogenator. More information about the membrane separators is provided in Appendix F. A stream of 99.9 mol% nitrogen is released to the atmosphere.

Distillation towers were sized using Aspen Tech after the desired separation scheme has been successfully modeled. All the columns were sized using bubble cap trays with a spacing of 2 feet to allow for potential frothing as a safety factor. In addition, all distillation towers in stages 3 and 4 along with piping are made with stainless steel, which does not exhibit ductile-to-brittle transitions. See Appendix E for our methods and more complete sizing information.

The membrane separation system requires 60,000 square meters of a polyvinyltrimethylsilane membrane. Polyvinyltrimethylsilane, which is a glassy polymer, is more robust and also separates hydrogen from nitrogen more effectively than softer polymers in the market. Our membranes will be installed as 1 meter long cartridges with a diameter of 10 centimeters. Each cartridge will have 10^6 hollow polymer fibers, each 100 microns in diameter. This being said, a total of 193 cartridges will need to be purchased for separation.

3.6 Stage 4: Separation of Heavy Components

Separation of the C2+ hydrocarbon feed from Stage 3 using the use of cryogenic distillation column schemes. The overall objective of this stage is to separate out the light components of our natural gas feed: hydrogen, nitrogen, and methane. Methane is sent to the market as IPQ natural gas. As shown in Figure 13, the C2+ stream will be sent to Stage 3 for further processing. This section presents the objective of the stage, steps through how the stage works, introduces the equipment required, then goes over sizing and operation specifics.

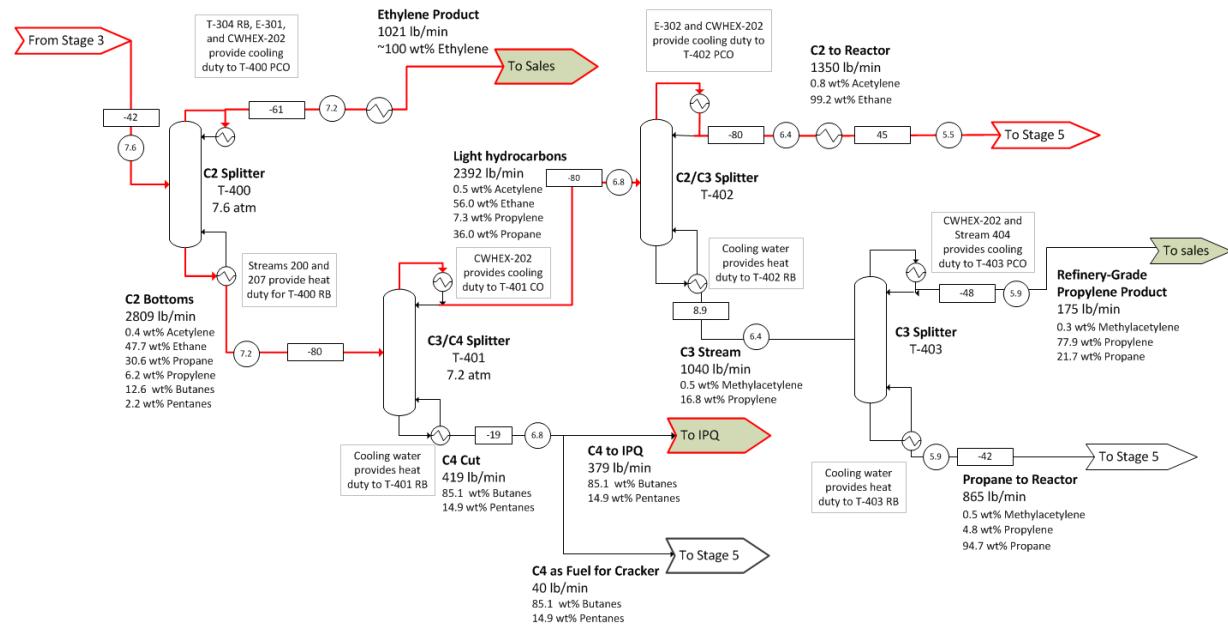


Figure 13: Stage 4 diagram, heavy component separation

Stage 4 is a continuation of Stage 3 in the sense that it continues the separation of hydrocarbons using cryogenic distillation columns. The C2+ stream from Stage 3 enters Stage 4 at a pressure of 7.6 atm and -42°C and enters the C2 Splitter (T-400) where our ethylene product is distilled.

The ethylene product stream leaves the top of the C2 Splitter at -61°C and 7.2 atm. The ethylene stream is then heated to 25°C using cooling water and enters the market via pipeline.

The C2 Bottoms stream exits the C2 Splitter at -80°C and 7.2 atm. This stream is fed directly into the C3/C4 Splitter (T-401) where a C4 Cut stream consisting of butanes and pentanes leave through the bottoms at a temperature of -19°C and 6.8 atm. About 10% of this stream is sent to be mixed in with our methane stream, which leaves as IPQ natural gas via pipeline. The rest is sent to the cracker in Stage 5 as fuel to heat the cracking reaction

The Light Hydrocarbons leave the C3/C4 splitter (T-402) at a temperature of -80°C and 6.8 atm and is fed into the C2/C3 Splitter. The C2/C3 splitter produces ethane with acetylene impurity at a temperature of -80°C and 6.4 atm. The cooling duty of the ethane stream is sent to distillation condensers downstream.

The bottoms of the C2/C3 splitter produces a C3 stream at -48°C at a pressure of 6.4 atm. This stream contains a mixture of primarily propane and propylene. This mixture is split by the C3 Splitter (T-403) into two streams. The distillate stream is refinery-grade propylene at a temperature of -48°C at a pressure of 5.9 atm. This refinery-grade propylene is approximately 78 wt% propylene and 22 wt% propane. This stream is sent out to the market via pipeline. The bottoms of the C3 splitter consists of a mixture of primarily propane at a temperature of -42°C and a pressure of 5.9 atm. This stream is sent to the hydrogenator in Stage 5.

Distillation towers in Stage 4 were also sized using Aspen Tech after the desired separation scheme has been successfully modeled. All the columns were sized using bubble cap trays with a spacing of 2 feet to allow for potential frothing as a safety factor. As mentioned earlier, all distillation towers and pipes in Stages 3 and 4 are made with stainless steel. See Appendix E for our methods and more complete sizing information on distillation towers.

3.7 Stage 5: Reaction

Stage 5 is where the hydrogenation and thermal cracking reaction steps take place. The hydrogenator uses hydrogen to convert alkynes into alkenes, and the reactor uses heat and steam to crack alkanes into alkenes. Stage 5 is depicted in Figure 14 below.

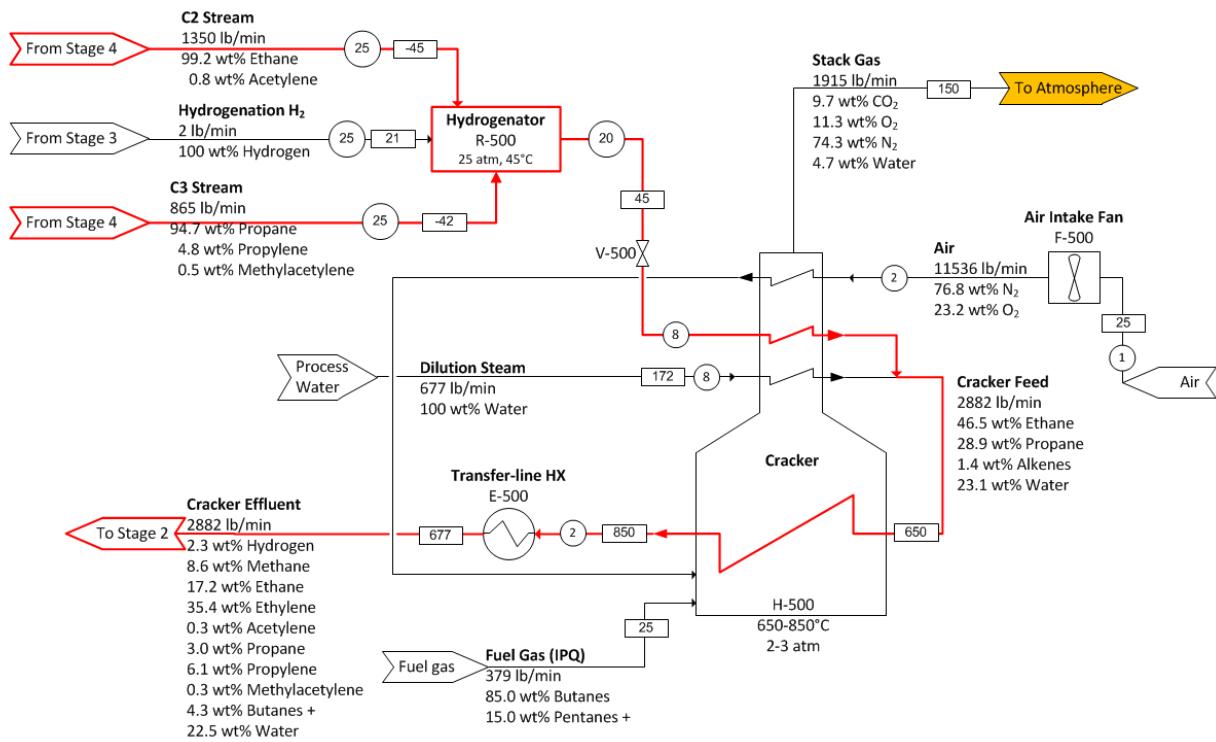


Figure 14: Stage 5 diagram, reactions

3.7.1 Hydrogenation

The first step in Stage 5 is hydrogenation. The purpose of the hydrogenator is to partially saturate the alkynes into alkenes through a chemical reaction called hydrogenation. This is done for two reasons. The alkenes produced in the reaction are more economically valuable than the alkynes from which they were formed. More importantly, it is difficult to separate the alkynes from their alkane counterparts through distillation. Without hydrogenation, the alkynes would form and cycle continuously through the process and accumulate. By hydrogenating them, they eventually leave the process.

The hydrogenation unit is a packed bed reactor and uses palladium supported on alumina as the catalyst with an extent of labeling of 10 wt% palladium. The reactor is 5 inches long and has a 2 ft diameter. The reaction is run at 45°C under a pressure of 25 atm. 48 pounds of catalyst are required for the 90% conversion. The pressure drop through the reactor causes the outlet pressure to be 19.7 atm. Although the hydrogenation reaction is strongly exothermic, the reactor itself is isothermal as the reacting species only account for 0.7 wt% of the feed. Calculations for these specifications are shown in Appendix G.

The mass flow into the hydrogenator is 2217 lb/min. The feed consists primarily of ethane and propane which do not participate in the reaction. Propylene is also present but does not react due to the selectivity of the catalyst. The remaining species are acetylene, propyne, and hydrogen in the specified 2:1 molar ratio of hydrogen to alkynes. The hydrogen is supplied by the membrane separator in Stage 2.

3.7.2 Thermal Cracking

Once most of the alkynes have been reduced, the gas from the hydrogenator is fed to one of four thermal (steam) crackers. The purpose of the cracker is to convert the alkanes in the feed to the desired alkene products (primarily ethylene and propylene). Thermal cracking was specified as MichiChem's preferred method for ethylene production.

The thermal cracking unit consists of four furnaces in parallel, such as the one illustrated in Figure 15. Each furnace has a radiant section (the firebox) through which the reactor coils wind. A butane/pentane mixture from the separation train is combusted in 100% excess air to heat the reactants in the coil. The fireboxes operate at approximately 1000°C, so most of the heat transfer into the cracker coils occurs through radiation.

The hot combustion gases from the radiant section move to the convection section where they are used to preheat the reactor feed and the air to 650°C. The combustion gas is then discharged to atmosphere via a stack.

The preheated hydrocarbon feed, which is primarily propane and ethane, is diluted with 0.3 pounds of steam per pound of feed before it enters the cracker coils (in order to improve selectivity to ethylene by decreasing hydrocarbon partial pressures). Inside the 2-inch diameter coils, the mixture is heated to a temperature of 850°C with just 0.45s residence time. To achieve the 0.45s residence time, which is optimal for ethylene selectivity, the total coil volume (between all 4 fireboxes) should be 8.8 m³.

Once the reactive species leave the radiant section of the furnace, the reaction needs to be immediately stopped in order to prevent ethylene from being consumed in undesired side reactions. The reaction is stopped by a quench that lowers the temperature, stopping the radical reactions. The quench occurs in a transfer-line heat exchanger that boils process water (coolant) to generate dilution steam to be added to the reactor. The reacted stream leaves the exchanger at 677°C.

Full calculations and further design considerations for the crackers and furnaces are available in Appendix H.

An instrumentation and process control scheme was developed for the crackers and furnaces and is described in the subsequent section.

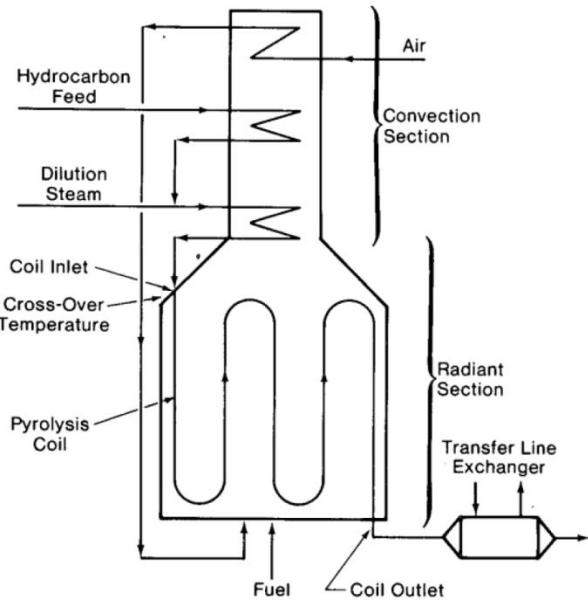


Figure 15: A simplified illustration of the parts of a thermal cracker. In reality, crackers can consist of several coils that run in parallel through the radiant section. [17]

3.8 Process Control – Cracker

Our team was asked to design a process control strategy for the crackers and furnaces. In implementing a control strategy on the cracker, it was first necessary to determine which process parameters were most essential to safely and properly operate the crackers and furnaces such that they produced the expected reaction yields. In descending order of importance, these parameters are:

1. Reactor coil outlet temperature
2. Steam-feed ratio
3. Quench outlet temperature (to ensure complete quenching)
4. Air-fuel gas ratio

In order to control these parameters, the instrumentation listed in Table 4 is required. Additional instrumentation that does not feed directly into any automatic controller is to be installed so that the process can be better monitored. An illustration of the placement of the instrumentation is shown in the piping and instrumentation diagram (P&ID) in Appendix O.

Table 4: Required instrumentation for crackers and furnaces

Instrument name	Instrument type	Measurement
FT 501	Orifice plate	Air intake flow rate
FT 409	Orifice plate	Fuel flow rate
AT 502	Analyzer	Stack gas NO _x emissions
FT 504	Orifice plate	Hydrocarbon feed flow rate
FT 505	Orifice plate	Steam flow rate
PT 506	Pressure gauge	Cracker inlet pressure
PT 507	Pressure gauge	Cracker outlet pressure
TT 507	Thermocouple	Cracker coil outlet temperature
TT 507B	Thermocouple	Post-quench temperature

The P&ID also shows the 4 controllers and 4 control elements used by those controllers. The details of these controllers and control elements are described in Table 5 and Table 6, respectively. Each controller will be discussed individually.

Table 5: Listing of automatic controllers used by crackers and furnaces

Controller	Description	Controlled variable	Manipulated variable
FFC 501	Air-fuel ratio control	Air flow (FT 501)/ Fuel gas flow (FT 409)	F-500 fan speed
FFC 505	Steam-feed ratio control	Steam flow (FT 505) / Hydrocarbon feed flow (FT 504)	Steam flow to cracker (via CV 505)
TC 507	Cracker coil outlet temperature control	Cracker coil outlet temperature (TT 507)	Fuel gas flow rate (via CV 409)
TC 507B	Quench outlet temperature control	Cracker product temperature after quench (TT 507B)	Process water flow rate (via CV 505W)

Table 6: Listing of final control elements used by the automatic controllers

Control element	Condition controlled
CV 505	Steam flow to cracker (excess steam vented)
CV 409	Fuel gas flow
CV 505W	Process water flow to quench exchanger E-500
F-500	Air intake flow rate

3.8.1 Reactor Coil Outlet Temperature Control

Perhaps the most important process parameter to control in an ethane cracking operation is the temperature of the reactor coil outlet, as it is a key determinant in the yield of ethylene. Since rate of reaction increases exponentially with temperature, the highest temperature in the reactor (the coil outlet) is the most important temperature to control. The temperature of the coil outlet is a function of the radiative heat transfer, which is most directly driven by the rate of combustion in the furnaces' fireboxes. As such, it was decided to control coil outlet temperature by manipulating the fuel gas flow rate. Controller TC 507 receives input from TT 507 (coil outlet temperature) and acts on control valve CV 409. The setpoint under normal process conditions should be 850°C. Since reaction rate is heavily dependent on temperature, tight alarm limits should be set at approximately 860°C (high alarm) and 835°C (low alarm).

Note that the reactor coil outlet temperature can also be affected by changes to that air-fuel gas ratio setpoint. When the combustion is set to run richer (less air), the ambient temperature of the firebox will rise until TC 507 backs down the fuel gas flow rate.

3.8.2 Steam-Feed Ratio Control

Another critical parameter for the assurance of high ethylene yield in the cracker is having an appropriate amount of steam to dilute the hydrocarbon feed. For our process, it is desired to have a mass flow rate ratio of 0.3 lb steam / lb hydrocarbon fed. This ratio can be maintained by the use of flow-flow ratio controller FFC 505. The controller takes as input the flow rates of the hydrocarbon feed (FT 504) and of the steam feed (FT 505). The ratio setpoint will be 0.3 under normal operating conditions. FFC 505 sends an output signal to CV 505, which controls the flow rate of steam to the cracker. For reasons to be discussed with the next controller, any excess steam from E-500 should be vented.

3.8.3 Quench Outlet Temperature Control

In order to preserve the high ethylene yield exiting the cracker coil outlet, the reaction must be sufficiently quenched immediately. Quenching occurs in transfer line heat exchanger E-500, which boils process water to provide the necessary cooling duty. It is important that the cracker products leaving the exchanger have been cooled enough to stop the radical reactions that would lead to degradation of the ethylene yield. To ensure sufficient quenching, TC 507B will take as input the quench outlet temperature (TT 507B) and will manipulate the process water (coolant) flow rate via control valve CV 505W.

Note that there are two control valves on Stream 505. In order to prevent accumulation of steam in the stream, CV 505 and CV 505W will communicate via the plant's distributed control system

(DCS). First, it is most important that there be enough steam to dilute the hydrocarbon feed, so TC 507B must never cause CV 505W to restrict the water flow rate below that required for dilution. In some instances, this requirement will cause the quench outlet temperature to fall below its setpoint; however, this error is entirely acceptable, as the cracker product must be cooled further in Stage 2A anyways. In cases where TC 507B requires a greater amount of steam production to keep the quench product below the allowable temperature maximum, accumulation of steam in Stream 505 will be avoided by venting the excess in CV 505.

3.8.4 Air-Fuel Gas Ratio Control

The final automatic controller for the cracker will be the air-fuel gas ratio controller, FFC 501. The amount of air needed for combustion of the fuel gas is directly proportional to the flow rate of fuel gas (which is set by TC 507); therefore, it is appropriate to use a ratio controller that takes as inputs the fuel gas flow rate (FT 409) and the air flow rate (FT 501). The controller sends its output to F-500, adjusting its power setting in order to manipulate the air intake rate. At steady state, the controller will maintain 100% excess air, as shown in the process flow diagrams (Appendix M).

3.8.5 Additional Instrumentation and Manual Control

In order to assure process safety, the pressure of the gas at the cracker inlet and outlet will be monitored by PT 506 and PT 507, respectively. The difference in these readings will be reported to the operators as the cracker's pressure drop, which will be 6 atm at steady state. These two pressure gauges will be able to provide much diagnostic information to the operators:

- If PT 507 suddenly drops, a cracker coil will have likely ruptured. As the pressure inside the coil exceeds the firebox pressure, there is no risk of oxygen getting into the process. The leaking product should combust in the firebox; however, the process will need to be shut down to fix the rupture.
- If PT 506 suddenly drops, there will have likely been an external leak. Hydrocarbons will have escaped the process, and the area would need to be evacuated.
- Over time, the small cracker coils will likely become plugged with deposits. A historical trend of the pressure differential will show this progression and will indicate when the cracker needs to be shut down in order to clean the coils.

From an environmental quality perspective, it was also decided to monitor the NO_x emissions in the furnaces' stack gases, as NO_x is prone to form under lean combustion (large excess air) at extremely high temperatures. AT-502 will measure and report the NO_x levels in the stack gas, but will not have any automatic control. There will be a high level alarm set for this data point corresponding to emissions limits, and the operator may correct for the high NO_x emissions by running the combustion richer (less air), which may be achieved by setting a lower setpoint on the air-fuel ratio controller FFC 501.

Although not explicitly stated here, there will be additional instrumentation throughout the cracker to further monitor its performance. There should be several thermocouples at strategic locations throughout the furnaces' fireboxes to ensure that the cracker is evenly and efficiently heating the hydrocarbon feed. There should also be flow meters on all streams so that leaks may be automatically detected. There should also be sufficient hydrocarbon and H₂S monitoring throughout the entire plant to ensure safety of the operators and of the community.

3.9 Plant Layout

The plant layout is one of the most important decisions of a process design team. The correct placement of equipment increases the inherent safety of the plant, decreases costs by minimizing pipe length and subsequently replacement and upkeep costs, and also is a great way to maximize heat integration by separating processes that operate at hot and cool temperatures to ensure efficiency. Our proposed plant layout is shown in Appendix P.

Safety was the foremost concern in the plant layout diagram and can be seen by the distance between equipment, the accessibility of each major process unit, and the separation of the impurity removal (Stage 1) from the rest of the plant. Stage 1 contains hazardous chemicals such as DGA and hydrogen sulfide. Stage 1 is separated from the rest of the plant to minimize the risk for operator exposure to these chemicals. Further, the control room is located centrally so that the operators will have fast access to all equipment; however, the loud compressors are kept as far away as reasonably possible.

To be safest, the equipment would be hundreds of yards of away from each other, but this is not economically feasible. Piping cost was minimized as much as safely possible by keeping major pieces of equipment about 50 feet apart, as was suggested by House [14]. Stages were arranged such that were almost always adjacent to any connected stages. For instance, Stages 2, 3, and 4 are located near each other, which helps to minimize the costs of the extensive heat integration that occurs between them. The hottest stage (Stage 5) is separated by a road from the coldest stages (Stages 3 and 4).

4 ECONOMIC ANALYSIS

The following sections describe the economic analysis that was performed for the ethylene from natural gas plant. The total capital investment (TCI) for this facility is \$443 MM. The annual sales are \$537.3 MM which exceeds the total production cost (TPC) of \$332.2 MM. Due to the sales being greater than the operating cost, the net present value (NPV) is a favorable \$87.9 MM and the project breaks even in 9 years. The analysis below describes the assumptions made for each cost associated with the project from initial design to after 10 years of operation.

4.1 Economic Analysis Overview

Of all of these values, only three are calculated directly: engineering costs, equipment costs, and piping costs. The calculations for these costs are shown in Appendix R.

4.2 Capital Costs

The Lindgren Group predicts a total capital investment (TCI) of \$443 MM. This number is derived from the fixed capital investment, working capital, and start-up costs. Overall, this is the cost incurred before the plant begins running.

4.2.1 Fixed Capital Investment

The fixed capital investment (FCI) for this project is \$340.8 MM and is comprised of the inside boundary limit (ISBL) and outside boundary limit (OSBL) costs. The ISBL cost is divided into

direct costs which account for \$69.4 MM and indirect costs that total \$165.6 MM and account for construction, taxes, and supervision support. Table 7 breaks these components into individual costs. The contingency cost, a subsection of the indirect cost, is money set aside for unforeseen difficulties such as construction setbacks.

Table 7: Breakdown of the fixed capital investment

Expense	Cost (k\$)
<i>Direct Cost</i>	69,385
Equipment	63,508
Piping	5,468
Engineering	408
<i>Indirect Cost</i>	165,658
Construction	113,270
Supervision	33,981
Taxes	4,530
Contingency (20% of direct cost)	13,877
<i>ISBL Cost (Direct + Indirect)</i>	235,043
<i>OSBL Cost (45% of ISBL)</i>	105,769
Fixed Capital Investment (ISBL + OSBL)	340,813

4.2.1.1 Inside Boundary Limits

The ISBL cost is estimated to be \$235 MM. It is the sum of the direct and indirect costs. Equipment and installation make up the direct costs while the indirect costs are for the needed support services such as construction, engineering, and supervision. Table 8 below summarizes the construction costs.

Table 8: Total construction costs. This total cost differs from the value given in Table 7 so that some calculations such as plant equipment and piping were not counted twice. More detail about the piping is given in Appendix K.

Component	% of Total Project	Cost (k\$)
<i>Civil & Structural</i>	13.3	34,610
<i>Insulation/Painting/Fire/HVAC</i>	3.6	9,408
<i>Plant Equipment</i>	24.3	63,508
Equipment	23.2	60,633
Installation	1.1	2,874
<i>Electrical</i>	6.7	17,510
Material	4.2	10,976
Installation	2.5	6,533
<i>Instrumentation</i>	13.5	35,282
Equipment	11.8	30,839
Installation	1.7	4,442
<i>Construction Management</i>	6.2	16,203
<i>Piping</i>	14.5	5,468
Material	7.2	2,715
Installation	7.3	2,752
<i>Engineering</i>	17.5	408
Process design	3.0	69
Civil/Mech/Inst Design	7.0	163
Piping Design	5.7	132
Other	1.8	41
<i>Miscellaneous</i>	0.4	253
Construction Total		182,655

4.2.1.2 Outside Boundary Limits

The OSBL cost is \$105.7 MM. As per MichiChem's budgeting protocol, the OSBL can range between 25% and 50% of the ISBL. This represents the costs of plant infrastructure such as roads, sewers, and additional low-cost equipment not anticipated during the design process. Because of the complexity of this facility, we estimate the OSBL to be 45% of the ISBL to account for additional difficulties encountered in the cryogenic processes.

4.2.2 Working Capital

We anticipate the need for \$68.1 MM in working capital. Although it is a large initial investment made at the beginning of year two, all of this money is recovered at the end of the plant life. MichiChem estimates the working capital to be 15-25% of the FCI as it accounts for raw material stock supply, product storage, accounts receivable, and other monthly operating expenses. The Lindgren Group estimates that the working capital for this project will be 20% of the FCI. While accounts receivable and accounts payable will be high, storage for raw materials

and finished products will be low. The majority of the raw materials and products are commodities and are transported via pipeline, so traditional road or railway shipping complications do not apply. More information about supply chain is given in Appendix Q.

4.2.3 *Startup Costs*

Startup costs for this facility are estimated to be \$34 MM which is 10% of the FCI. This cost covers the startup procedure which includes multiple steps. The system must be first be inerted, particularly the ethylene cracker, for safety reasons. Additional safety and operability checks must be done, and this expense covers piping and equipment that require tuning. Finally, the system is not ideal upon startup, and adjustments will likely be needed before the plant can run at full capacity and make the products to specification.

4.2.4 *Total Capital Investment*

The TCI is the total money spent before the process is fully operational. It is the sum of all capital investments including the fixed capital, working capital, and startup costs. Table 9 summarizes this information and shows a TCI of \$443 MM.

Table 9: Summary of total capital investment

Capital Investment	Cost (k\$)
<i>Fixed Capital</i>	340,813
<i>Working Capital</i>	68,162
<i>Startup Cost</i>	34,081
Total Capital Investment	443,057

4.3 Production Costs

The total production cost (TPC) for the proposed facility is \$332.2 MM. This is the summation of all costs incurred while the plant is operational. It includes not only raw materials and labor, but also plant overhead and general expenses. The following sections explain each component of this expense.

4.3.1 *Direct Production Cost*

The direct production cost totals \$260.8 MM. This is the cost associated with everything directly relating to the production of saleable materials. These costs are summarized in Table 10. Raw materials, utilities, waste, and labor are addressed below. Maintenance is assumed to be 10% of the FCI and supplies is assumed to be 15% of maintenance. These costs cover all personnel and materials needed to keep the plant fully operational.

Table 10: Summary of direct production costs

Component	Cost (k\$)
<i>Raw materials</i>	125,883
<i>Utilities</i>	93,712
<i>Waste</i>	55
<i>Labor</i>	2,042
Supervision (17.5% of labor)	357
Lab costs (15% of labor)	306
<i>Maintenance (10% of FCI)</i>	34,081
<i>Supplies (15% of Maintenance)</i>	5,112
Direct Production Total	260,887

4.3.1.1 Raw Materials

The raw materials cost accounts for the majority of the direct production costs, totalling \$125.9 MM annually. The sole raw material required for this process is the wellhead gas. According to the U.S. Energy Information Administration, the average cost of wellhead gas in 2012 was \$2.66/MCF [15]. We assume that since this is a commodity material, a contract will lock the price in for the lifetime of the plant.

4.3.1.2 Utilities

Utilities cost \$93.4 MM of the production costs of this process. Table 11 shows the sources of these costs. Details for each utility component are presented in Appendix L.

Table 11: Sources of utility costs

Utility	Consumption	Rate	Annual Cost (k\$)
<i>Process Water</i>	148,000	1000 kg	0.04 \$/1000 kg
<i>Cooling Water</i>	21,455,612	Kgal	0.43 \$/K gal
<i>Electricity</i>			0.057 \$/kWh
Compressors	1,362,491,406	kWh	77,662
Pumps	15,527,928	kWh	885
Fans/Blowers	82,515,678	kWh	4,703
<i>Refrigeration</i>	15667.2	GJ	901
Utility Total			93,383,976

4.3.1.3 Waste

Wastewater is the only waste produced in this process. This wastewater is produced in Stage 2 by the phase separators and dehydrators. At a disposal cost of \$1.43/Kgal, the annual production of 39,000 Kgal of wastewater costs \$55,770.

4.3.1.4 Labor

Labor is one of the three costs calculated directly for this analysis. This cost totals \$2 MM. The engineering labor is calculated directly at a cost of \$85.50/hr. The number of operators required per shift can be estimated. Table 12 represents an estimation of labor required for the types of equipment in our process. [16]

Table 12: Estimated labor required per piece of equipment, adapted from Table 6-13

Type of Equipment	Workers/unit/shift
Blowers/Compressors	0.1
Towers/Columns	0.2
Reactors	0.5
Heat Exchangers	0.1

The total estimate for the entire plant is nine operators per shift. It is mentioned that these estimates can shift down with new controls systems and automated equipment [16]. Equipment purchased for this process is the newest available, offering up-to-date systems that increase automation and decrease labor. With this assumption, this plant requires seven operators per shift at \$35.75 per hour for a total labor cost of \$2 MM per year.

4.3.2 General Expenses

At a cost of \$71.3 MM, general expenses cover a variety of items. For this analysis, plant overhead and property taxes and insurance qualify as general expenses. Other general expenses include plant administration, sales and marketing, and research and development. Table 13 shows these expenses. Administration is estimated to cost \$11.4 MM, 3% of the TPC. Sales/marketing and research/development costs are anticipated to be low – 2% and 5% respectively – for this project due to the commodious nature of the products.

Table 13: Summary of general expenses

Expense	Cost (k\$)
<i>Administrative</i>	11,400
<i>Sales/Marketing</i>	19,000
<i>Research/Development</i>	19,000
<i>Overhead</i>	21,888
<i>Property Taxes/Insurance</i>	13,632
General Expenses Total	71,288

Taxes and insurance cost \$13.6 MM and account for 4% of the FCI. These charges are constant and are independent of production. Plant overhead costs \$21.9 MM annually and is assumed to cost 60% of the total cost of operating labor, supervision, and maintenance. This too is present regardless of production and accounts for everyday building expenses such as building electricity and janitorial services.

4.3.3 Total Production Cost

The TPC for this project is \$332.2 MM. This is the sum of the costs of the raw materials, utilities, labor, taxes, and general expenses. The breakdown of these costs is shown in Table 14 below. Although the costs for this facility are great, the sales revenue described in the following section offsets these costs for a positive NPV.

Table 14: Summary of total production costs

Cost	(k\$)
<i>Direct Cost</i>	260,887
<i>General Expenses</i>	71,288
TPC Total	332,175

4.4 Sales Revenue

Annual sales for this facility are estimated to be \$537.3 MM each year. Of the saleable products made by this plant, ethylene yields the most profit at \$290 MM and IPQ natural gas is the second highest seller at \$110.8 MM annually. The side products, refinery-grade (R-grade) propylene, hydrogen, naphtha, hydrogen sulfide, and low pressure steam, account for the remaining \$136.5 MM. MichiChem requires that 500 MM pounds of ethylene are made each year. The IPQ natural gas consists mainly of methane because this method reduced the need for extraneous cryogenic separation processes. Refinery-grade (R-grade) propylene must be 50% propylene. Our product is 77.9 wt% pure in propane. As described before, the hydrogen sulfide is sold to a sulfur processing plant. The sale price is based solely on the hydrogen sulfide content of the product, although this process purifies it to 80 wt% hydrogen sulfide. Naphtha is easily separated from the feed, making it a low-maintenance product. Table 15 shows this information.

Table 15: Summary of saleable products

Component	Price	Annual Production	Annual Sales (k\$)
Ethylene	0.58 \$/lb	500.0 MM lb	290,00
IPQ Natural Gas	3.90 \$/MMBTU	2.84×10^7 MMBTU	110,760
Propylene (R-grade)	0.65 \$/lb	85.7 MM lb	55,705
Hydrogen	1 \$/lb	36.0 MM lb	36,000
Naphtha	1 \$/gal	42.5 MM gal	42,500
Hydrogen Sulfide	0.14 \$/ton	13,500 ton	2
Steam (low pressure)	6.62 \$/tonne	356,535 tonne	2,360
PRODUCTS TOTAL			537,327

4.5 Economic Projection

The anticipated NPV for this project is \$87.9 MM. The discounted cash flow rate of return (DCFRoR) is 14.6% which is above MichiChem's minimum acceptable rate of return (MARR) of 11%. The discounted payback period is 9 years. Although the NPV is positive, the long discounted payback period and relatively low DFCROR cause us to challenge the real economic

feasibility of this project. For this reason, we recommend that MichiChem waits two years to evaluate any market change and then re-evaluates the project.

4.5.1 Net Present Value

The NPV for this project is expected to be \$87.9 MM. This accounts for many factors including state and federal taxes (4% and 48% of the revenue respectively), depreciation, and the 11% MARR. The calculations involving depreciation use the 7-year MACRS schedule. Full calculations for this number are provided in Appendix R.

Figure 16 shows a discounted cumulative cash flow diagram. The drops before year zero show the construction costs. The drop in year 0 shows the working capital and startup costs. The project begins at year 0 but does not make a profit in its first year. Over the first year, the plant only produces half of its total capacity but incurs all production costs, resulting in monetary losses. However, after the first year of production, the plant runs at full capacity. After seven years, the depreciation allowance runs out, resulting in higher taxes and a reduced cash flow. The project breaks even in eight years. At the end of the project lifetime, the working capital is returned, resulting in a net present value of \$87.7 MM.

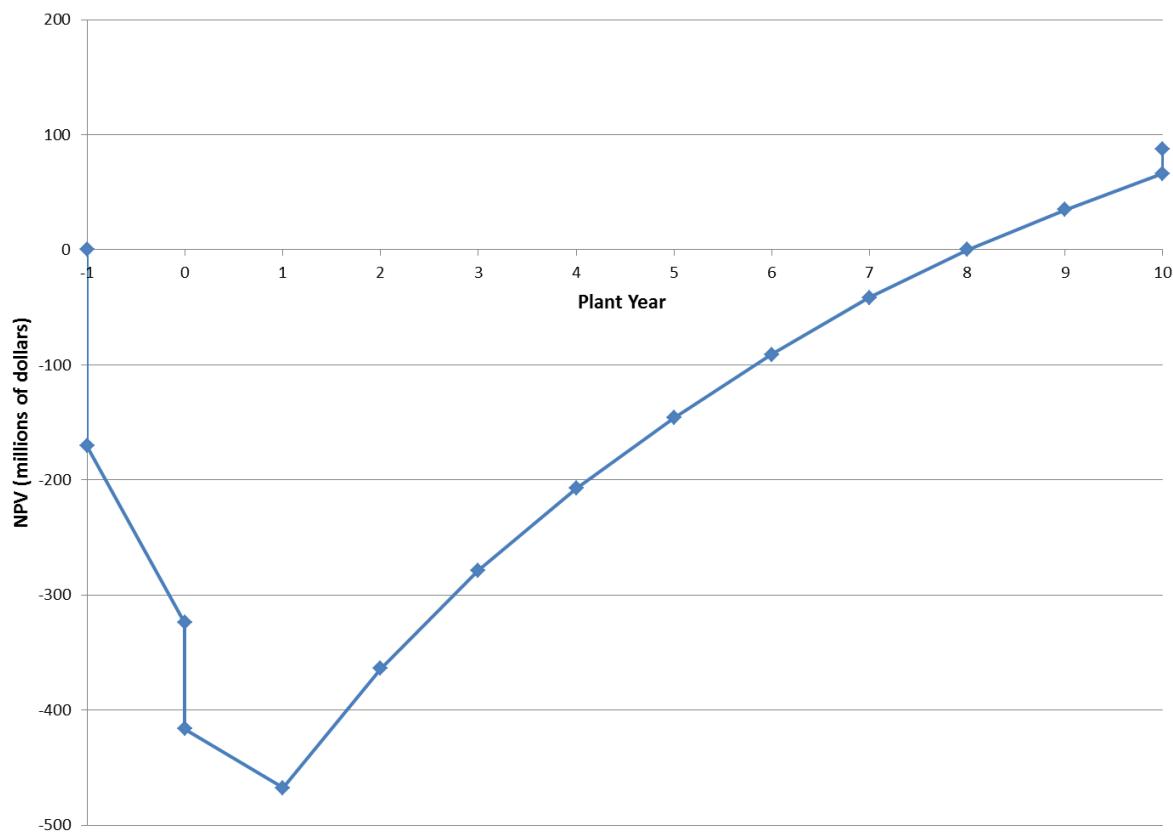


Figure 16: Cumulative cash flow diagram for the ethylene production process

4.5.2 Discounted Cash Flow Rate of Return

The discounted cash flow rate of return (DFCRoR) is 14.6%. This is the interest rate which causes the project to achieve an NPV of \$0 at the end of the plant lifetime. This makes it the highest interest rate that will allow the project to break even. Since this number is greater than the MARR, the project is profitable.

4.5.3 Discounted Payback Period

The discounted payback period is eight years of operation. This means that the project recovers all capital and operating costs and begins making money after eight years. This is two year before the end of the project lifetime, so the process makes money for two years.

4.6 Sensitivity Analysis

As this project has an NPV of only \$87.9 MM, a variety of factors could dramatically impact the economic outcome. Figure 17 is a Pareto chart showing the direct production costs. Together, raw materials and utilities account for 84% of the production costs, so effects on both of these costs will be evaluated. Main revenue drivers will be evaluated as well.

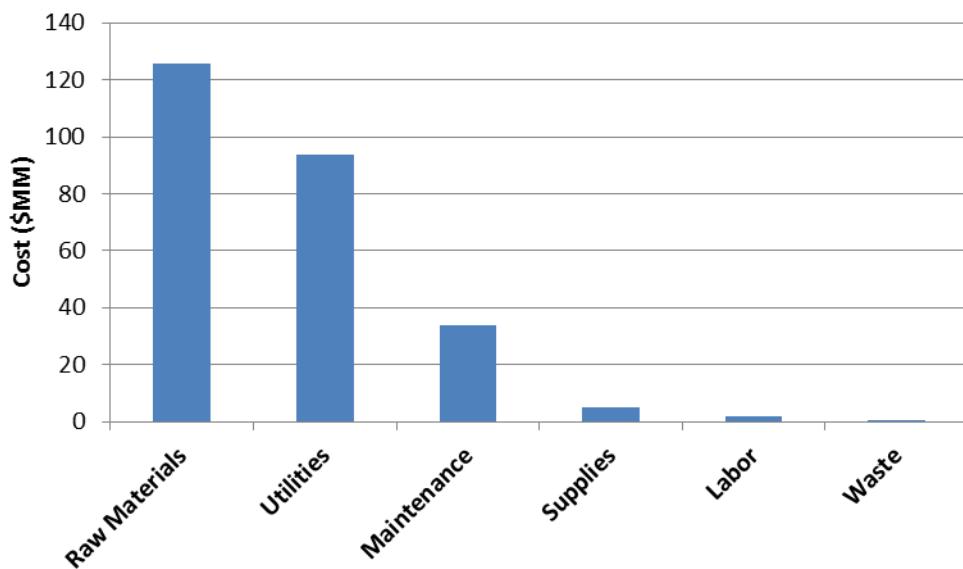


Figure 17: Pareto chart showing components of the direct production cost

4.6.1 Raw Materials

The cost of raw materials accounts for 48% of the direct production cost. As wellhead gas is the only raw material for this process, the total cost is entirely dependent on the cost of the wellhead gas. According to the EIA, wellhead gas is at its lowest price since 1999 [15]. For a more accurate prediction of future wellhead gas prices, the cost of gas over the past 10 years (2003-2012) is averaged. This results in a cost of \$5.30/mcf. If this were the price at which MichiChem purchased its natural gas, the raw material cost would increase from \$125.9 MM to \$250.8 MM, resulting in an NPV of -\$282.0 MM.

4.6.2 Utilities

Utilities are the source of 35.8% of the direct production cost, costing \$93.7 MM annually. When broken into individual components as shown in Figure 18, it is obvious that electricity accounts for the vast majority of the utility cost.

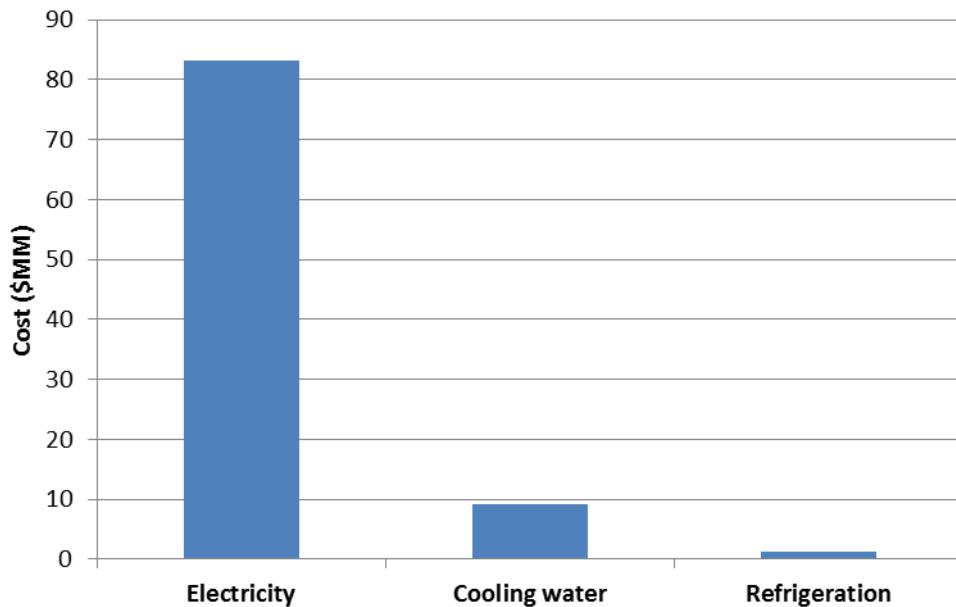


Figure 18: Pareto chart showing the breakdown of utility costs

4.6.2.1 Cost of Electricity

As electricity is responsible for the bulk of the utility costs, the cost of electricity has a strong effect on the NPV. For example, if the cost of electricity were reduced by 30% to \$0.04/kWh, the NPV would almost double, reaching \$161.6 MM. Conversely, if the price of electricity increases by \$0.02/kWh, the project breaks even after 10 years. As it is unlikely that the cost of electricity will change noticeably during the project lifetime, other key cost and revenue drivers are evaluated.

4.6.2.2 Compressor 201

When further inspecting the electricity costs, it is apparent that C-201 is the most expensive piece of equipment to operate, costing \$70.8 MM annually. Minimizing the operating cost of this compressor would strongly affect the NPV. If the cost of the compressor were halved, the NPV would increase to \$192.9 MM. Reducing this cost would be best achieved by investigating other methods to operate the compressor.

4.6.3 Revenue Drivers

Ethylene and IPQ natural gas together comprise almost 75% of the sales from this process. The effects of price changes to these products will be evaluated.

4.6.3.1 Ethylene

Ethylene is the product responsible for the highest percentage of the revenue stream. At a cost of \$0.58/lb, the annual production of 500 million pounds yields \$290 MM in sales. If the price of ethylene were to rise to \$0.60/lb, the revenue from ethylene would increase to \$300 MM. As a result, the NPV would become \$113.5. Conversely, if the price of ethylene were to drop to \$0.51/lb, the project would break even at the end of the plant lifetime.

4.6.3.2 IPQ Natural Gas

The profitability of the process is overall most dependent on natural gas; however, changes in the price of IPQ natural gas alone do not strongly affect the NPV. Even an increase from \$3.90/MMBTU to \$4.00/MMBTU only increases the NPV to \$95.2 MM.

Since the prices of wellhead gas and IPQ natural gas are naturally linked, it is most beneficial to examine their effects together. If the prices increase proportionally (that is, if the wellhead price doubles, then the IPQ natural gas price also doubles), the NPV is adversely affected. If they decrease proportionally, the NPV increases. This makes sense since the wellhead gas is the source of more products than just the IPQ natural gas.

5 ENVIRONMENT, HEALTH, AND SAFETY

Several hazards to the environment and to plant workers exist in our process. Measures to mitigate these hazards are summarized here.

5.1 Environment and Health

Our main concerns for the environment exist in the streams that we release into the air. The gas sweetening process removes carbon dioxide and hydrogen sulfide from the inlet gas. After removal, these compounds are separated. The carbon dioxide is released into the atmosphere with only trace amounts of hydrogen sulfide. While carbon dioxide is a greenhouse gas, current permitting allows us to release it, and the trace amount of hydrogen sulfide falls within the legal limit.

Rather than having the hydrogen sulfide sent off as waste, we can sell it at 30% of the market value of sulfur. This stream is 80% pure (weight basis), making it an attractive option to companies that processes this gas into elemental sulfur or sulfuric acid.

The final set of air emissions from our process—the stack gases from combustion in the fireboxes—is not toxic but does involve some environmental considerations. The extremely high combustion temperatures in the fireboxes can cause the formation of NO_x gases [17] which contribute to acid rain and tropospheric ozone. NO_x levels should be monitored, and if they exceed emission limits, emissions must be mitigated using such measures as selective catalytic reduction (SCR). The combustion gases will be discharged up the stack at 150°C, which will give the stack gas enough buoyancy to carry away from the plant and should sufficiently superheat the water so that it does not condense at low elevations. [18]

5.2 Worker Safety

The main concern for worker safety comes from the extreme temperatures and high pressures that the process demands. In the cryogenic distillation section, the process reaches temperatures as low as -243°C. Equally as dangerous, the cracker firebox reaches up to 1000°C. If the process equipment and piping is sufficiently insulated so as to isolate operators from the extreme temperatures, accidental contact with dangerous temperatures can be avoided, and the process is made more energy-efficient at the same time. Most of the process runs at low to moderate pressure, but the hydrogenator and absorber run at 25 atm and 37 atm, respectively. By following specific design parameters for pressure vessels and installing relief valves, we can ensure that the equipment remains safe.

Another concern in our process is the ubiquity of highly flammable hydrocarbons. Monitors should be in place throughout the plant to determine if and where leaks occur so that the gas can be contained and the leak can be fixed. Additionally, the system should be inerted prior to startup and during the shutdown process. Further, workers should be cautious of creating any inadvertent ignition source that could set off an explosion in a potential gas-leak environment; operators should use specially rated spark-resistant phones and radios and should use extreme caution when welding. An advisable extra precaution for our hydrocarbon-based plant would be to include flame-retardant clothing (FRC) in the personal protective equipment (PPE) requirement.

While all plant emissions are within legal limits, certain measures still need to be taken to ensure that nitrogen and hydrogen sulfide do not harm the plant workers. Our process emits high-purity nitrogen gas to the atmosphere, and nitrogen (or another inert) will be used to inert vessels and pipelines during shutdown and startup. These concentrated areas of nitrogen represent a possible hazard to workers. Nitrogen gas is not toxic in and of itself; however, when pure nitrogen is released locally (either at the nitrogen stack or in an inerted vessel), it displaces the oxygen in the air, leading to asphyxiation after just a few breaths. Any worker working near the nitrogen stack tip or in an inerted vessel should use a self-contained breathing apparatus (SCBA). [19] Hydrogen sulfide, on the other hand, is extremely toxic. Although H₂S will only be emitted in low concentrations, it is being processed in high concentrations, and precautions need to be taken in case of a leak. The plant should be equipped with H₂S detection, and all workers should wear personal H₂S meters at chest level.

This discussion has so far addressed the safety hazards specific to our process; however, there are numerous safety considerations common to all chemical and petrochemical plants. The design of the process and equipment, even if it follows codes and guidelines, can only ensure a certain degree of plant safety. Properly-designed control systems can provide an additional level of protection; however, it is ultimately up to the plant workers themselves to behave safely. The only way to ensure a safe workplace is to have all employees and management buy into a “safety culture” wherein safety is truly the top priority. All plant employees should hold each other accountable for abiding by safety rules, and everybody should strive for a continual improvement of the safety record. Further, safety is neither passive nor static—plant workers must actively think about safety as they operate the plant and should always be looking for new ways to make the plant a safer place.

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7 LIST OF APPENDICES

Appendix A: Absorber/Stripper

Appendix B: Phase Separator

Appendix C: Dehydrator

Appendix D: Refrigeration

Appendix E: Distillation

Appendix F: Membrane Separator

Appendix G: Hydrogenator

Appendix H: Steam Cracker and Firebox

Appendix I: Heat Exchangers

Appendix J: Compressors, Fans, Blowers, and Pumps

Appendix K: Piping Information

Appendix L: Utility

Appendix M: Heat Integration

Appendix N: Process Flow Diagrams

Appendix O: Piping and Instrumentation Diagram

Appendix P: Plant Layout

Appendix Q: Supply Chain

Appendix R: Economics

Appendix A: Absorber Stripper

A.1 Absorption Tower

A.2 Stripper

A.1 Absorption Tower

The amine absorption tower is one of the most widely used processes to remove H₂S and CO₂ from the gas stream. The column has been sized to match the specifications given for plant B, shown below, for temperature, lean and rich solution loading, pressure, all specified temperatures, and tray size [8].

Plant	A	B-1	B-2
Gas Feed Rate, MMscfd	6	121	83
Solution Flow rate, gpm	172	556	426
Solution Concentration, wt% DGA	50	60	56.5
Feed Gas Analysis			
H ₂ S vol%	5.48	0.5–1.25	0.74
CO ₂ vol%	6.52	1.5–3.75	3.46
Outlet Gas Analysis			
H ₂ S gr/100 scf	0.205	<0.25	0.01–0.05
CO ₂ vol%	—	<0.01	0.0093
Lean Solution Loading			
H ₂ S, gr/gallon	2		~21
CO ₂ mole/mole amine	0.04		0.09
Rich Solution Loading			
H ₂ S mole/mole amine	0.09		0.06
CO ₂ mole/mole amine	0.18		0.33
Absorber			
No. of trays	25		20
Pressure, psig	140		550
Lean Solution Temp., °F	120		88
Rich Solution Temp., °F	156		171
Stripper			
No. of trays, stripping	21		16
No. of rays, reflux	4		4
Pressure, psig	13		7.25
Reboiler temperature, °F	255		250

Sources: Plant A data from Harbison and Dingman (1972), Plant B-1 data from Holder (1966),
Plant B-2 data courtesy Fluor Daniel (1995)

Figure A-1: Operating Data for aqueous DGA plants treating natural gas [8].

Trayed vs. Packed column

Both tray and packed columns can be used for amine sweetening absorption towers [3]. Oftentimes, the deciding factor between a tray and packed column for amine absorption systems is individual needs, as both offer benefits for different systems. Figure A-1 shows a general overview for choosing between the two contactor designs [8]. From this guide, as well as plant data obtained from Kohl's *Gas Purification*, tray columns have been found to be better for our absorption tower for the following reasons. Tray columns can perform better than packed columns when the following conditions are met:

- Moderate to high pressures

- Column diameters from 3 to 10 feet
- Internal tower cooling

Our process will be at moderate pressure and models plant B from Kohl's Gas Purification so tray columns will be used for the absorption tower.

Conditions of Application	Staged Columns		Rating of Column Internals			
	Perforated, or Valve Trays	Bubble Cap or Tunnel Trays	Differential Columns Randomly Packed	Systematically Packed	Downcomer-less	Pseudo-Equilibrium Disc and Donut
Low pressure (<100 mm Hg)	2	1	2	3	0	1
Moderate pressure	3	2	2	1	1	1
High pressure (>50% of critical)	3	2	2	0	2	0
High turndown ratio	2	3	1	2	0	1
Low liquid rates	1	3	1	2	0	0
Foaming systems	2	1	3	0	2	1
Internal tower cooling	2	3	1	0	1	0
Solids present	2	1	1	0	3	1
Dirty or polymerized solution	2	1	1	0	3	2
Multiple feeds and sidestreams	3	3	1	0	2	1
High liquid rates (scrubbing)	2	1	3	0	3	2
Small diameter columns	1	1	3	2	1	1
Columns with diameter 3–10 ft	3	2	2	2	2	1
Large diameter columns	3	1	2	1	2	1
Corrosive fluids	2	1	3	1	2	2
Viscous fluids	2	1	3	0	1	0
Low ΔP (efficiency no concern)	1	0	2	2	0	3
Expanded column capacity	2	0	2	3	2	0
Low cost (performance no concern)	2	1	2	1	3	3
Available design procedures	3	2	2	1	1	1

Notes:

Rating key: 0 - Do not use
 1 - Evaluate carefully
 2 - Usually applicable
 3 - Best selection

Staged columns: Tray columns with separate liquid and vapor flow paths.
Common types: Bubble cap, sieve, valve.
Proprietary types: Angle, Uniflux, Montz, Linde, Thorman, Jet.
Differential columns: True countercurrent flow of gas and liquid.
Randomly packed: Raschig rings, saddles, slotted rings, Tellereites, Maspac.
Systematically packed: Flexipac, Goodloe, Hyperfil, Sulzer, Glitch Grid.
Pseudo-equilibrium stages: Countercurrent flow of gas and liquid with discrete trays.
Downcomerless trays: Perforated, Turbogrid, Ripple.
Low pressure drop trays: Disc and donut, shower deck.
Special devices (not rated in table):
 Venturi scrubber, turbulent contact absorber, marble bed absorber, horizontal spray chamber, cocurrent rotator.
Based on data of Frank, 1977

Figure A-2: A guide to choosing column internals in a gas-liquid contactor. [8]

Prevention of Foaming in the Absorption Tower

When an absorption tower is improperly designed for this type of process, foaming can result. Foaming results in a reduction in impurity removal, high pressure drops, and higher amine losses

by increasing the formation of unwanted salts [8]. The prevention of foaming can be done several ways [8]:

- The temperature difference of the lean solution and feed should be greater than 10° F
- The minimum contact temperature should be greater than 50 to 60 °F to ensure the higher amine viscosity will not initiate foaming

Our temperature difference is slightly below 10° F but the minimum contact temperature is well above the minimum (50 °F) entering at 80°C which allows the assumption that minimal foaming will occur and not be detrimental to the performance of the absorption tower.

Sizing of the Absorption tower

Absorption towers are approximately 20 trays is specified [8]. Figure A-1 shows the general standard for spacing between trays for an amine absorption tower is eighteen inches with an addition four feet for the bottom and top [13]. This gives the total height of the absorption tower at 34 feet.

The diameter of the absorption tower can be sized two different ways. The first is to approximate the diameter using Figure A-2 to estimate the required diameter at 550 psi and 112.77 MMSCFD. Using this graph, the diameter should be about 105" [13]. However, this figure is a very general diagram to approximate what the inner diameter should be, and more rigorous calculations were performed below to find the diameter of the column.

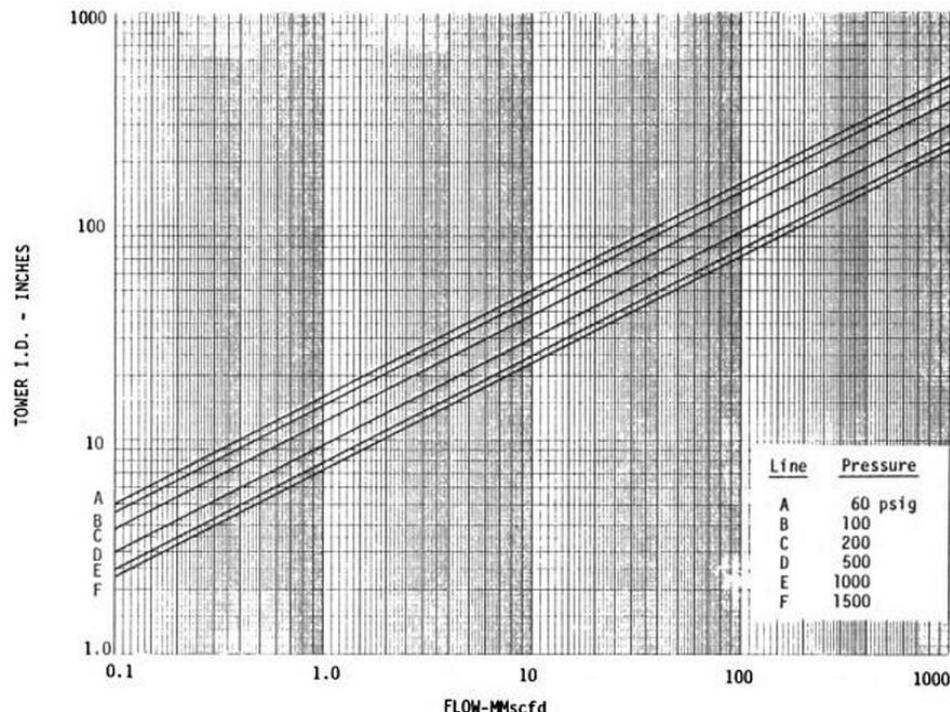


Figure A-3: Approximate Diameter required for amine tray-type absorbers [13].

One of the most important features of any absorption tower is the velocity of the gas. The gas velocity should be as close to flooding as possible to maximize throughput while maintaining a steady state absorption tower. The Souders-Brown equation below approximates the gas velocity.

$$v_g = K * \left[\frac{\rho_{amine} - \rho_{gas}}{\rho_{gas}} \right]^{.5}$$

K is a constant that changes for different liquids and gases. For amine absorption towers, K is set equal to 0.25 [8]. By reducing this velocity by an additional 50%, the column avoids foaming and flooding [8]. For our process, the velocity of gas through the column is 35 feet per minute. The amount of raw gas needed for the process is known, and thus the volumetric flow rate can be easily calculated. The diameter of the column can then be calculated by the well-known equation below where Q is the volumetric flowrate, A is the area, and V is the velocity.

$$Q = A * V$$

The diameter is calculated at 97" which is close to the general approximation of 105" from Figure A-2.

Energy requirements

The binding of H₂S (675 btu/lb) and CO₂ (850 btu/lb) to the DGA is a highly exothermic reaction. This reaction in the absorber produces 73650 btu/min. This heat causes a temperature profile in the absorption column similar to that shown in Figure 9. The temperature of the lean amine and rich amine was specified by the plant data the process is modeled from, while the exit vapor stream is estimated from the Souders-Brown equation. The balance on the energy entering and exiting the absorber system is shown in Table A-1.

Absorber	
Lean amine Temp (F)	88
Bottoms Temp (F)	156.5
Enter Gas Temp (F)	82
Exit Gas Temp (F)	88
Heat from reaction (btu/min)	73647.11
Heat for entering gas (btu/min)	-13413.41
Lean amine (btu/min)	-60242.75
% Error	0.012

Table A-1: Energy balance around the absorber

Materials Selection

Oilfield Processing by Manning discusses materials of choice for absorption towers in amine processes. The external shell is suggested to be carbon steel as well as lugs or clips that connect the exterior to the interior. Internals subject to high velocities or in active areas such as demisters, trays, and bolts should be constructed with stainless steel [13]. The materials selection was accounted for in the costing of the equipment.

A.2 Stripping Tower

The regenerator is run at low pressure and high temperature to reverse the reaction between the acid gas and the amine solution. The stripping tower has been designed to emulate the regenerator from plant B in figure 1, with 0.5 atm pressure, and a reboiler temperature of 250° F.

Sizing of the Stripping Tower

The tower has been sized to 20 total trays with spacing between the trays set at 24" based on the industrial average [13]. The total height of the regenerator is 46 feet, leaving 3 feet for the top and bottom of the tray tower.

The diameter has been sized using the Souder-Brown equation like the absorber, resulting in a vapor velocity of 8.25 feet per second. The diameter can be calculated from the vapor velocity and a volumetric flow rate of 6480 ft^3/min from the same equation as used for the absorption tower. Therefore, the minimum diameter is 49 inches.

$$Q = A * V$$

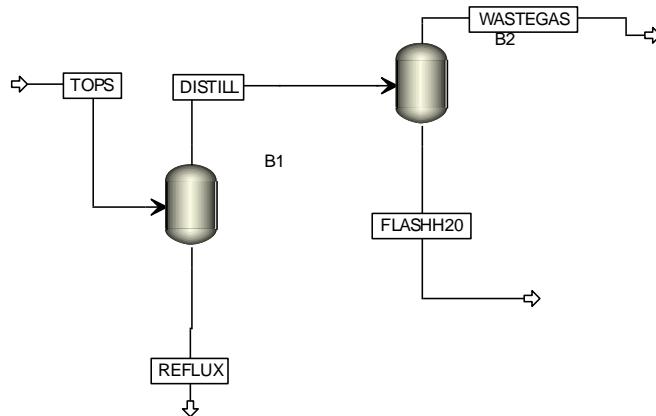
Energy Balance

The energy balance on the stripping tower requires finding the necessary reboiler duty and condenser duty, as well as the heat required by the reverse DGA reaction. The total amount of acid gas to be removed is assumed at steady state to be equal to the amount that reacted in the absorption tower. Thus, the heat of reaction 73650 btu/min and will require the same amount to force the reaction backward. Manning's quick approximations measure the duty at 640,000 btu/min as seen by the calculation below [13]:

$$Q \left(\frac{btu}{min} \right) = 638250 = 30000 * \frac{gpm}{60}$$

The more rigorous calculation by Aspen (below) shows total enthalpy requiring 571150 btu/min to remain at steady state. The relative closeness is a good check on whether the condenser pressures are correct or not. The condenser can therefore be sized at 770 ft² from the approximation below [13].

$$5.2 * gpm = ft^2 \text{ for reflux condenser} = 770$$



regenerator condenser					
Stream ID	DISTILL	FLASHH2O	REFLUX	TOPS	WASTEGAS
Temperature	F	100.0	35.0	100.0	220.0
Pressure	psia	14.70	146.96	14.70	7.35
Vapor Frac		1.000	0.000	0.000	1.000
Mole Flow	lbmol/hr	159.531	8.817	1676.690	1836.221
Mass Flow	lb/hr	5833.618	170.413	31198.382	37032.000
Volume Flow	cuft/hr	64786.475	2.648	505.734	1.81538E+6
Enthalpy	MMBu/hr	-10.760	-1.100	-207.122	-183.491
Mole Flow	lbmol/hr				
WATER		8.747	8.654	1664.832	1673.579
CO2		53.159	< 0.001	0.011	53.170
DGA		0.131	0.126	11.283	11.414
H2S		97.495	0.036	0.563	98.058

Figure A-5: Aspen data for the energy balance around the stripping tower

The reboiler duty can be readily done by hand. Manning's shortcut approximation for reboiler duty is:

$$Q \left(\frac{btu}{min} \right) = \frac{72000}{60} * 135 = 162000$$

The actual amount when factoring in heating for makeup water, distillate return, the feed flow rate, and the heat for reaction is shown in the table below. Each of these is calculated to reach 250 °C (reboiler temperature) and their overall heat duty is 203918 btu/min. The square feet required for a kettle reboiler is approximated at 11.3 gpm = 240 ft² from Manning's correlations. [13]

Table A-2: Energy balance around stripping tower accounting for makeup water heating

Manning estimate	btu/min	162034.9
Heat needed for reaction	btu/min	73647.1
Low pressure steam	btu/min	1211
Distillate return	btu/min	77995.95
Feed	btu/min	51064
Regenerator heat requirement	btu/min	203918.
Error from Manning estimation to calculated heat	% error	20.5

Materials Selection

The selection of materials for the stripping tower is the same as the absorption tower.

Oilfield Processing by Manning discusses materials of choice for absorption towers in amine processes. The external shell is suggested to be carbon steel as well as lugs or clips that connect the exterior to the interior. Internals subject to high velocities or in active areas such as demisters, trays, and bolts be stainless steel within the absorption and stripping towers [13]. As is the case with the absorption tower, the stripping tower material selection was accounted for in the costing of the tower.

Absorption and Stripping Tower specifications

Equipment #	Equipment	Specifications
T-100	Tower	Diameter
		97 Inches
		Number of Trays
		20 Trays
		Tray Spacing
		1.5 Feet
		Pressure
		37 atm
		Height
		34 Feet
		Material
		CS/SS
T-101	Tower	Diameter
		49 Inches
		Number of Trays
		20 Trays
		Tray Spacing
		1.5 Feet
		Pressure
		0.5 Atm
		Height
		34 Feet
		Material
		CS/SS

Appendix B: Phase Separation Design

- B.1 Objective and Operation Selection
- B.2 Aspen Thermodynamics Model
- B.3 Phase Separator Design Criteria
- B.4 Sizing a Three-Phase Separator
- B.5 Sizing a Horizontal Two-Phase Separator
- B.6 Sample Calculations for Sizing PS-200
- B.7 Sample Calculations for Sizing PS-201
- B.8 Master List of Phase Separators

B.1 Objective and Operation Selection

Phase separation occurs in both Stage 1 and Stage 2 of our process. In the impurity removal stage (Stage 1), phase separators separate liquid and gas from partially condensed streams. In the liquid removal stage (Stage 2) the phase separator is used to separate out all the water and naphtha in the hydrocarbon stream before Stage 3 since water can freeze and clog up our distillation columns. In addition, phase separators are used in the refrigeration stage to separate partially condensed refrigerant.

Use of a separator vessel will be used because it is most commonly used in natural gas refineries and is more economical than alternative methods of separation such as adsorption, absorption and membrane to separate out water and naphtha.

B.2 Aspen Thermodynamics Model

An Aspen simulation was conducted to understand expected flow rates and temperatures of our desired separation. The thermodynamics of the phase separation were modeled in Aspen using the Peng-Robinson equation of state. The Aspen model for Stage 2a's water and naphtha removal was drawn as shown in Figure B-1, below.

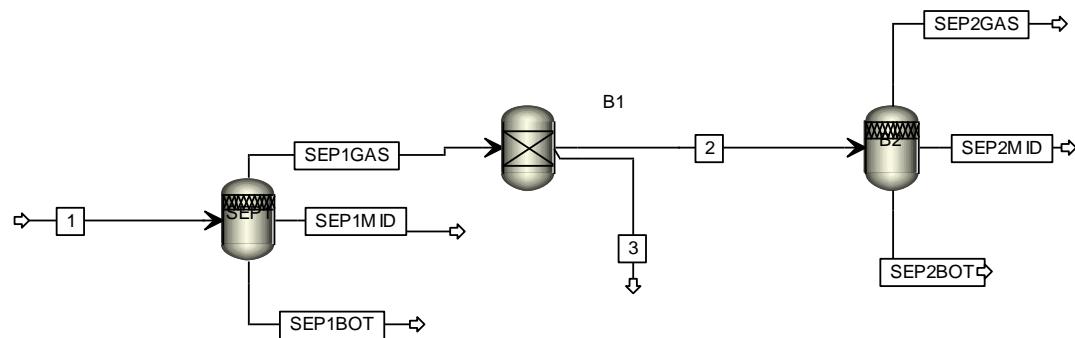


Figure B-1: Aspen model used to determine behavior of water and naphtha removal system at varying temperatures and pressures. A splitter with 100% water split (B1) models the absorbent while three-phase separators model the phase separation drums.

As was discussed in the report, the temperatures and pressures and temperatures were varied until an appropriate balance was struck between how much naphtha was being recovered, how much water was knocked out in the first tank, and how much ethylene and propylene product was condensed into the naphtha.

The results from Aspen for the selected conditions are shown in Table B-1. Mass fractions could be calculated from this information, which is later used in scale-up.

Table B-1: Aspen results for selected conditions in water removal stage

	1	2	3	SEP1BOT	SEP1GAS	SEP1MID	SEP2BOT	SEP2GAS	SEP2MID
Temperature C	10.00	1.00	1.00	1.00	1.00	1.00		-20.00	-20.00
Pressure bar	25.00	12.16	12.16	12.16	12.16	12.16	8.11	8.11	8.11
Vapor Frac	1.00	1.00	0.00	0.00	1.00	0.00		1.00	0.00
Mole Flow kmol/hr	117.80	111.03	0.06	3.92	111.09	2.79	0.00	109.10	1.93
Mass Flow kg/hr	2897.08	2660.41	1.06	70.63	2661.47	164.98	0.00	2557.82	102.58
Volume Flow cum/hr	88.19	192.97	0.00	0.08	193.05	0.26	0.00	266.62	0.16
Enthalpy Gcal/hr	-2.07	-1.71	0.00	-0.27	-1.71	-0.09		-1.68	-0.06
Mole Flow kmol/hr									
N2	3.70	3.70	0.00	0.00	3.70	0.00	0.00	3.70	0.00
H2	1.50	1.50	0.00	0.00	1.50	0.00	0.00	1.50	0.00
HEPTANE	0.30	0.03	0.00	0.00	0.03	0.27	0.00	0.00	0.03
HEXANE	0.40	0.10	0.00	0.00	0.10	0.30	0.00	0.02	0.08
N-PENTAN	0.80	0.47	0.00	0.00	0.47	0.34	0.00	0.24	0.23
ISOPENT	0.50	0.32	0.00	0.00	0.32	0.18	0.00	0.18	0.14
N-BUTANE	2.90	2.40	0.00	0.00	2.40	0.50	0.00	1.94	0.46
ISOBUTAN	0.50	0.43	0.00	0.00	0.43	0.07	0.00	0.37	0.06
PROPANE	8.70	8.27	0.00	0.00	8.27	0.43	0.00	7.88	0.39
ETHANE	14.00	13.81	0.00	0.00	13.81	0.19	0.00	13.66	0.15
METHANE	66.50	66.37	0.00	0.00	66.37	0.13	0.00	66.30	0.08
ETHYLENE	7.00	6.94	0.00	0.00	6.94	0.06	0.00	6.90	0.04
PROPYLEN	7.00	6.69	0.00	0.00	6.69	0.31	0.00	6.42	0.27
WATER	4.00	0.00	0.06	3.92	0.06	0.02	0.00	0.00	0.00

B.3 Phase Separator Design Criteria

The first phase separator will separate out 3-phases: hydrocarbon vapor, water, and naphtha. The second phase separator will separate out 2-phases: naphtha and hydrocarbon vapor. Thus, we will be designing both a two-phase separator and a three-phase separator for our ethylene plant.

Criteria for our phase separators taken are to:

- Provide sufficient time to allow the immiscible vapor, naphtha, and water phases to separate by gravity.
- Provide sufficient time to allow for the coalescence and breaking of emulsion droplets at the oil-water interface.

Vessel Orientation Selection

In industry, there are two major setups for phase separation: horizontal and vertical, as shown in Figure B-2. Additionally, a spherical separator is a third setup used occasionally for phase separations that involve high pressures.

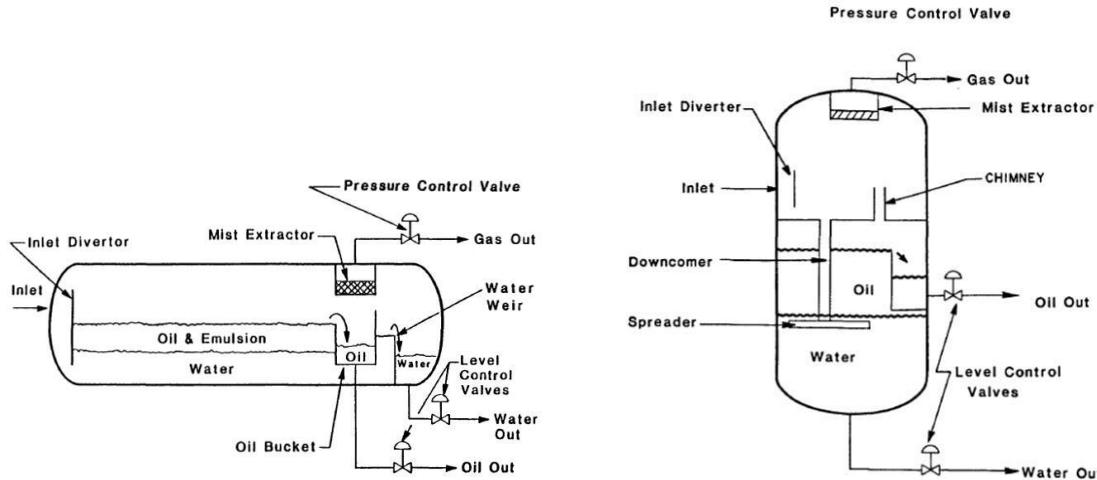


Figure B-2: Schematics for a bucket and weir three-phase separator design (left) versus a vertical three-phase separator. [20]

Vertical separators occupy less floor space, and are ideal if space is an issue. Vertical separators are also better suited for wellstreams with low to intermediate gas-to-oil ratios. On the other hand, horizontal separators are better suited and less expensive when separating wellstreams with high gas-to-oil ratios. A more complete table of advantages and disadvantages is shown in Table B-2.

Table B-2: Comparison of the advantages, disadvantages, and ideal use of vertical, horizontal, and spherical phase separators. [21] [22]

Type	Advantages	Disadvantages	Ideal use
Vertical	<ul style="list-style-type: none"> • Easier to clean • Saves space • Provides better surge control • Liquid level control is not critical • Lower tendency for re-evaporation of liquid into gas phase 	<ul style="list-style-type: none"> • Takes a longer diameter separator for a given gas capacity compared to a horizontal separator • More expensive to fabricate • Difficult and more expensive to ship 	Low to intermediate gas-to-oil ratio where a relatively large liquid flowrate is expected.

Horizontal	<ul style="list-style-type: none"> Handles high gas-to-oil ratios since design permits higher gas velocities. Costs less than the vertical separator Easier and cheaper to assemble and ship. Requires less piping for field connections Reduces turbulence and foaming Several separators can be stacked, minimizing space requirements 	<ul style="list-style-type: none"> Generally larger space requirements Liquid level control more critical Much harder to clean 	High gas-to-oil ratio and for liquid separations. Good for a diverse range of situations
Spherical	<ul style="list-style-type: none"> Very inexpensive Good for low to intermediate gas-to-oil ratios. Very compact and easy to ship and install Better clean-out 	<ul style="list-style-type: none"> Limited liquid settling section and difficult to use for three-phase separation Liquid level control is very critical 	Intermediate or low gas-to-oil ratios, preferably two-phase separations under high pressure.

Horizontal separators are ideal for PS-200, and PS-201 because the mass flow rate of liquid is significantly lower than the mass flow rate of the vapors being separated. For instance, in stage 2a, we only aim to separate out water and naphtha, which consist of approximately 12% of our input vapor feed. A horizontal separator is the best choice for both our three-phase separator and two-phase separator, visually represented in Figure B-3.

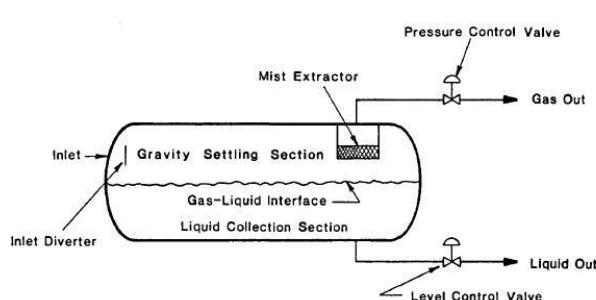


Figure 4-1. Horizontal separator schematic.

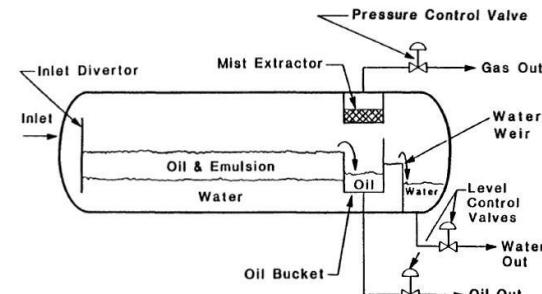


Figure 5-3. Bucket and weir design.

Figure B-3: Comparison of a two-phase horizontal separator (left) and a three-phase horizontal separator (right) [20]

Vertical separators are ideal for PS-100, PS-101, PS-202 and PS-203 because the mass flow rate of liquid is significantly lower than the mass flow rate of the vapors being separated. For instance in Stage 1, PS-100 aims to separate out 2.2 lb/min of entrained natural gas from 1275 lb/min of the riche amine liquid. A vertical separator is visually represented in Figure B-4.

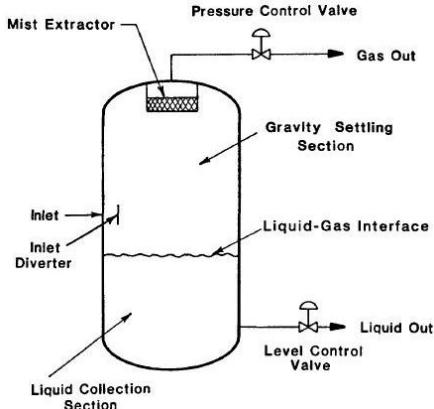


Figure B-4: Vertical separator schematic [20]

In both vertical and horizontal phase separators, mist extractors and inlet diverters will be used to physically aid in separating the vapor and liquid phases of our streams. For the three-phase separator, a weir will be used to separate the oil and water phases. Since the time required to separate water and oil is the limiting rate for three-phase separation, it is expected that the three-phase separator will be larger than the two-phase separator, to accommodate the longer phase separation time (i.e. residence time) required for separation.

B.4 Sizing a Three-Phase Separator

To size our horizontal three-phase separator, such as PS-200, basic sizing principles will typically involve gas-liquid separation and liquid-liquid separation fundamentals. The feed will enter just above the vapor-liquid interface on one end of the horizontal three-phase separator. As mentioned earlier, our final phase separator must:

- Provide sufficient time to allow the immiscible vapor, naphtha, and water phases to separate by gravity.
- Provide sufficient time to allow for the coalescence and breaking of emulsion droplets at the oil-water interface.

Phase Separation Time

The phase separation time, also known as residence time, is the effective time available for each phase's droplets to be separated from the other phases. Phase separation times based on years of experimental data and operational experience has been summarized by the American Petroleum Institute (API) Specification 12J document. [23] [24] A summary of typical phase separation times is shown in Table B-3.

Table B-3: Phase separation times for various water-oil mixtures at various conditions [23]

Oil Gravities	Separation Time (minutes)
Above 35°API	3 to 5
Below 35°API	
Temperature > 37°C	5 to 10
27°C < Temperature < 37°C	10 to 20
15°C < Temperature < 27°C	20 to 30
0°C < Temperature < 15°C	30 to 40

Additionally, API gravity (°API) which is inversely proportional to the specific gravity of the oil that needs to be separated out from water can be calculated using the following equation:

$$API \text{ gravity} = \frac{141.5}{SG} - 131.5 \quad (\text{B-1})$$

$$SG = \frac{\rho_{oil}}{\rho_{water}} \quad (\text{B-2})$$

To estimate phase separation time, one would first calculate API gravity using equations B-1 and B-2, then use Table B-3 to determine the typical separation time. Conceptually, these tables and equations tell us that it takes longer to separate oil and water if their densities are closer to each other. As the density of oil deviates from the density of water, the easier, and thus faster, the separation occurs.

Determining Total Volume Required

The equations below allow us to relate our light phase (naphtha) and heavy phase (water) phase separation times with volume and volumetric flow rates.

$$\tau_{heavy \text{ phase}} = \frac{V_{heavy \text{ phase}}}{\dot{V}_{heavy \text{ phase}}} \quad (\text{B-3})$$

$$\tau_{light \text{ phase}} = \frac{V_{light \text{ phase}}}{\dot{V}_{light \text{ phase}}} \quad (\text{B-4})$$

$$\tau_{vapor \text{ phase}} = \frac{V_{vapor \text{ phase}}}{\dot{V}_{vapor \text{ phase}}} \quad (\text{B-5})$$

Using equations B-3, B-4 and B-5, we can determine the volume requirements for the heavy and light phase separations levels. The following specifications will be used to determine the total volume required for effective separation to occur:

- Phase separation times for the heavy phase, light phase, and vapor phase will be equal ($\tau_{heavy \text{ phase}} = \tau_{light \text{ phase}} = \tau_{vapor \text{ phase}}$) since this is a continuous process. Phase separation times will be estimated using Table B-3.
- $\dot{V}_{vapor \text{ phase}}$, $\dot{V}_{light \text{ phase}}$, and $\dot{V}_{heavy \text{ phase}}$ will match the flow rates calculated by Aspen.

Required volumes of heavy phase, light phase, and vapor phase necessary for the horizontal phase separator can be determined from the specifications and equations introduced above.

Length-to-Diameter Ratio of Phase Separation Unit

The length-to-diameter ratio of a phase separation unit is dependent on the vessel operating procedure, as shown in Table B-4.

Table B-4: Length-to-diameter ratio guidelines [25]

Vessel operating pressure (psia)	Length/Diameter ratio
$0 < P < 250$	1.5 to 3.0
$250 < P < 500$	3.0 to 4.0
$500 < P$	4.0 to 6.0

Number of Phase Separators for Process

To determine the number of phase separators for our process, we must define the diameter of our tank. To reduce turbulence of fluids, phase separators should be large but small enough such that the water and naphtha can be effectively separated out from the bottom of the separator. One can either define the number of parallel phase separators desired for the process or the diameter of the process to determine the final size. It is easier to just define the number of parallel phase separators since dealing with a fraction of a phase separator is a hassle.

Equation B-6 coupled with a L/D ratio from Table B-4 allow us to determine the final length and diameter of our phase separator.

$$V_{total} = \sum \frac{\pi D^2}{4} L \quad (\text{B-6})$$

From an economics standpoint, the diameter of our phase separator is ultimately limited by transportation constraints; the maximum diameter of our separation unit should be 14 feet. As shown in Figure B-5, phase separators can be quite large.



Figure B-5: Two large phase separators with diameters of ~10 feet in industry. [26]

B.5 Sizing a Horizontal Two-Phase Separator

Sizing a horizontal two-phase separator, such as PS-201, is simpler than sizing a horizontal three-phase separator. This is because the final phase separator only needs to provide sufficient time to allow the naphtha to condense from the vapor phase. Just like the three-phase separator, the feed will enter just above the vapor-liquid interface on one end of the horizontal two-phase separator.

All the steps, except the steps necessary to determine the phase separation time, apply for a two-phase separator. The phase separation time for a two-phase separator is typically about 1 minute, to allow enough time for the desired naphtha to separate enough from the vapor. [27]

B.6 Sample Calculations for Sizing PS-200

In our calculations, water is the heavy phase and naphtha is the light phase. From Aspen simulations, we are given that:

$$\dot{V}_{water} = 0.082 \frac{m^3}{hr}$$

$$\dot{V}_{naphtha} = 0.264 \frac{m^3}{hr}$$

$$\dot{V}_{vapor} = 193.052 \frac{m^3}{hr}$$

From Equations B-1 and B-2 we calculate an API of 94.9.

$$SG = \frac{\rho_{oil}}{\rho_{water}} = \frac{\left(\frac{\dot{m}_{naphtha}}{\dot{V}_{naphtha}} \right)}{\rho_{water}} = \frac{\left(\frac{164.980542 \frac{kg}{hr}}{0.26377856 \frac{m^3}{hr}} \right)}{1000 \frac{kg}{m^3}} = 0.625$$

$$API\ gravity = \frac{141.5}{SG} - 131.5 = \frac{141.5}{0.625} - 131.5 = 94.9$$

From Table B-3, the phase separation time required for PS-200 is 3 to 5 minutes; this means that it will take 3 to 5 minutes to separate naphtha and water after they condense. This phase separation time may seem small; however it is an easy separation of very different substances. To be conservative in our design, a phase separation time of 5 minutes will be used.

Equations B-3, B-4, and B-5 were used to determine the volume of water and naphtha that should be present in the P-200 tank (or parallel tank system) at a given time. Recall $\tau_{water} = \tau_{naphtha} = \tau_{vapor}$.

$$V_{water} = \tau_{water} \dot{V}_{water} = (5\ minutes) \left(0.08198748 \frac{m^3}{hr} \right) \left(\frac{1\ hr}{60\ minutes} \right) = 0.0068\ m^3$$

$$V_{naphtha} = \tau_{naphtha} \dot{V}_{naphtha} = (5\ minutes) \left(0.26377856 \frac{m^3}{hr} \right) \left(\frac{1\ hr}{60\ minutes} \right) = 0.0220\ m^3$$

$$V_{vapor} = \tau_{vapor} \dot{V}_{vapor} = (5\ minutes) \left(193.051744 \frac{m^3}{hr} \right) \left(\frac{1\ hr}{60\ minutes} \right) = 16.0876\ m^3$$

Adding up these volumes allow us to determine the total volume required for the phase separator to operate properly:

$$V_{total} = V_{water} + V_{naphtha} + V_{vapor} = 16.1164\ m^3$$

Since the pressure of our phase separator is 12 atm (176 psi), Table B-4 indicates that the length-to-diameter ratio of our phase separator should be between 1.5 and 3.0. Since 16 m^3 is a reasonable volume to work with, one phase-separator is sufficient to achieve the phase separation desired.

Thus, the final volume and dimensions of our phase separator can be calculated using the rules of thumb given in Table B-4 as follows:

$$V_{total} = 16.1164 \text{ m}^3 = \frac{\pi D^2}{4} L$$

$$\frac{L}{D} = 4.0$$

Solving the system of equations give us **D = 1.9 m and L = 5.7 m**. Thus, a three-phase separator with a diameter of 1.9 meters and length of 5.7 meters is sufficient to separate out the naphtha and water from the hydrocarbon vapor.

B.7 Sample Calculations for Sizing PS-201

From Aspen simulations, we are given that:

$$\dot{V}_{naphtha} = 0.162 \frac{\text{m}^3}{\text{hr}}$$

$$\dot{V}_{vapor} = 266.617 \frac{\text{m}^3}{\text{hr}}$$

Since $\tau_{naphtha} = \tau_{vapor} = 1 \text{ minute}$, the volume of the two-phase separator can be calculated as follows:

$$V_{naphtha} = \tau_{naphtha} \dot{V}_{naphtha} = (1 \text{ minute}) \left(0.162 \frac{\text{m}^3}{\text{hr}} \right) \left(\frac{1 \text{ hr}}{60 \text{ minutes}} \right) = 0.0027 \text{ m}^3$$

$$V_{vapor} = \tau_{vapor} \dot{V}_{vapor} = (1 \text{ minute}) \left(266.617 \frac{\text{m}^3}{\text{hr}} \right) \left(\frac{1 \text{ hr}}{60 \text{ minutes}} \right) = 4.4436 \text{ m}^3$$

$$V_{total} = V_{naphtha} + V_{vapor} = 4.4463 \text{ m}^3$$

Since the pressure of our phase separator is 8 atm (118 psi), Table B-4 indicates that the length-to-diameter ratio of our phase separator should be between 1.5 and 3.0. Since 4.4 m^3 is a reasonable volume to work with, one phase-separator is sufficient to achieve the phase separation desired.

Thus, the final volume and dimensions of our phase separator can be calculated as follows:

$$V_{total} = 4.4463 \text{ m}^3 = \frac{\pi D^2}{4} L$$

$$\frac{L}{D} = 3.0$$

Solving the system of equations give us **D = 1.2 m and L = 3.7 m**. Thus, a two-phase separator with a diameter of 1.2 meters and length of 3.7 meters is sufficient to separate out the naphtha and the hydrocarbon vapor.

B.8 Master List of Phase Separators

Table B-5 summarizes the dimensions of all phase separators in our process.

Table B-5: Summary of the volume and dimensions of all phase separators in the process

Equipment	Volume (m ³)	Diameter (m)	Length (m)
<i>Horizontal Separators</i>			
PS-200	16.1	1.9	5.7
PS-201	4.4	1.2	3.7
<i>Vertical Separators</i>			
PS-100	8.4	1.3	6.5
PS-101	0.63	0.5	2.8
PS-202	10	1.5	5.9
PS-203	4.1	1.1	4.3

Appendix C: Dehydration Bed Design

The procedure for designing the adsorbent bed was laid out by Kohl and Nielsen [8]:

1. Select the adsorbent material based on constraints.
2. Determine the allowable gas superficial velocity that corresponds to an acceptable pressure drop. Calculate bed cross sectional area given the result from (2).
3. Select a cycle time 8-12 hours and calculate the amount of adsorbent needed based on degenerated capacity of the adsorbent.
4. Determine the bed length based on (3) and the length of unused bed (LUB).

Applying the procedure to this adsorbent bed yields:

1. Only molecular sieves could ensure that the outlet gas would have a dew point less than -100°C. Given the low tolerance to water in the distillation feed, molecular sieves were the appropriate sorbent choice. 8x12 mesh (1/16") spheres were chosen as they should be the easiest to model.
2. Pressure drop was calculated using a modified Ergun equation [8]:

$$\frac{\Delta p}{L} = \left(\frac{f_t C_t G^2}{\rho D_p} \right) * 10^{-10}$$

Where $\frac{\Delta p}{L}$ = pressure drop (in psi) per foot of bed length

f_t = friction factor, read from a chart based on the Reynold's number

C_t = pressure drop coefficient, read from chart

G = superficial mass velocity ($\text{lb}/\text{hr}/\text{ft}^2$)

ρ = fluid density, as determined by ASPEN (lb/ft^3)

D_p = effective particle diameter (ft)

There is an 8 psi difference between the bed inlet pressure and the separation train inlet. There is some room for pressure drop, but only a reasonable amount. The pressure drop equation was evaluated at several cross sectional areas for the molecular sieve packing, and the correlation in Figure C-1, below, was observed.

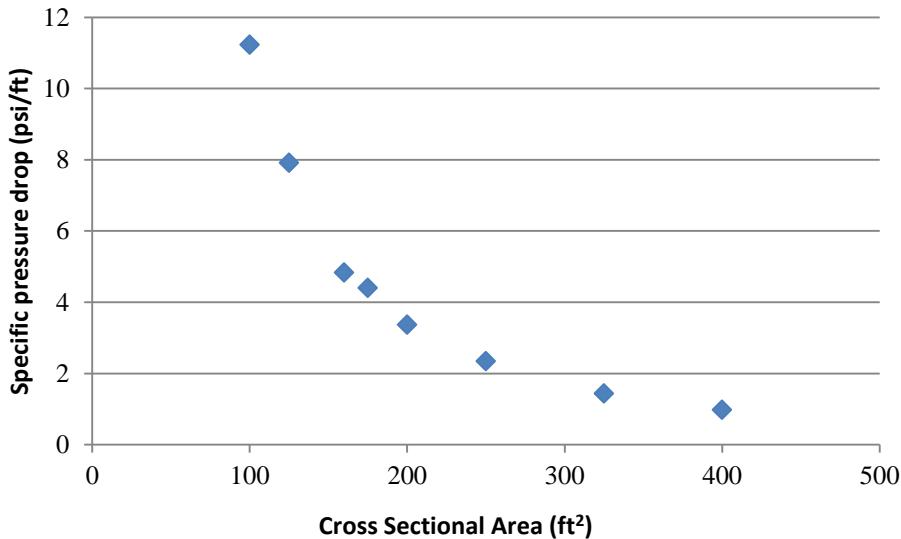


Figure C-1: Pressure drop decreases as bed cross section increases.

Ultimately, a 200 ft² cross section was chosen, corresponding to a pressure drop of 3.37 psi/ft.

3. A cycle time of 8 hours was chosen since this would result in a shorter, cheaper bed. Degenerated molecular sieve adsorbent is expected to have a capacity of 0.13 lb water/lb of adsorbent and a bulk density of 43 lb/ft³.

$$9.74 \frac{\text{lb } H_2O}{\text{min}} * \frac{1 \text{ lb adsorbent}}{0.13 \text{ lb } H_2O} * \frac{60 \text{ min}}{\text{h}} * \frac{8 \text{ h}}{\text{cycle}} * \frac{1 \text{ ft}^3}{43 \text{ lb}} = 836 \frac{\text{ft}^3 \text{ adsorbent}}{\text{cycle}} = LES$$

4. Calculate the length of the mass transfer zone via the correlation:

$$MTZ = \left(\frac{v}{35} \right)^{0.35} z$$

Where $z = 0.85$ for the selected sieve type

v = superficial velocity = $\dot{m}/\rho/A$

$$MTZ = \left(\frac{6675 \frac{\text{lb}}{\text{min}}}{0.767 \frac{\text{lb}}{\text{ft}^3} * 200 \text{ ft}^2} \right)^{0.35} * 0.85 = 0.907$$

$$l_{bed} = LUB + LES = 0.5MTZ + LES = 4.63 \text{ ft}$$

$$\Delta p = 4.63 \text{ ft} * 3.37 \frac{\text{psi}}{\text{ft}} = 15.6 \text{ psi}$$

Therefore, for an 8-hour rotating schedule, two molecular sieve-packed beds of cross section 200 ft² and length of 5 ft are needed.

Appendix D: Refrigeration System Design

- D.1 Overview
- D.2 Objective and Selecting a Suitable Refrigeration Process
- D.3 Refrigerant Selection
- D.4 Refrigeration Process Selection
- D.5 Heat Exchanger Selection
- D.6 Refrigeration Unit Design
- D.7 Refrigeration Unit Efficiency
- D.8 Refrigeration Unit Heat Exchange

D.1 Overview

This section will describe the methods taken in designing and sizing units within our cryogenic refrigeration system.

D.2 Objective and Selecting a Suitable Refrigeration Process

The objective of the cryogenic refrigeration stage is to take the water and naphtha-free stream from the phase separators and absorbent bed and liquefy it for distillation. Due to the need to reach cryogenic temperatures, refrigeration cycles with multiple stages will be necessary. There are many technology options and factors that will affect our decision when selecting a suitable liquefaction process.

D.3 Refrigerant Selection

The liquefaction of our natural gas stream requires heat exchange between a refrigerant cold enough to affect liquefaction. There are many types and combinations of refrigerants, but they can be categorized into two broad categories: mixed refrigerants (MRs) or pure component refrigerants (PCRs). Pure components refrigerants are often used because of their simplicity and easy operation. Mixed refrigerants, however, are more efficient at cooling than pure refrigerants if its cooling curve matches the gas being liquefied, as demonstrated in Figure D-1.

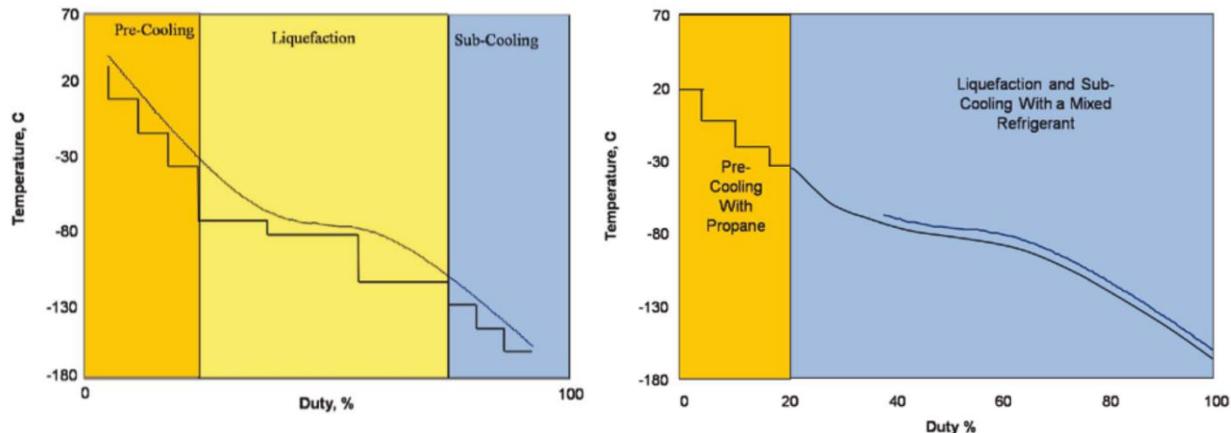


Figure D-1: Liquefaction process using pure component refrigerants (left) and mixed refrigerants (right) [28]

Though more complicated, our liquefaction system will use a mixed refrigerant due to its improved efficiency over pure component refrigerants.

Composition of Mixed Refrigerant

The selection of an optimal mixed refrigerant composition is not clearly defined or stated in the literature. [29] As reported by Baek, a mixed refrigerant that consists of approximately 20 wt% nitrogen, 35 wt% methane, and 45 wt% propane is a close-to-ideal composition because its cooling curve matches the gases being liquefied more than pure component refrigerants.

D.4 Refrigeration Process Selection

The selection of natural gas liquefaction refrigeration processes depend primarily on the flow rate of gas needed to be liquefied and whether there are any space restrictions. The space restrictions of usually tailored toward floating plants, so our land based process will not be limited by that constraint. As shown in Figure D.2, as the flow rate of natural gas required to be liquefied increases, the refrigeration design also must be modified due to economic constraints.

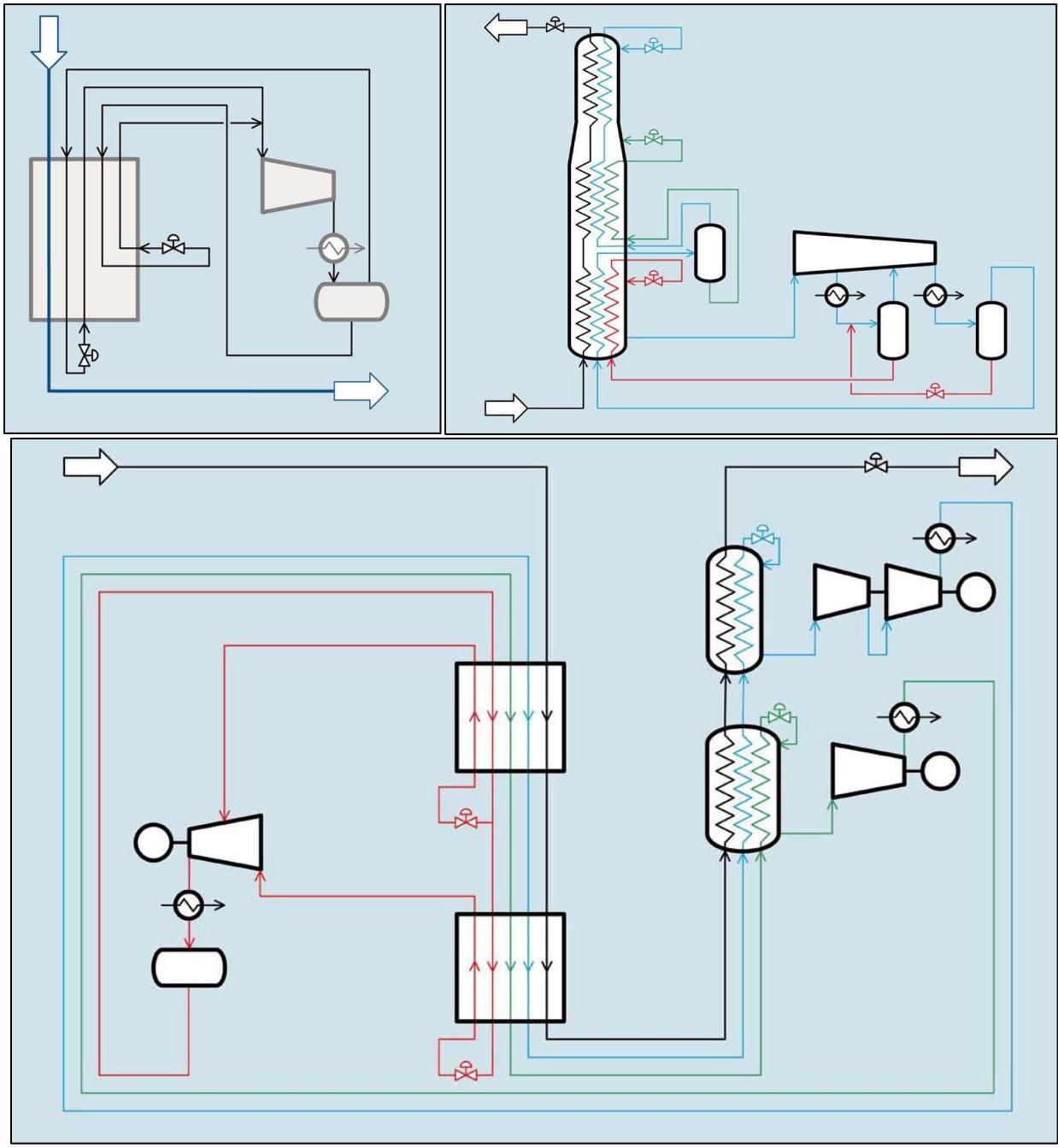


Figure D-2: Representative natural gas liquefaction schematics for a small refrigerator (top left), a medium-sized refrigerator (top right) and a large refrigerator (bottom). Table D-1 shows rough definitions for how refrigerator sizes correspond with plant capacity. [30]

Table D-1: Rough definitions for small, medium, and large plant sizes [30]

Refrigerator Size	Plant Capacity (metric tons per year)
Small	< 0.5
Medium	0.2 – 1.0
Large	3 – 12

As shown in Figure D-2, small refrigeration units typically use a basic single flow liquefaction process (see Figure D-2) where the cycle gas stream is compressed to high pressure and temperature, cooled to ambient temperatures, then flashed to a colder temperature. This flashed refrigerant is separated into liquid condensate and vapor in the flash tank. The vapor is used directly as cooling duty while the liquid condensate is flashed into a vapor to even lower temperatures and used as cooling duty.

Medium and large refrigeration units use the same principles of compressing and expanding refrigerant to achieve colder temperatures. As shown in Figure D-2, medium sized refrigeration units typically use a multi-stage process and large refrigeration units typically use a cascade refrigeration process.

Since our ethylene plant plans to liquefy approximately 6500 lb/min of hydrocarbons (or approximately 1.5 metric tons per year), then either a medium or large refrigeration unit for our process would be the most economical. A design that takes aspects of both medium and large sized refrigeration units will be designed and implemented.

D.5 Heat Exchanger Selection

When liquefying natural gas hydrocarbon streams, two types of heat exchanger units are often used: the plate-fin heat exchanger (PFHEX) and the coil-wound heat exchanger (CWHEX). The CWHEX is the core equipment used with medium or large refrigeration units. Additionally, the CWHE is great at providing a large heating surface per shell, and is tolerant against thermal shocks due to its design. PFHEXs are the preferred heat exchangers in small refrigeration units. Since our plant will use a medium refrigeration unit, a CWHEX, shown in Figure D-3, will be used for liquefaction.

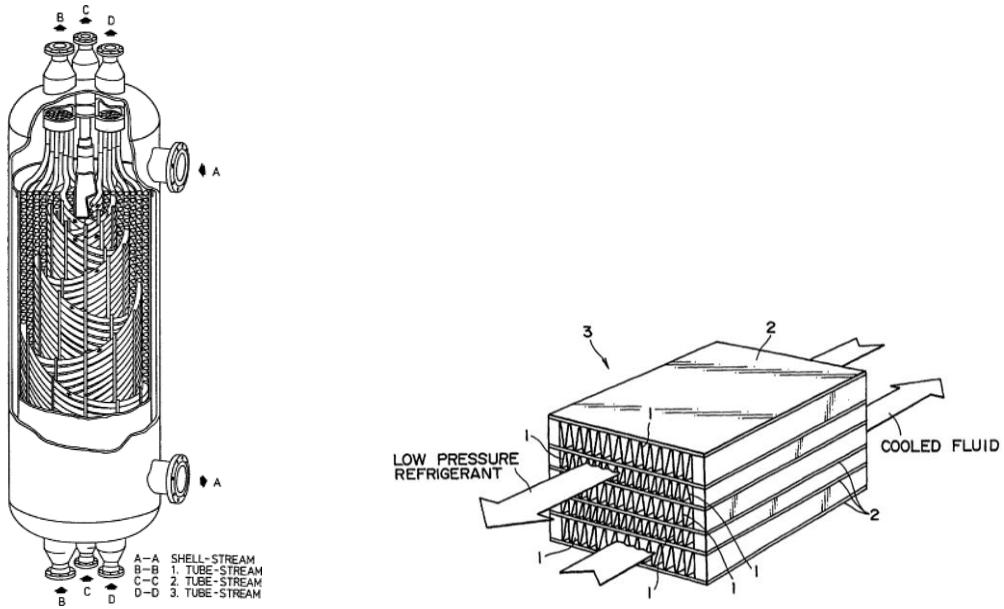


Figure D-3: A coil-wound heat exchanger (CWHEX), left, and plate-fin heat exchanger (PFHE), right. [31] [32]

D.6 Refrigeration Unit Design

From our decisions so far, we have specified the following for our refrigerator design:

- Use of mixed refrigerant to better match cooling curves
- Use of a multi-stage/cascade process to reach cryogenic temperatures
- Use of a coil-wound heat exchanger (CWHEX) for heat transfer

In general, typical refrigeration units for plants our size uses several heat exchangers, Joule-Thompson valves, and vapor-liquid phase separators hooked into a cascade system, as shown in Figure D-4. [33]

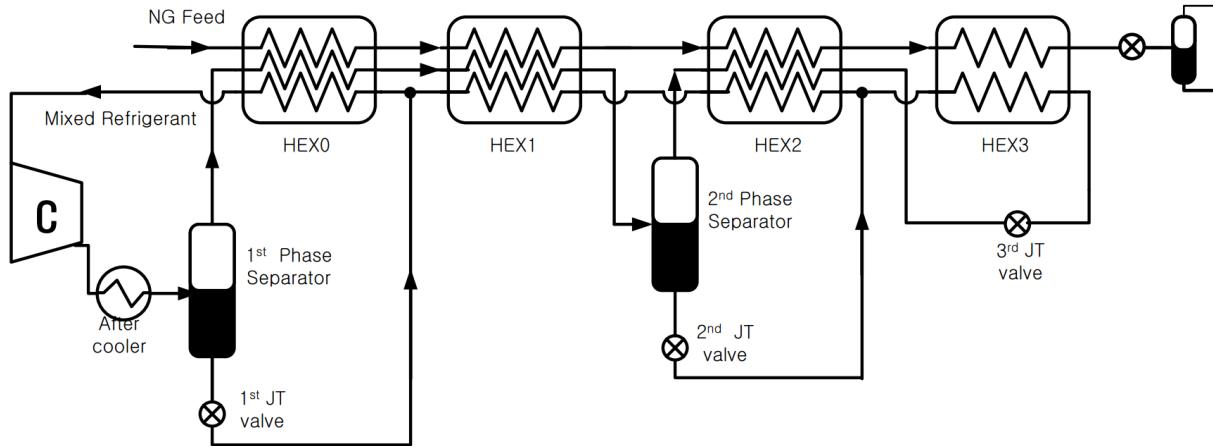
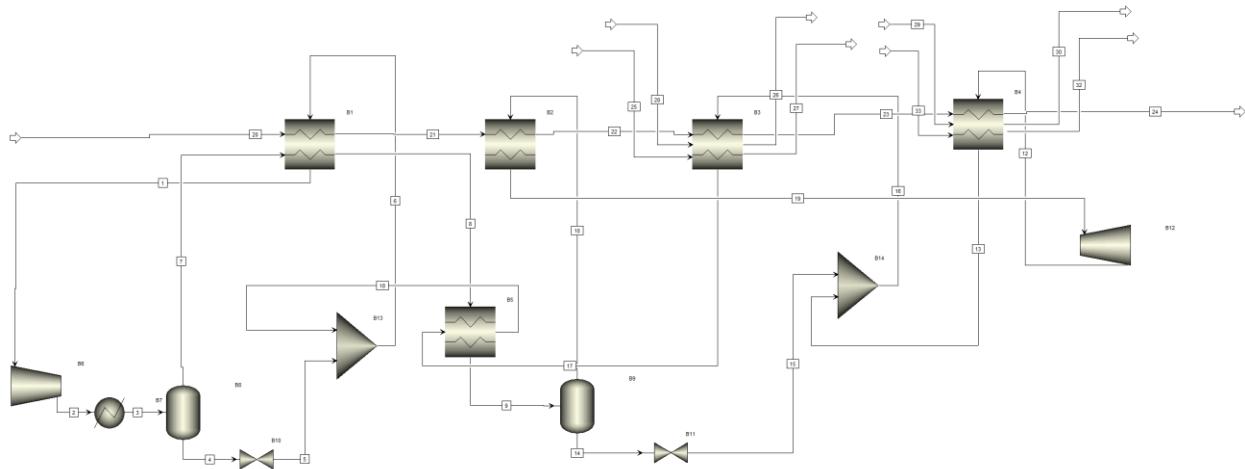


Figure D-4: Schematic of a typical cryogenic refrigeration unit. [29] (HEX = heat exchanger, JT = Joule-Thompson)

Since our refrigeration system will need to liquefy a large volume of natural gas, our system will need to be efficient. By replacing the 3rd Joule Thompson valve with an expander the liquefaction cycle efficiency can be increased. [29] Since both an expander and compressor are present in this cycle, the energy generated by the expander can be used to reduce utility required to power the compressor, ultimately creating a turbo-expanded process. [34] The use of a turbo-expander will further improve the efficiency of our process. The compressor in the refrigeration stage aims to pressurize a gas flow rate of 122 kg/hr of refrigerant from 1.5 atm to 30 atm. An efficiency of 80% was assumed for both the compressor and turbine. The advantage of this turbo-expander process is that energy generated by the turbine partially powers the energy used by the compressor. Figure D-5 shows a schematic of the Aspen simulation we used to model our refrigeration system.



D.7 Refrigeration Unit Efficiency

Energy enters the system in the form of shaft work for the compressor-turbine system heat from the natural gas feed. Energy exits the system in the form of heat from interstate cooling within the compressor.

$$\eta = \frac{\text{useful energy out}}{\text{energy put into system}} = \frac{W_{\text{cooling of natural gas}}}{W_{\text{compressor}} - W_{\text{turbine}}}$$
$$= \frac{0.23 \times 10^8 \frac{\text{Btu}}{\text{hr}}}{2.43 \times 10^8 \frac{\text{Btu}}{\text{hr}}} = 0.095$$

Thus, our cryogenic refrigerator has an efficiency of 9.5%. It is recommended to MichiChem Corp. that the efficiency of our cryogenic refrigeration system be improved in future studies and designs before funding the project.

D.8 Refrigeration Unit Heat Exchange

Heat exchange between the designed refrigeration unit and the natural gas feed must be designed so that our desired liquefaction duty will occur for both the hydrocarbon feed into the cryogenic separation system and distillation condensers. A minimum approach temperature of 10°C was assumed for feed temperatures higher than -30°C. A minimum approach temperature of 2.5°C was assumed for temperatures lower than -30°C. [30] Aspen was used to close energy balances for our multi-stream coil-wound heat exchangers.

Appendix E: Distillation Design

- E.1 Separation Alternatives
- E.2 Multicomponent Separation Design
- E.3 Modeling and Sizing the Distillation Column
- E.4 Cryogenic Equipment Considerations

E.1 Separation Alternatives

There are several methods that can be implemented to separate our hydrocarbon stream into valuable products of acceptable purity.

- Gas absorption (scrubbing)
- Adsorption (pressure swing)
- Membrane separation
- Cryogenic distillation

For each method, its background, uses in industry, and economics will be briefly discussed.

Current Industrial Practices

Absorption occurs when molecules are taken up by a fluid. For the ethylene production process, gas would be absorbed into a liquid. In industry, gas absorption is commonly used to remove harmful particulates or CO₂ from exhaust gas. [35]

Adsorption (Pressure Swing)

Adsorption occurs when molecules adhere to a solid surface. For the ethylene process, gas would be adsorbing onto a surface. Since gases tend to be more attracted to solid surfaces under higher than ambient pressures, target gases can be removed by adsorbing them onto solid surfaces at high pressure, then released by decreasing the pressure. This process is known as pressure swing adsorption (PSA). [36]

Adsorbents for PSA systems should have the following properties:

- High selectivity for certain gases
- High porosity (high surface areas)
- Reusability

In industry, common adsorbents include activated carbon, silica gel, alumina, and zeolites. PSA is used in many applications such as the purification of water, catalysis of reactions, extraction of nitrogen from air, and the removal of water from gases and liquids. The costs of adsorbents are determined primarily by their selectivity, porosity and reusability. Absorbents that exhibit high selectivity, high porosity, and reusability cost more.

Membrane Separation

A membrane is a semipermeable barrier that allows the passage of select gases, vapors, or liquids at different rates. Each gas in the feed has a permeation rate through the membrane which depends on several factors, including:

- Size of molecules
- Affinity of molecules to membrane material
- Permeation driving forces (concentration or pressure differences)

Membranes provide a cost-effective purification of hydrogen and methane and are used in industry for [7]:

- Hydrogen separation
- Separating nitrogen from air
- CO₂ and water removal from natural gas
- Organic vapor removal from air or nitrogen streams

The cost of membranes is determined primarily by the permeability and selectivity for a specific gas in a mixture. It is ideal to have high permeability and high selectivity; however for most membranes, increasing permeability will decrease selectivity.

Cryogenic Distillation

Cryogenic distillation, like any other distillation process, takes advantage of the different boiling points of gases in a gas mixture. In ethylene production, cryogenic distillation would be used to separate the cracker effluent into hydrogen, ethylene, methane, and other products. [37]

Cryogenic distillation is useful for separating large quantities of gas mixtures. Since distillation requires the fluid to be in the liquid and gas phases, a large amount of energy is required to achieve cryogenic temperatures. The economics of cryogenic distillation depend on the amount of gas undergoing separation. This alternative is preferable for large volumes of gas as it offsets the large amount of energy required for cryogenic distillation.

E.2 Multicomponent Separation Design

Since designing a multicomponent distillation scheme is extremely open ended, the following steps were taken to guide us toward our final design:

1. Determine separation sequences
2. Decide on the fate of potential byproduct streams
3. Understand general rules of thumb of column design
4. Estimate column operating conditions
5. Model, simulate, and size distillation column
6. Select suitable construction materials for distillation
7. Tabulate and optimize heat integration.
8. Determine refrigeration and/or heating required outside of heat integration
9. Model, simulate, and size refrigeration units.
10. Conduct costing analysis on overall separation process

Separation Sequence

When designing our multicomponent distillation system, we first started creating a separation sequence by defining heavy and light component splits. These splits were determined by ordering the components by increasing boiling points, as shown in Table E-1, and then determining logical or favorable locations for splitting. For instance, easier separation can be

achieved if there is a large difference in boiling points between the tops and bottoms streams. In addition, the following rules of thumb for determining separation sequences were taking into consideration:

1. Direct sequences that remove components one-by-one in the distillate are favored.
2. Equal-molar separation of the feed between the distillate and bottoms are favored.
3. Difficult separations should be the last to be separated.
4. Desired high-purity products should be the last to be separated.

Our proposed distillation scheme is shown below in Figure E-1.

Table E-1: Boiling points of components

Component name	Aspen Alias	Boiling Point (°C) at 1 atm
Hydrogen	H2	-252.7
Nitrogen	N2	-195
Methane	CH4	-161.5
Ethylene	C2H4	-103.7
Ethane	C2H6	-88.6
Acetylene	C2H2	-84
Propylene	C3H6-2	-47.7
Propane	C3H8	-42.1
Methyl-acetylene	C3H4-2	-23.2
Isobutane	C4H10-2	-13
1-Butene	C4H8-1	-6.3
1,2-Butadiene	C4H6-3	-4.4
n-Butane	C4H10-1	-1
Vinyl-acetylene	C4H4	5.5
2-Methyl-butane	C5H12-2	30
n-Pentane	C5H12-1	36.1
n-hexane	C6H14-1	68.7
Benzene	C6H6	80.1
n-Heptane	C7H16-1	98.4

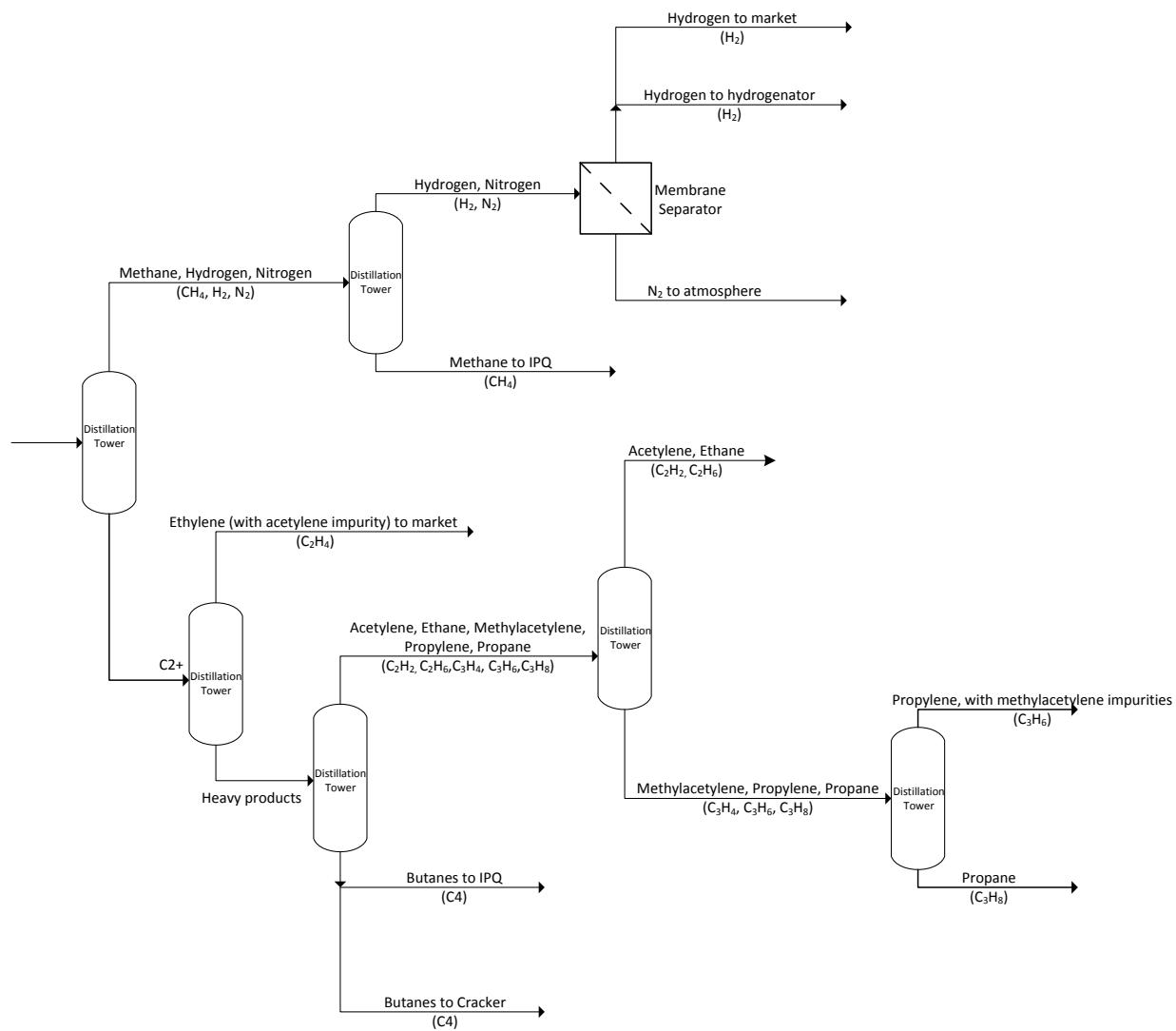


Figure E-1: Proposed distillation scheme and fate of streams

Fate of Streams

There are three different fates that product and byproduct streams can take in our process:

- Recycle
- Market

- Purge or waste

To determine whether potential byproducts should be recycled, we looked into the potential for them to create our required products: ethylene and IPQ natural gas. Since ethane and propane can be cracked into ethylene it was determined that these products would be recycled.

To determine whether potential byproducts should be sold to the market, we compared their respective prices with an estimated cost of separation. If there is economic potential, then operations were added to produce those side products. We decided that propylene, ethylene, hydrogen gas, and naphtha will be sold to the market.

If a component does not pass the two criteria stated above, then it can either be purged or, if hazardous, then sent a waste treatment plant for treating. We decided that nitrogen gas will be purged to the atmosphere.

General Rules of Thumb

There are several design considerations for designing distillation columns that needs to be met to maximize safety and economic potential; this will allow us to understand what types of columns are feasible from both an economic standpoint and a practical standpoint.

The criteria listed in Table E-2, below, indicate constraints and specifications that were taken into account in each distillation column design. [38]

Table E-2: Tower specifications for optimal operation

Specification	Value	Comments
Tray Spacing	~2 feet	Easy access for maintenance
Pressure drop	~0.1 psi/tray	Allow fluids to flow
Tray Efficiencies	~60 to 90%	Vapors between trays not well mixed
Reflux Ratio	R/Rmin = 1.2 to 1.5	Economic optimum
Number of Stages	N/Nmin = 2	Economic optimum
Tower Height	~175 ft max	Wind and foundation consideration
Height/Diameter ratio	<20, max 30	Structural consideration

Estimating Optimal Operating Conditions

Since we are designing a process that produces 500 million pounds of ethylene per year, this will be the specification that determines flow rates every other stream in our process. To obtain initial estimates for operating conditions, we used the boiling point of components to determine rough temperatures where streams will be completely liquefied. Estimated flow rates were based off the assumption that 100% separation was possible.

To obtain estimated optimal operating conditions, a DSTWU column uses the Gilliland's, Winn's, and Underwood's methods to calculate staging and reflux ratio optiums under the assumption of constant molar overflow and constant relative volatilities, as shown in Table E-3. [39]

Table E-3: Estimated optimal operating conditions from DSTWU using the Peng-Robinson thermodynamic model

	T-300,T-301, T-302,T-303	T-304	T-400	T-401	T-402	T-403
DSTWU (Specifications)						
Pressure leaving	7.6	7.2	7.2	6.8	6.4	5.9
Light Key Recovery	n/a	n/a	1.0	1.0	1.0	0.9
Heavy Key Recovery	n/a	n/a	0.0	0.0	0.0	0.1
DSTWU (Optimums)						
Feed Stage	n/a	n/a	26.3	23.8	25.5	23.0
Number of Trays	n/a	n/a	50.0	47.0	54.2	40.0
N_{\min}	30.0	25.0	26.2	24.0	9.5	20.9
R_{\min}	0.2	3.5	3.5	0.2	0.0	20.6

The Winn-Underwood-Gilliland method (also known as Fenske-Underwood-Gilliland or FUG method). These methods can be manually implemented, however more appropriate thermodynamic and interaction models can provide more accurate physical properties. Thus, computer simulators such as Aspen should be used instead. The algorithm used by Aspen is shown in Figure E-2.

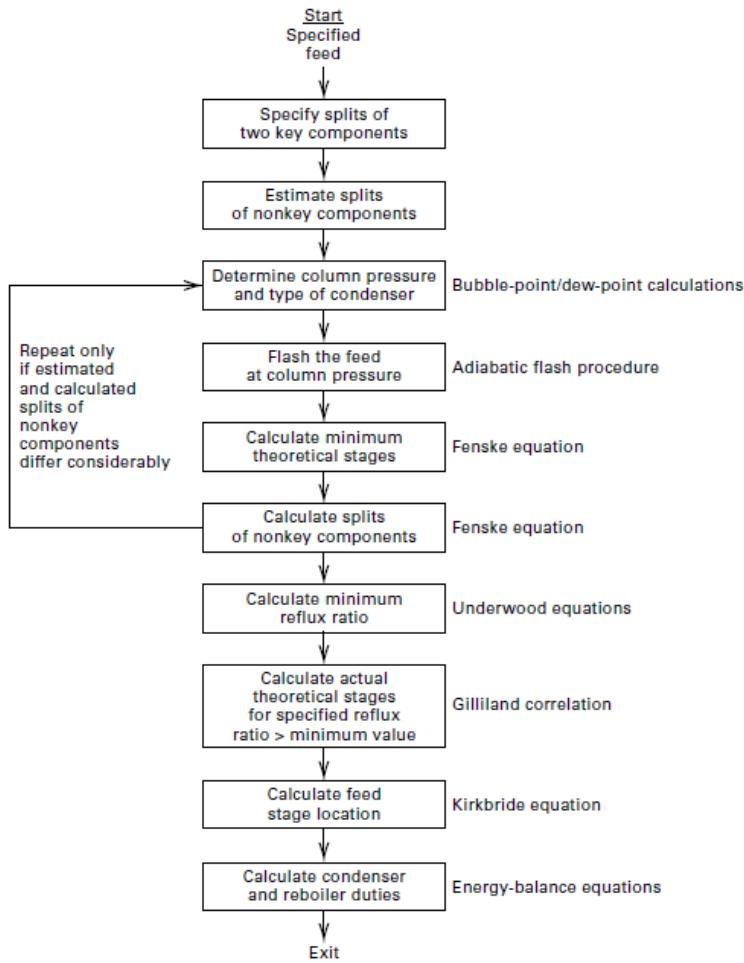


Figure E-2: Fenske-Underwood-Gilliland method algorithm. [40]

E.3 Modeling and Sizing the Distillation Column

After estimates of optimal conditions were carried out by the DSTWU method in Aspen, the optimal conditions were entered as specifications into the RadFrac distillation model, which is more rigorous and accurate for simulating distillation. The sizing values computed by DSTWU and the actual input specifications for the RadFrac model is shown in Table E-4. Additionally, Table E-4 also shows that the specifications computed by DSTWU fall within a few major rules of thumb.

Table E-4: DSTWU Approximations and RadFrac Specifications. Notice that major rules of thumb fall within specifications.

	T300	T301	T400	T401	T402	T403
RadFrac (Specifications)						
Pressure Drop (atm)	0.4	0.4	0.4	0.4	0.4	0.5
Trays	50	50	52	48	50	40
Tray spacing (ft)	2	2	2	2	2	2
Column diameter (ft)	10.3	12.1	13.2	9.3	7.2	10.7
Reflux Ratio	0.3	5.0	5.0	0.3	0.5	26.0
DSTWU (Approximations)						
Light Key Recovery	n/a	n/a	1	1	1	1
Heavy Key Recovery	n/a	n/a	0	0	0	0
Feed Stage	n/a	n/a	26	24	25	23
N	n/a	n/a	n/a	n/a	54	40
N _{min}	30	25	26	24	9	21
R _{min}	0.25	3.50	3.50	0.18	0.05	20.58
Pressure leaving	7.6	7.2	7.2	6.8	6.4	5.9
Rules of Thumb						
L/D < 20	10	8	8	10	14	8
Height <150 ft						
0.01 psi (0.0068 atm) pressure drop per tray	0.013	0.016	0.015	0.017	0.004	0.006

E.4 Cryogenic Equipment Considerations

In this section, a few considerations specific to cryogenic equipment and will be discussed.

Materials Selection

Since properties of solids at cryogenic temperatures are considerably different from those at ambient temperatures, many materials will be unsuitable for use at cryogenic conditions. The choice of materials will be dictated by mechanical properties, cost, ease of fabrication, and so on. [41] As shown in Table E-5, metals such as aluminum, copper, nickel, and 18-8 type stainless steels do not exhibit ductile-to-brittle transitions at cryogenic temperatures, indicating that its use in cryogenic applications is favorable. Thus, our distillation columns, pipes, tanks, and other devices such as sensors for control systems will be made from these materials. Additionally, notice that polymers that can potentially come in contact with materials or equipment at cryogenic temperatures should not be used for a variety of factors such as its increase in brittleness.

Table E-5: Structural properties of materials at cryogenic conditions

Material	Examples	Properties
Face-centered-cubic (FCC)	Al, Cu, Ni, Stainless Steels (18-8 type)	No ductile-to-brittle transition at low temperatures
Body-centered-cubic (BCC)	Fe, martensitic steels (low carbon, 400-series)	Ductile-to-brittle transition at low temperatures
Hexagonal-close-packed (HCP)	Zn, Zr	Properties intermediate of FCC and BCC
Polymers		Increase in strength and brittleness at low temperatures Decrease in impact resistance

Insulation

Since cryogenic distillation is so energy intensive, measures must be taken to minimize heat leak to the surrounding atmosphere. Heat leak into a storage tank or transfer system, such as a truck tank occurs by either radiation and/or conduction through the insulation, or by conduction through inner shells, connected pipes, etc. Cryogenic insulation systems, also known as cryostats are designed to reduce heat leak to the environment by equipment operating at cryogenic temperatures, pipes, or tanks storing cryogenic liquid. [41] [42] [43]

Radiation shields such as multilayer insulation is effective in reducing heat losses due to radiation. Powder insulation, though about 10 times less effective than multilayer insulation, is used to insulate within awkward structural complexities such as in corners and edges that are otherwise difficult to insulate.

Storage tanks for large volumes ($>1000 \text{ m}^3$) is often insulated with un-evacuated perlite that is pressurized with boil-off gas from the tank's liquid. Transport vehicles often contain an inner vessel that holds liquid surrounded by vacuum perlite or multilayer insulation, all enclosed within the outer vessel. The outer vessel is often extremely reflective, again, to minimize radioactive heat leak.

Appendix F: Membrane Separation Design

- F.1 Overview
- F.2 Economics of Membrane vs. Burn
- F.3 Unit Operation
- F.4 Hydrogen-Selective Membrane Options
- F.5 Physical Structure of Polymer Membranes
- F.6 Membrane Design Equations
- F.7 Sample Calculation for M-302

F.1 Overview

Since hydrogen and nitrogen have extremely low boiling points, it is difficult and expensive to liquefy these two components for distillation. Instead of distillation, we will be using a membrane separation system to retrieve valuable hydrogen as feed for the downstream hydrogenator unit. Excess hydrogen produced will be sold to the market.

F.2 Economics of Membrane vs. Burn

$$-286 \frac{kJ}{gmol} \left(\frac{1 \text{ gmol}}{2.02 \text{ g}} \right) \left(\frac{1000 \text{ g}}{kg} \right) \left(\frac{1 \text{ kg}}{2.2 \text{ lb}} \right) = -64356 \frac{kJ}{lb} * \frac{\$3.90}{1 * 10^6 \text{ btu}} = \frac{\$0.24}{lb}$$

From the simple calculation above, it is obvious that we should sell hydrogen to the market rather than burn it since its energy-worth from burning is significantly lower than its standalone value to the market.

F.3 Unit Operation

Membranes are an integral part of many industrial processes because its simple operation is often more environmentally sustainable and cost-effective compared to other separation technologies. Significant applications are in gas separations and water purification. The unit operation is simple to describe. As shown in Figure F-1, the high pressure feed enters the membrane unit where molecules with higher permeability through the membrane will exit as the permeate. The retentate contains molecules that were not able to travel through the membrane.

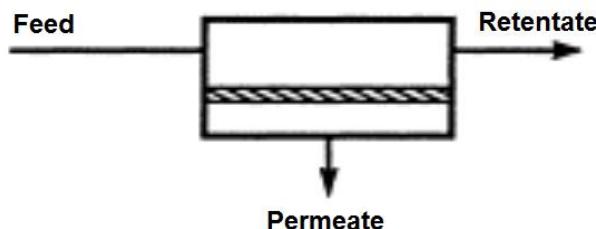


Figure F-1: Unit operation diagram for a membrane separator [44]

F.4 Hydrogen-Selective Membrane Options

As shown in Table F-1, properties of five hydrogen-selective membranes are shown. Each membrane has advantages and disadvantages. Research organizations and companies continue to work to develop better versions of each. For our purposes,

Table F-1: Comparison of properties between five hydrogen-selective membranes [45]

	Dense Polymer	Microporous Ceramic	Dense Ceramic	Porous Carbon	Dense Metallic
Operating Temperature	<100°C	200 – 600°C	600 – 900°C	500 – 900°C	300 – 600°C
H ₂ Selectivity	Low	Moderate	Very high	Low	Very high
H ₂ Flux	Low	High	Moderate	Moderate	High
Known Poisoning Issues	HCl, SO _x , CO ₂		H ₂ S	Strong vapors, organic carbon	H ₂ S, HCl, CO
Example Materials	Polymers	Silica, alumina, zirconia, titania, zeolites	SrCeO ₃ BaCeO ₃		Palladium alloys, Pd-Cu, Pd-Au
Transport Mechanism	Solution/diffusion	Molecular sieving	Solution/diffusion	Surface diffusion, molecular sieving	Solution/diffusion

F.5 Physical Structure of Polymer Membranes

Membranes consist of two major layers: a non-porous membrane and a porous support. The non-porous membrane is where the separation occurs. The porous support, whose purpose is for mechanical integrity, is often about 40 to 200 times thicker than the non-porous membrane.

F.6 Membrane Design Equations

The “well-mixed” model will be used in our membrane separation design and assumes that the flux is driven by the retentate and permeate properties, which are assumed constant along the length of the membrane. [46] Design equations for this model are shown below:

$$\frac{n_P y_{P_{H_2}}}{A_m} = \frac{\frac{P_{H_2}}{l_m} \left(x_{R_{H_2}} - \frac{(P_P)}{P_F} y_{P_{H_2}} \right)}{\left(1 - x_{R_{H_2}} \right) - \frac{P_P}{P_F} (1 - y_{P_{H_2}})} \quad (\text{F-1})$$

$$\frac{y_{P_{H_2}}}{1 - y_{P_{H_2}}} = \frac{\alpha_{H_2, N_2}^* \left(x_{R_{H_2}} - \frac{P_P}{P_F} y_{P_{H_2}} \right)}{\left(1 - x_{R_{H_2}} \right) - \frac{P_P}{P_F} (1 - y_{P_{H_2}})} \quad (\text{F-2})$$

$$\theta = \frac{n_P}{n_F} = \frac{x_{F_{H_2}} - x_{R_{H_2}}}{y_{P_{H_2}} - x_{R_{H_2}}} \quad (\text{F-3})$$

where:

- n_P = molar flow rate of permeate stream
- $y_{P_{H_2}}$ = mole fraction of H_2 in permeate stream
- n_F = molar flow rate of feed stream
- $x_{F_{H_2}}$ = mole fraction of H_2 in feed stream
- $x_{R_{H_2}}$ = mole fraction of H_2 in retentate stream
- P_{H_2} = permeability of hydrogen through membrane
- l_m = membrane thickness
- P_P = pressure of permeate stream
- P_F = pressure of feed stream
- A_m = membrane area
- α_{H_2,N_2}^* = separation factor between H_2 and N_2
- θ = minimum reject concentration (i.e. cut)

F.7 Sample Calculation for M-302

The following algorithm was conducted in Microsoft Excel:

1. List some values of $x_{R_{H_2}}$.
2. Calculate $y_{P_{H_2}}$ using equation F-2 using goal-seek.
3. Calculate θ with equation F-3. Pay attention that $0 \leq \theta \leq 1$. The initial input of $x_{R_{H_2}}$ will have to be manipulated so θ spans a number of values between 0 and 1.
4. Calculate the required area of the membrane using equation F-1.

Using the algorithm with the following specifications shown in Table F-2, results that relate the membrane cut, output purities, and required surface area is shown Table F-3.

Table F-2: Membrane design specifications

Variable	Value	Units
n_F	250	lb-mol/min
$x_{F_{H_2}}$	0.339	-
P_F	7.2	atm
P_P	1.1	atm
α_{H_2,N_2}^*	38.9	-
l_m	1.0×10^{-7}	m
P_{H_2}	2.5×10^{-8}	barrer

Table F-3: Results of the “well-mixed” membrane model calculations.

$y_{P_{H_2}}$	θ	A_m (m^2)
0.25	1.44	536447
0.47	0.64	168891
0.65	0.37	66960
0.78	0.24	28860
0.85	0.15	12847
0.90	0.07	4102

As shown in Table F-3, notice that the required membrane area is lowest when the ratio between the permeate flow rate and feed flow rate is low. Since we are confined to a feed flowrate of 159.6 lb/min (736 lb-mol/min) and retentate flow rate of 83.4 lb/min (110 lb-mol/min), the required cut is then 0.15, which corresponds to an area of 13000 m

Appendix G: Hydrogenator Calculations

- G.1 Catalyst Weight Sample Calculation
- G.2 Polymath Calculation
- G.3 Polymath Conversion Graph
- G.4 Hydrogenator Length Calculation
- G.5 Heat Effects in the Hydrogenator
- G.6 Catalyst Cost

G.1 Catalyst Weight Sample Calculation

The following calculation is the set up to putting the differential equation into Polymath to determine the catalyst weight for a 90% conversion of alkynes to alkenes.

$$\frac{dx}{dw} = \frac{-r_A'}{F_{A_0}}$$

$$-r_A' = \frac{k_3 P_c}{1 + K_{ac} P_c} + \frac{k_4 P_c P_H}{(1 + K_{ac} P_c)^2} + \frac{2k_5 P_c^2 P_H + k_1 P_c P_H^2}{(1 + K_{ac} + P_c)^3}$$

$$P_A = C_A RT = P_{A_0} \left(\frac{1-x}{1+ex} \right) y$$

$E = y_{A_0} \delta \rightarrow y_{A_0} \approx 0$ because acetylene fraction is extremely low
 $\rightarrow E = 0$

$$P_A = P_{A_0} (1-x)y$$

$$y = \frac{P}{P_0} = (1-\alpha w)^{1/2} \longrightarrow \alpha \text{ accounts for pressure drop}$$

$$\alpha = \frac{2\beta_0}{A_c (1-\phi) \rho_c P_0}$$

$$\beta_0 = \frac{G(1-\phi)}{g_c \rho_0 D_p \phi^3} \left[\frac{150(1-\phi)\mu}{D_p} + 1.75 G \right] \rightarrow \text{Ergun equation}$$

$G = \frac{\dot{m}}{A_c}$ → \dot{m} is 226.2 lb/min. By giving the reactor a 2 ft diameter ($A_c = 3.14 \text{ ft}^2$), the maximum line velocity is not exceeded.

$$G = 720 \frac{\text{lb}}{\text{min} \cdot \text{ft}^2}$$

$\phi = 0.3$ → conservative void fraction estimate

$$\mu = 0.001 \frac{\text{lb m}}{\text{ft min}} \quad \left. \begin{array}{l} \text{estimated based on} \\ \text{properties of air} \end{array} \right\}$$

$$\rho_0 = 2.17 \frac{\text{lb m}}{\text{ft}^3} \quad \left. \begin{array}{l} \text{estimated based on} \\ \text{properties of air} \end{array} \right\}$$

$$D_p = 0.01 \text{ ft} \rightarrow \text{according to manufacturer}$$

$$g_c = 115.826 \frac{\text{lb m} \cdot \text{ft}}{\text{min}^2 \cdot \text{lb}_f} \rightarrow \text{conversion factor}$$

$$\beta_0 = 2405 \frac{\text{lb f}}{\text{ft}^3} = 1.137 \frac{\text{atm}}{\text{ft}}$$

$$\rho_c = 2.8 \frac{\text{g}}{\text{mL}} \rightarrow \text{based on density of alumina}$$

$$\alpha = 0.00379 \frac{1}{\text{lb m}}$$

Using Polymath, we obtain a graph of conversion as a function of catalyst weight. A 90% conversion requires 48 lbs of catalyst.

G.2 Polymath Calculation

This is the code entered into Polymath to calculate the amount of catalyst. The comments on the right explain the purpose of each number or calculation.

Polymath DEQ Program

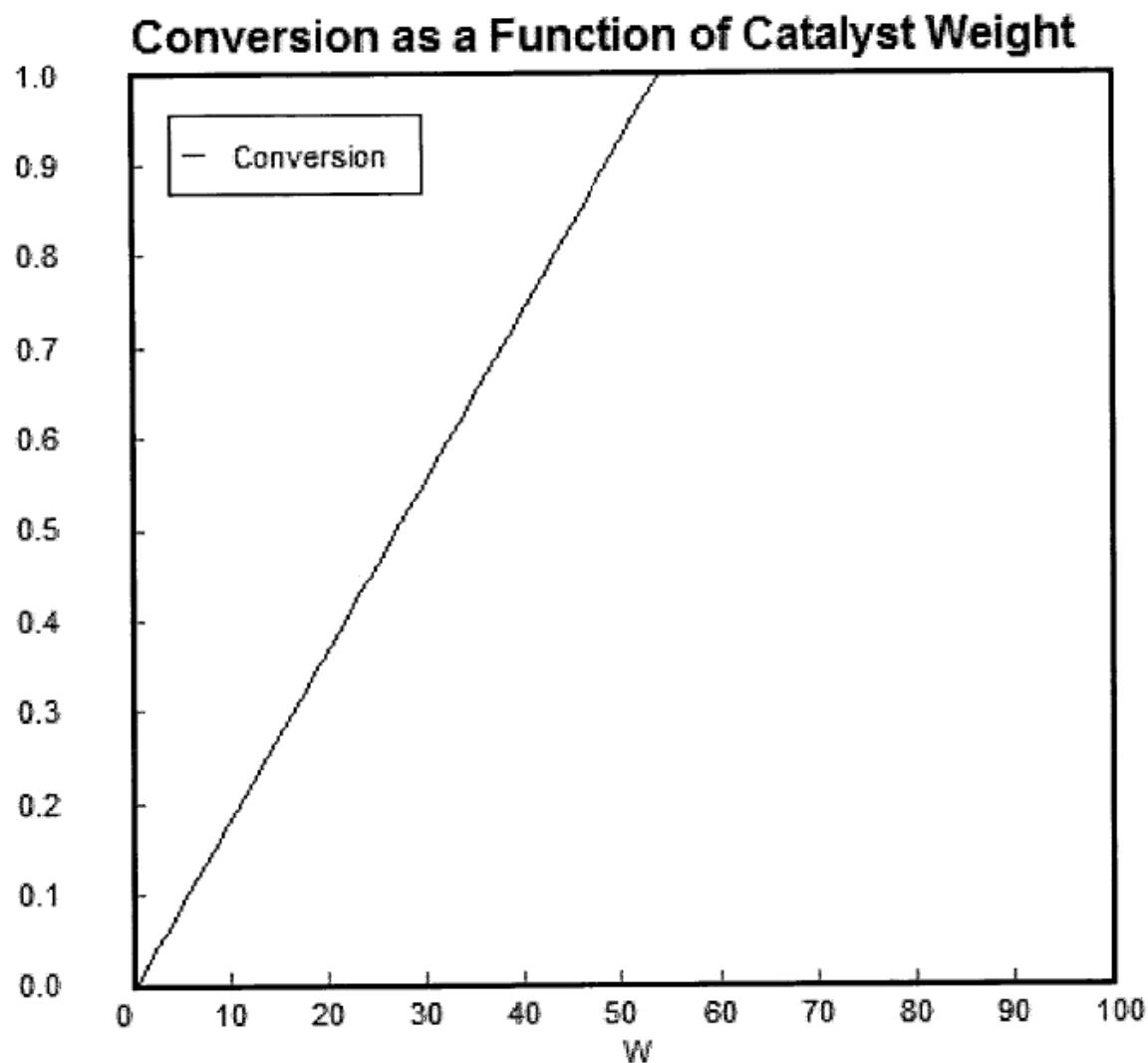
No Title

File: \\storage.adsroot.itcs.umich.edu\home\windat.v2\Desktop\Hydrogenation kinetics.pol

```
d(x) / d(W) = -r*453.6*.1/F/106.42          # The regular expression is -r/F. The additional factors change the units  
                                                # from mols of palladiumto pounds of catalystbased on a 10 wt%  
                                                # catalyst.  
  
r=-k3*Pc/(1+kac*Pc)-k4*Pc*Ph/((1+kac*Pc)^2)-((2*k5*Pc^2*Ph)+(k1*Pc*Ph^2))/((1+kac*Pc)^3)  
k1=12.63/1000  
k3=8.352/1000          # r is the rate expression given by Borodzindki et al. The k values are  
k4=44.38/1000          # divided by 1000 to get the units from mol to kmol.  
k5=567/1000  
kac=63.9          # kac has units of pressure, not of mols, so the conversion factor is  
                   # not needed  
  
Pc=P0*y*(1-x)*0.0065          # Partial pressure in kPa of alkynes based on the mol fraction.  
Ph=P0*y*(1-x)*0.0065*2          # Partial pressure of hydrogen is twice that of alkynes due  
                                # to the 2:1 molar feed ratio.  
  
F=0.00367          # Total molar flowrate in kmol/s  
  
x(0) = 0          # There is no conversion when the catalyst weight is 0.  
  
T=45+273          # The reaction temperature is 45C.  
  
P0=2533          # The initial pressure is 25 atm, but the calculation is done  
                   # in kPa.  
  
y=(1-alpha*W)^0.5          # y accounts for the pressure drop in the reactor.  
alpha=0.00379          # alpha is based on particle diameter and the cross sectional area  
                   # of the reactor.  
  
W(0) = 0          # We evaluate the conversion from 0 to 100 lbs of catalyst to find  
W(f) =100          # the weight for a 90% conversion.
```

G.3 Polymath Conversion Graph

Polymath constructed a graph of conversion as a function of catalyst weight. By finding where the conversion reaches 0.9, the weight is determined. The required weight is 48 pounds.



G.4 Hydrogenator Length Calculation

The following work calculates the length of the hydrogenator, given the diameter.

For this reactor, we chose a 2ft diameter. The bulk density of the catalyst is $0.6 \frac{\text{lb}}{\text{mL}}$ or $37.46 \frac{\text{lb}}{\text{ft}^3}$ according to the manufacturer. To obtain the desired 90% conversion, 48 lbs of catalyst are needed. With this information, the length of the reactor can be determined.

$$l = \frac{V}{A}$$

$$V = \frac{W}{P} = \frac{48 \text{ lb}}{37.46 \frac{\text{lb}}{\text{ft}^3}} = 1.28 \text{ ft}^3$$

$$A = \pi \left(\frac{d}{2}\right)^2 = \pi (1)^2 = 3.14 \text{ ft}^2$$

$$l = 0.407 \text{ ft} = 5 \text{ in.}$$

D.5 Heat Effects in the Hydrogenator

The following calculation proves that the hydrogenator can be considered isothermal.

$$T_{out} = \frac{X[-\Delta H_{rxn}^{\circ} + \sum \Theta_i C_p i T_o + X \Delta C_p T_a]}{\sum \Theta_i C_p i + X \Delta C_p}$$

This equation gives the outlet temperature of a reactor based on the heat of reaction and heat capacities of the nonreacting species. While the hydrogenation reaction is strongly exothermic, we propose that the reactor remains isothermal due to the small amount of material participating in the reaction. With this assumption, $\Delta C_p = 0$. The equation becomes:

$$T_{out} = \frac{X[\Delta H_{rxn}^{\circ} + \sum \Theta_i C_p i T_o]}{\sum \Theta_i C_p i}$$

If we can show that the heat capacity term dominates the numerator, then $T_{out} = T_o$ and the reactor is isothermal.

$$-\Delta H_{rxn}^{\circ} = H_f^{\circ}(\text{reactants}) - H_f^{\circ}(\text{products})$$

$$H_f^{\circ}(C_2H_2) = 8541 \frac{kJ}{kg}$$

$$H_f^{\circ}(H_2) = 0 \frac{kJ}{kg}$$

$$H_f^{\circ}(C_3H_8) = 1345 \frac{kJ}{kg}$$

$$-\Delta H_{rxn}^{\circ} = 7196 \frac{kJ}{kg}$$

The nonreacting species are ethane and propane.

$$\Theta_{ethane} = \frac{1327 \frac{lb}{min}}{17 \frac{lb}{min} \text{ reacting}} = 78$$

$$C_p_{ethane} = 1.8 \frac{kJ}{kg K}$$

$$\Theta_{propane} = \frac{916 \frac{lb}{min}}{17 \frac{lb}{min} \text{ reacting}} = 54$$

$$C_p_{propane} = 1.7 \frac{kJ}{kg K}$$

$$T_o = 318 K$$

$$\sum \Theta_i C_p i T_o = 73840 \frac{kJ}{kg}$$

$\sum \Theta_i C_p i T_o \gg -\Delta H_{rxn}^{\circ}$ so $T_{out} = T_o$. Reactor is isothermal.

G-6 Catalyst Cost

The hydrogenator catalyst is 10 wt% Palladium on alumina. The cost was estimated as follows:

$$\text{Palladium: } 0.1 * 48 \text{ lb} * \frac{\$1571}{100 \text{ g Pd}} * \frac{453.59 \text{ g}}{\text{lb}} = \$34,204$$

$$\text{Alumina: } 0.9 * 48 \text{ lb} * \frac{\$159}{\text{lb}} = \$6,859$$

$$\text{Total cost} = \text{Palladium} + \text{Alumina} = \$41,063$$

Appendix H: Steam Cracker and Furnace Design

H.1 Coil Design

H.2 Furnace Design Considerations

H.3 Furnace Energy Balance

H.1 Coil Design

There are two criteria that must be satisfied when designing the cracker coils.

1. The coils need to have a residence time of 0.45s to ensure maximum ethylene selectivity
2. The coils need to have a surface area that will accommodate the correct amount of radiation flux.

In order to meet the first criterion, the plug flow reactor design equation can be applied:

$$V_{coil} = \dot{V}_{feed} \tau = \frac{\dot{m}_{feed} \tau}{\bar{\rho}}$$

where:

$$\begin{aligned} V_{coil} &= \text{Coil volume (ft}^3\text{)} \\ \dot{V}_{feed} &= \text{Feed volumetric flow rate (ft}^3/\text{s)} \\ \tau &= \text{Residence time} = 0.45\text{s} \\ \dot{m}_{feed} &= \text{Feed mass flow rate} = 48.0 \text{ lb/s} \\ \bar{\rho} &= \text{Average coil fluid density} = 0.07 \text{ lb/ft}^3 \end{aligned}$$

Therefore, the total coil volume between the four fireboxes must be $309 \text{ ft}^3 = 8.75 \text{ m}^3$.

For simplicity, the coils will be modeled as carbon steel cylindrical pipes that wind through the fireboxes. Zimmermann suggests that a typical firebox will be able to irradiate the coils with a flux between $50\text{-}90 \text{ kW/m}^2$ surface area. Typical cracker coils range from 25-180 mm in diameter. [9]

Ultimately, a coil diameter of 2 inches (0.051 m) was chosen because this diameter was small enough to yield sufficient surface area-to-volume ratio to allow for sufficient radiation flux; however, the diameter was large enough that the required length of coil to achieve the necessary 8.75 m^3 in volume was reasonable.

Once the diameter was set at 2-inches, the total coil length could simply be determined based on the known coil volume, given the cylinder volume formula.

$$V_{coil} = \pi \left(\frac{D}{2}\right)^2 l_{coil} \rightarrow l_{coil} = \frac{V_{coil}}{\pi \left(\frac{D}{2}\right)^2} = 4297 \text{ m}$$

The surface area can then be calculated as:

$$A_{coil} = \pi D l_{coil} = 686 \text{ m}^2$$

According to Aspen, the power required to heat the reactants and provide the heat of reaction is $54,840 \text{ kW}$. The necessary flux for a 2-inch pipe would therefore be $\frac{54,840 \text{ kW}}{686 \text{ m}^2} =$

80.0 kW/m^2 . This flux is within the typical flux for a cracker, so this coil design is feasible. Each of the four fireboxes would therefore contain a total of 1074 m of 2-inch coil.

H.2 Furnace Design Considerations

This section will address some of the design details of the furnace.

Coil Shape

Albright reports that typical firebox dimensions are on the order of 10 m × 10 m base, and 10 m in height [17]. The main line of steam-hydrocarbon mixture splits into multiple coils upon entering the top of the firebox. A common coil shape is a U-shape that turns around at the bottom of the firebox and leaves back out the top, after recombining with the other coils [9]. For a 10m tall firebox, each coil would be 20 m in length. Given that each firebox must accommodate 1074m of coil, there would be 54 coils per firebox.

Coil and Burner Configuration

Recall from before that the required radiation flux into the coils is 80.0 kW/m^2 , which is on the higher end of what is typically achievable in a cracker. In order to be able to achieve the higher flux, there would need to be sufficient spacing between the coils such that there would not be much shadowing.

The suggested firebox base dimensions are 8m by 5m. There could be 5 rows of 11 coils. The rows would be offset so that the inner rows would still have exposure to the burners. A sample of this layout is shown in Figure H-1, below.

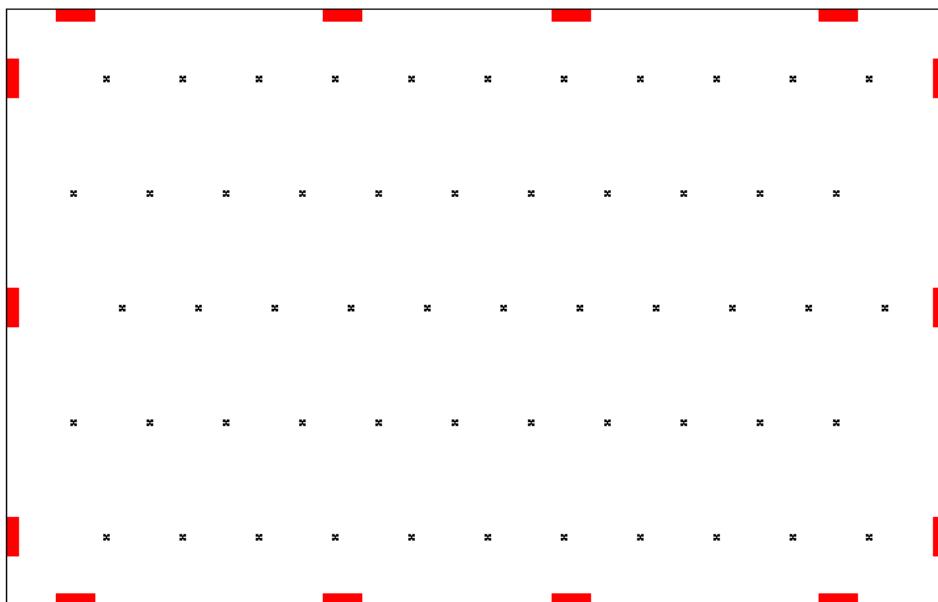


Figure H-1: A proposed staggered layout of U-coils in the firebox. The red indicates a burner. The coils are offset so that the inner coils still have access to the radiation from the burners.

Insulation

Albright recommends the use of ceramic fiber to insulate the firebox. These alumina- and silica-based fibers are able to withstand temperatures in excess of 1000°C. For firebox temperatures near 1000°C, 6-inch thick insulation is recommended. [17]

H.3 Furnace Energy Balance

Thermodynamic modeling in Aspen shows that the net change in enthalpy of all streams exiting the furnace compared to all streams entering the furnace is 7830 MJ/min. Assuming adiabatic operation of the furnace (i.e., good insulation), the duty supplied to the furnace must therefore be 7830 MJ/min. If complete combustion is assumed, the butane/pentane fuel gas will provide the system with the lower heating value of the fuel. The duty provided by the fuel is calculated in Table H-1, below.

Table H-1: A spreadsheet used in determining the necessary flow rate of butane/pentane fuel mix to provide required duty

Fuel flow	378.5	lb/min	
x	m (lb/min)	ΔH_c (MJ/lb)	H (MJ/min)
C4H10	0.7476	282.9651442	20.760
C4H6	0.08413	31.84495192	20.230
C4H8	0.01923	7.278846154	20.450
C5H12	0.14904	56.41105769	20.613
	TOTAL		7830

The value of fuel flow, which was multiplied by known mass fractions (x) to determine flow rates of each fuel, was guessed until the total duty was 7830 MJ/min.

Appendix I: Heat Exchangers

Two different heat exchange methods were used to change stream temperatures. The first was a shell and tube heat exchanger, utilized when it was cost effective or possible to do so. To optimize the plant and minimize costs, heat integration was used between stages as much as possible. If there was no stream that could economically cool the desired stream, the more expensive option, refrigerant cooling, was used.

Shell and Tube Heat Exchanger

Heat exchangers duties and sizes were calculated from equations given in *Fundamentals of Momentum, Heat, and Mass Transfer* [47]. To minimize time spent on sizing heat exchangers, excel spreadsheets were used and an example on E-100 can be seen below.

Table I-1: Sample Excel spreadsheet used to calculate sizing specifications for heat exchangers

Shell/tube lean-water						
Heat Exchanger 102	1-pass		Water Cost (\$/min)		0.22	
$Q=UA*\Delta T_{LM}$						
			Natural Gas			
Ttubein (F)	95	TH2		95	M (lb/min)	4835
Ttubeout (F)	82.4	TH1		82.4	Cp (btu/lb*f)	0.24
Tshellin (F)	33.8	TC2		33.8	Q (Btu/min)	14620
Tshellout (F)	58	TC1		58	Water	
ΔT_{LM}	17.8				M (lb/min)	644
U (btu/min*ft^2 F)	.025				Cp (btu/lb*f)	1
A (ft^2)	36195				Q (btu/min)	15584

The temperatures were specified by MichiChem by the MichiSite Data spreadsheet on the temperature of the cooling water. The process stream temperatures were specified by the equipment requirements. Sample calculations from the spreadsheet are shown below. U is the overall heat transfer coefficient for various fluid combinations and a listing of coefficients for various conditions can be found in Welty [47].

$$\Delta T_{LM} = \frac{\Delta T_2 - \Delta T_1}{\ln \left(\frac{\Delta T_2}{\Delta T_1} \right)}$$

Q is calculated by:

$$Q_{hot} = C_{p_{hot}} * m_{hot} * (T_{in} - T_{out})$$

The mass flow rate of the cooling stream is found by the following equation:

$$Q_{water} = Q_{hot} = C_{p_{water}} * m_{water} * (T_{wout} - T_{win})$$

$$m_{water} = \frac{Q_{amine}}{C_{p_{water}} * (T_{wout} - T_{win})}$$

The heat exchanger was sized by the following equation solved for area, including a 10% safety factor to ensure optimal performance.

$$Q_{hot} = U * \frac{A}{1.10} * \Delta T_{LM}$$

The table below highlights the total area for the heat exchangers, as well as the type and material chosen.

Table I-2: Full list of Heat Exchangers used in plant process

Equipment #	Equipment	Specification
E-100	Heat Exchanger	Shell/tube Material CS Area 3698.9 m^2
E-101	Heat Exchanger	Shell/tube Material CS/SS Area 113.4 m^2
E-102	Heat Exchanger	Shell/tube Material CS/SS Area 251.0 m^2
E-103	Heat Exchanger	Shell/tube Material CS/SS Area 86.7 m^2
E-104	Heat Exchanger	Shell/tube Material Steel Area 1075 3.7 m^2
E-200	Heat Exchanger	Shell/tube Material CS Area 8.9 m^2
E-201	Heat Exchanger	Shell/tube Material CS Area 59.0 m^2
CWHEX-200	Heat Exchanger	Area 8536.1 m^2 Material CS

Equipment #	Equipment	Specification		
CWHEX-201	Heat Exchanger	Area	4668.6	m^2
		Material	CS	
CHWEX-202	Heat Exchanger	Area	6921.7	m^2
		Material	CS	
CHWEX-203	Heat Exchanger	Area	3137.3	m^2
		Material	CS	
CHWEX-204	Heat Exchanger	Area	7843.3	m^2
		Material	CS	
E-300	Heat Exchanger	Shell/Tube		
		Area	196.9	m^2
		Material	SS	
E-301	Heat Exchanger	Shell/Tube		
		Area	3748.7	m^2
		Material	SS	
E-302	Heat Exchanger	Shell/Tube		
		Area	1603.7	m^2
		Material	SS	
E-400	Heat Exchanger	Shell/Tube		
		Area	443.1	m^2
		Material	SS	
E-401	Heat Exchanger	Shell/Tube		
		Area	11469.2	m^2
		Material	SS	
E-500	Transfer line h-ex	Shell/tube		
		Area	6.6	m^2
		Material	CS	

Appendix J: Compressors, Fans, Blowers, and Pumps

J.1 Compressors

J.2 Blowers and Fans

J.2 Pumps

J.1 Compressors

A centrifugal compressor achieves compression by applying inertial forces to the gas using rotating impellers. As shown in Figure J-1, when gases enter the impeller, it is forced through the rotating impeller blade in the diffuser where it experiences a decrease in velocity and increase in pressure. The increase in pressure will depend on the diameter and rotation speed of the impeller. In addition, the maximum pressure increase possible per impeller is ultimately limited by material the impeller is made out of. [48] Each impeller is able to perform a 100 to 130 psi increase. [49] Since gases get hot when compressed, multiple stages of impellers in series will require interstage cooling, as shown in Figure J-1. Whenever interstage cooling is used, one must also be sure that the gases inside the compressor do not condense else costly damage can occur.

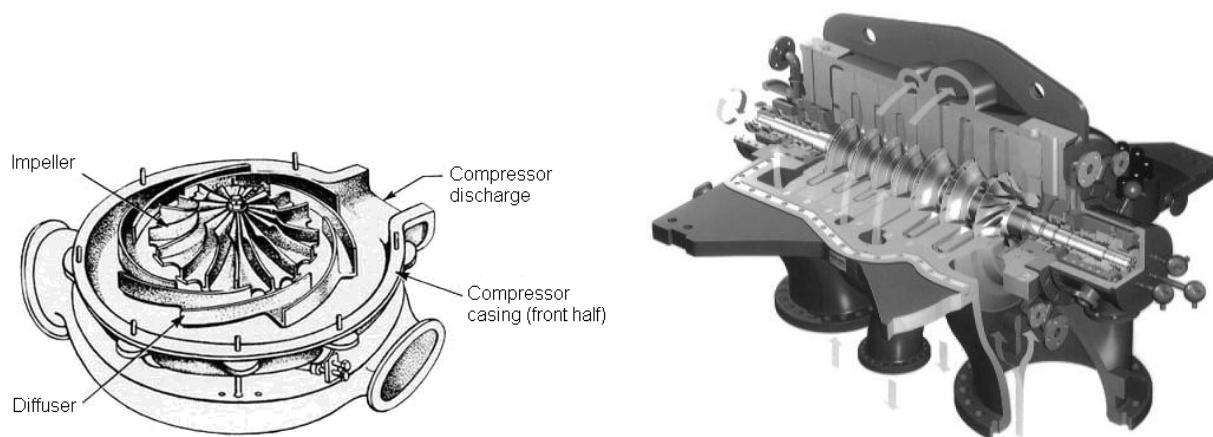


Figure J-1: Representative images for a centrifugal compressor (left) and a multistage centrifugal compressor with interstage cooling (right). Arrows in the image on the right represent paths of cooling fluid within the compressor block. [48]

The capital and operating costs of these compressors are very high in industry, and so it is important to correctly size a compressor to increase pressure the desired amount while not using extra energy. To size the compressors, equations from Plant Design and Economics for Chemical Engineers by Peters and Timmerhaus were used [50]. Most compressor calculations are based on polytrophic paths that approach adiabatic, with the equation of state $p v^k$ being constant. Due to the large flow rates of the MichiChem process, multi-stage compressors were used with the equations for the adiabatic head, the adiabatic power, and discharge temperature. The table below shows sample calculations of C-100 in stage 1A for the cooling water rate necessary, and the power required from the following parameters; entering temperature, exiting temperature, k, entering and exiting pressure, the number of stages, and overall mass flow through the system.

Table J-1: Multi-stage compressor calculations, example spreadsheet

Description	Variables	Units	Values	Compressor Cooling Rate
Gas constant	R'	kJ/(kg*k)	0.345	KJ/s 6908.191
Entering T	T1	K	298.000	BTU/s 6547.701
Specific Heat	Cp	kJ/kg C	1.934	BTU/min 392862.077
	Cv	kJ/kg C	1.531	
Cp/Cv	K	none	1.263	
Discharge P	P2	kPa	3799.680	Cooling Water Flow Rate
Entering P	P1	kPa	690.000	lb/min 9821.551926
# of stages	N	integer	9.000	
Mass flow	M	kg/sec	36.536	
Adiabatic Head	Had	N*m/kg	75.042	Raw Gas Volumetric Flow Rate
Power required	Pad	KW	2741.765	M^3/sec 5.283
Exit T	T2	K	309.993	M^3/hr 19019.360

The power necessary for the compressor to run is calculated by the following equation [50]:

$$P_{ad} = M * N * \frac{K}{K - 1} * T_1 * 2.78 * 10^{-4} * \left(\left(\frac{P_2}{P_1} \right)^{\frac{K-1}{K}*N} - 1 \right)$$

The equation for power is assuming equal division of compression work between the stages and intercooling of the gas after each stage back to the original inlet temperature. It also assumes the overall system of the compressor and cooling water is adiabatic. All of the variables above are constants that have been specified from literature or MichiChem's process requirements. The Volumetric flow rate can be calculated by calculating the density of gas in Aspen using Peng-Robinson.

$$T_2 = T_1 * \frac{P_2^{\frac{k-1}{k*Nst}}}{P_1}$$

T_2 , calculated above, is the temperature that is theoretically reached at the end of each stage if there were no cooling. Therefore, the inter-stage cooling requirement is calculated the same way a heat exchanger cooling water flow rate is calculated:

$$C_p * M * (T_2 - T_1) = Q * N = M_{water} * C_{p,water} * (T_{2,water} - T_{1,water}) * 1.1$$

The only unknown in the equation is M_{water} which can be calculated. The safety factor of 1.1 allows for 90% efficiency of cooling.

When sizing the compressor, the most important factors are a compressor that can operate at the desired exit pressure, and one large enough to handle the required volumetric flow rate. The table

of compressors below were sized by the equations above, and then costed by the methods in Appendix R.

Table J-2: A full list of compressors and their specifications

Equipment #	Equipment	Specification		
C-100	Compressor	Material	SS	
		Volumetric Flow	5.3	M^3/s
		Stages	9	
		Outlet Pressure	37.5	atm
		Power	2740	kWhr/hr
C-101	Compressor	Material	1075	CS
		Volumetric Flow	1.5	m^3/s
		Stages	3	
		Outlet Pressure	15	atm
		Power	1980	kWhr/hr
C-200	Compressor	Material	CS	
		Volumetric Flow	21	m^3/s
		Stages	2	
		Outlet Pressure	12.5	atm
		Power	8333	kWhr/hr
C-201	Compressor	Material	SS	
		Volumetric Flow	22649.6	ft^3/hr
		Stages	5	
		Outlet Pressure	30	atm
		Power	152206	kWhr/hr
C-300	Compressor	Material	SS	
		Volumetric Flow	11347	ft^3/hr
		Stages	1	
		Outlet Pressure	10	atm
		Power	567	kWhr/hr
C-301	Compressor	Material	SS	
		Volumetric Flow	8667	ft^3/hr
		Stages	1	
		Outlet Pressure	6.2	atm
		Power	1.63	kWhr/hr
C-302	Compressor	Material	SS	
		Volumetric Flow	2133	ft^3/hr
		Stages	1	
		Outlet Pressure	6.4	atm
		Power	113.5	kWhr/hr
C-303	Compressor	Material	SS	
		Volumetric Flow	31	ft^3/hr
		Stages	1	
		Outlet Pressure	5.9	atm
		Power	454	kWhr/hr

Equipment #	Equipment	Specification	
C-500	Compressor	Material	CS
		Volumetric Flow	0.4 m^3/s
		Stages	1
		Outlet Pressure	25 atm
		Power	574 kWhr/hr

J.2 Blowers and Fans

Blowers and fans are sized the same way for equipment costing. Blowers were used when there was larger than $\frac{1}{2}$ atmosphere increase in pressure up to 3 atmosphere's increase in pressure. Fans were up to a $\frac{1}{2}$ atmosphere pressure increase.

Both Blowers and fans are sized according to the blower inlet's volumetric flow rate, and its power is calculated by the equation below, where Q is the volumetric flow rate and ΔP is the change in pressure. The efficiency of both blowers and fans were considered to be 70% efficient.

$$Power = Q * \Delta P * .7$$

Material selections were considered by the individual streams needs. A full list of all blowers and fans for the plant can be seen below.

Table J-3: A full list of fans and blowers and their specifications

Equipment #	Equipment	Specification	
B-100	Blower	Material	CS
		Volumetric Flow	17.35 ft^3/min
		DP	2 atm
		Power	2.7 kWhr/hr
F-100	Fan	Material	1075 CS
		Volumetric Flow	54.9 m^3/min
		DP	0.5 atm
		Power	0.85 kWhr/hr
F-500	Fan	Material	CS
		Volumetric Flow	73 m^3/s
		DP	1 atm
		Power	10108 kWhr/hr

J.3 Pumps

Pumps were sized based on the volumetric flow rate inlet of the pump. The power estimation for each pump was found by the same estimation as for blowers and fans, and is shown below. Pumps were also assumed to be running 70% efficient.

$$Power = Q * \Delta P * .7$$

The table below gives the specifications for the pumps used in this process.

Table J-4: A full list of pumps and their specifications

Equipment #	Equipment	Specification	
P-100	Pump	Material Volumetric Flow Outlet Pressure Power	CS 0.523 M^3/min 37.5 atm 33.11997549 kWhr/hr
P-200	Pump	Material dP Volumetric Flow Power	CS 5.5 atm 0.0122 m^3/s 9.30 kWhr/hr
P-300	Pump	Materials Volumetric Flow dP Power	SS 6169.0 ft^3/hr 35.8 atm 1855 kWhr/hr
P-500	Pump	Material dP Volumetric Flow Power	CS 8 atm 0.0050 m^3/s 5.59 kWhr/hr

Appendix K: Piping Information

- K.1 General Method
- K.2 Pressure Drop in Liquids
- K.3 Pressure Drop in Gases
- K.4 Sample Calculation – Sizing and Pressure Drop for Liquid
- K.5 Sample Calculation – Sizing and Pressure Drop for Liquid
- K.6 Master Piping List

K.1 General Method

A general method for pipe sizing and pressure drop calculation is as follows:

1. Determine flows and composition within pipe. Ascertain fluid density and viscosity.
2. Determine the pipe material from the compatibility chart (Table K-1).
3. Determine the pipe length from the plant layout diagram.
4. Consult recommended fluid velocity guidelines (Table K-2) and select the nominal pipe size that yields the appropriate fluid velocity.

$$D_{min} = \sqrt{\frac{4\dot{m}}{\rho v_{max}\pi}}$$

where:

- D_{min} = minimum allowable diameter (ft)
 \dot{m} = mass flow rate (lb/s)
 ρ = fluid density (lb/ft³)
 v_{max} = maximum allowable velocity (ft/s)

5. Check the pressure drop across the pipes.
6. Select pumps and compressors, if necessary.

Pipelines that carried product out of the process or raw material into the process were assumed to be 1000 ft in length and had tolerances for larger pressure drops. Pressure drops larger than 0.5 atm required motive force addition.

Table K-1: Pipe material compatibility [51]

Service	Conditions	Material
Water	All	CS
Mixed hydrocarbons	> -30°C	CS
Amines	All	SS
Hydrogen gas [52]	> -30°C	Cu
Air	All	CS
Cryogenic substance	< -30°C	SS

Table K-2: Suggested line velocities [53]

Fluid	Line velocity (ft/s)
Air	67
Ethylene	100
Hydrogen	67
Natural gas	100
Hydrocarbon liquid	6
Steam	67
Water	5

K.2 Pressure Drop in Liquids

To calculate the pressure drop for liquids, first calculate the Reynolds number $Re = \frac{\rho v D}{\mu}$. Use the Moody's chart in Figure K-1 to find the friction factor f . Stainless and carbon steel piping have a roughness on the order of 10^{-5} .

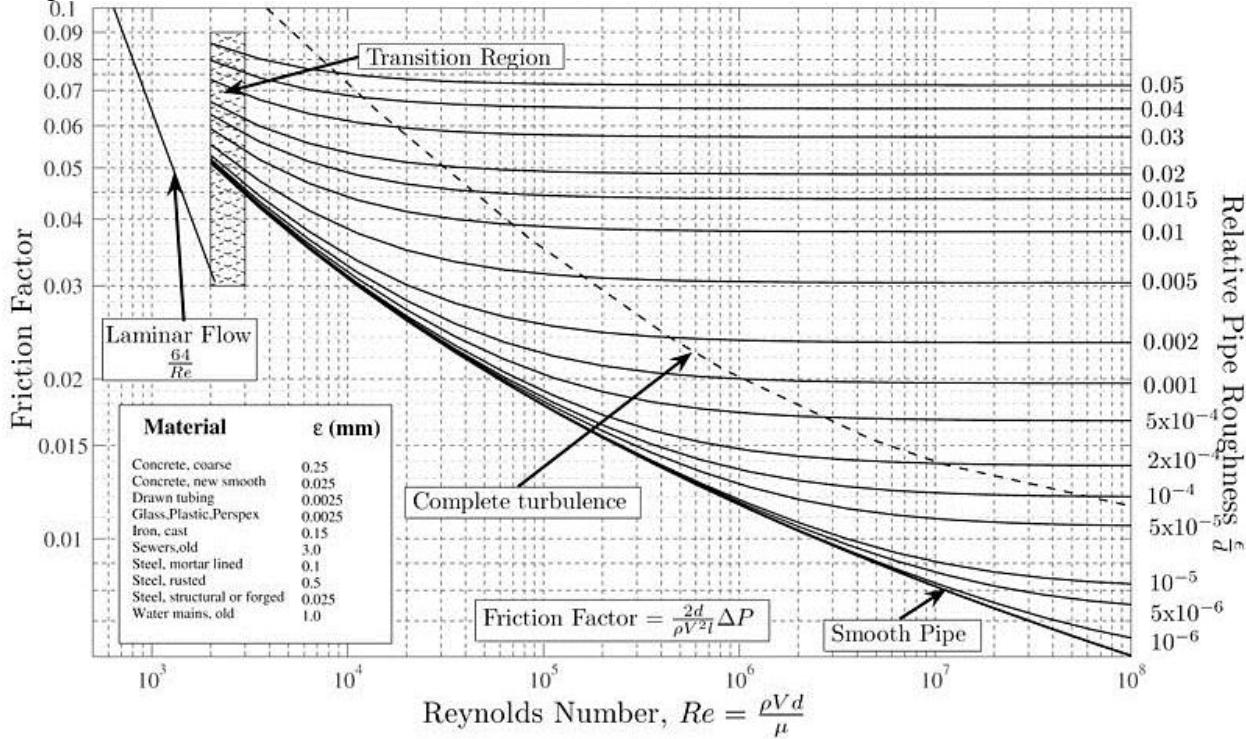


Figure K-1: Moody's Chart [54]

The pressure drop can then be calculated using the following equation:

$$\Delta p = 4f\rho \frac{\Delta L}{D} \frac{v^2}{2}$$

where:

- Δp = pressure drop (Pa)
- f = friction factor (dimensionless)
- ρ = fluid density (kg/m^3)
- ΔL = length of the pipe (m)
- D = diameter of pipe (m)
- v = average velocity in the pipe (m/s)

For liquids, pumps will provide the motive force. There are different types of pumps such as centrifugal, piston, gear, and much more.

K.3 Pressure Drop in Gases

For pressure drop, the following equation can be used only if the pressure changes no more than 10%.

$$p_1^2 - p_2^2 = \frac{4f\Delta LG^2 RT}{DM}$$

where:

- p_1 = initial pressure (Pa)
- p_2 = final pressure (Pa)
- f = friction factor (dimensionless)
- ρ = density (kg/m^3)
- ΔL = length of the pipe (m)
- G = flow ($\text{kg}/\text{s}/\text{m}^2$)
- R = gas constant (J/mol-K)
- T = temperature (K)
- D = diameter of pipe (m)
- M = molecular weight (kg/mol)

The pressure drop may be found by rearranging:

$$\Delta p = p_1 - p_2 = p_1 - \sqrt{p_1^2 - \frac{4f\Delta LG^2 RT}{DM}}$$

For gases, a few options are available to provide the motive force, as summarized below.

Table K-2: Options for providing motive force for gases.

Type	Optimal Use
Fans	Low delivery pressure ($\Delta p < 3\text{psi}$)
Blowers	Moderate pressure ($3\text{psi} < \Delta p < 30\text{psi}$)
Compressors	High pressures ($\Delta p > 30\text{psi}$)

K.4 Sample Calculation – Sizing and Pressure Drop for Liquid

Below is a worked out example for the pipe sizing and pressure drop calculation for Stream 201, wastewater. Steps are numbered as described in the procedure in Section K.1.

1. Flow = 10.7 lb/s water
 $\mu = 4 \text{ lb}/\text{ft}\cdot\text{h}$
 $\rho = 62.3 \text{ lb}/\text{ft}^3$ (fluid properties from Aspen, Peng-Robinson method)
2. For water, use carbon steel; roughness = 5×10^{-5}
3. Length = 1000 ft (leaving process)
4. $v_{max, water} = 5 \text{ ft/s}$

$$D_{min} = \sqrt{\frac{4(10.7 \frac{lb}{s})}{62.3 \frac{lb}{ft^3} \left(5 \frac{ft}{s}\right) \pi}} = 0.209 \text{ ft} = 2.51 \text{ in} \rightarrow 4 \text{ in nominal size}$$

This corresponds to a velocity of $v = \frac{\dot{m}}{\rho \pi (\frac{D}{2})^2} = 1.97 \frac{ft}{s}$

$$5. \quad Re = \frac{\rho v D}{\mu} = 3.69 \times 10^4$$

$$f = 0.022$$

$$\Delta p = 4f\rho \frac{\Delta L v^2}{2D} = 32100 \frac{lb}{ft^2} = 0.47 \text{ atm}$$

6. Since this is a wastewater stream that already has sufficient pressure, this is an acceptable pressure drop.

K.5 Sample Calculation – Sizing and Pressure Drop for Gas

Below is a worked out example for the pipe sizing and pressure drop calculation for Stream 203, PS-200 vapor product.

1. Flow = 111 lb/s mixed hydrocarbon

$$\mu = 0.024 \text{ lb/ft-h}$$

$\rho = 0.82 \text{ lb/ft}^3$ (fluid properties from Aspen, Peng-Robinson method)

2. For water, use carbon steel; roughness = 5×10^{-5}

3. Length = 30 ft

4. $v_{max, HC} = 100 \text{ ft/s}$

$$D_{min} = \sqrt{\frac{4(111 \frac{lb}{s})}{0.82 \frac{lb}{ft^3} \left(100 \frac{ft}{s}\right) \pi}} = 1.31 \text{ ft} = 15.8 \text{ in} \rightarrow 18 \text{ in nominal size}$$

This corresponds to a velocity of $v = \frac{\dot{m}}{\rho \pi (\frac{D}{2})^2} = 76.8 \frac{ft}{s}$

$$5. \quad Re = \frac{\rho v D}{\mu} = 1.42 \times 10^4$$

$$f = 0.014$$

$$\Delta p = p_1 - p_2 = p_1 - \sqrt{p_1^2 - \frac{4f \Delta L G^2 R T}{D M}} = 0.035 \text{ atm}$$

6. This is a negligible pressure drop.

K.6 Master Piping List

The results of this pipe sizing procedure are shown below for all major lines in the plant. Note that there were only significant pressure drops on product streams that had excess pressure head to lose.

Line #	Service	Material	Dia. (in)	Length (ft)	Qty.
100	NG	SS	24	50	1
101	NG	CS	18	100	1
102	DGA/Water	SS	6	30	1
103	NG	SS	1	30	1
104	DGA/Water	SS	6	45	1
105	DGA/Water	CS	6	75	1
106	CO2 H2S	1075 CS	4	45	1
107	Water/DGA	CS	1	20	1
108	CO2 H2S/water	1075 CS	1	45	1
109	CO2 H2S	1075 CS	4	30	1
110	CO2 H2S	1075 CS	6	45	1
111	CO2 H2S	1075 CS	1	50	1
112	CO2 H2S	1075 CS	4	75	1
113	CO2 H2S	1075 CS	4	55	1
114	NG	SS	24	75	1
115	DGA	CS	1	15	1
116	Water	CS	1	15	1
200	Mixed HC (g)	CS	24	425	1
201	Water	CS	4	1000	1
202	Mixed HC (l)	CS	2	1000	1
203	Mixed HC (g)	CS	18	30	1
204	Mixed HC (l)	CS	2	1000	1
205	Mixed HC (g)	CS	24	140	1
207	Mixed HC (g)	CS	18	30	1
208	CH+N2	SS	17	60	3
209	CH+N2	SS	17	60	3
210	CH+N2	SS	8	60	1
211	CH+N2	SS	15	60	1
212	CH+N2	SS	18	60	2
213	CH+N2	SS	7	60	4
300	CH4,H2,N2	SS	20	50	5
301	C2+	SS	15	50	1
302	H2/N2	SS	17	50	3
303	CH4	SS	19	1000	3
304	H2/N2	Copper	19	20	2
305	H2/N2	Copper	20	20	2
306	H2/N2	Copper	20	20	2
307	N2	Copper	13	20	1

Line #	Service	Material	Dia. (in)	Length (ft)	Qty.
308	H2/N1	Copper	11	20	1
309	H2/N2	Copper	8	20	1
310	H2/N2	Copper	8	20	1
311	H2/N2	Copper	16	20	2
312	H2	Copper	8	1000	1
313	H2/N2	Copper	2	20	1
400	Ethylene	SS	20	1000	1
401	C2+	SS	19	20	5
402	C2-C4	SS	19	20	4
403	C4+	SS	16	20	1
404	C2	SS	16	20	2
405	C3	SS	18	100	2
406	C3	SS	18	1000	1
407	C3	SS	18	100	1
408	C4+	CS	9	1000	1
409	C4+	CS	12	100	1
501	Air	CS	18	30	16
503	Mixed HC (g)	CS	6	100	1
504	Mixed HC (g)	CS	3	30	4
505-liq	Water	CS	4	1000	1
505-gas	Steam	CS	12	45	4
506	Mixed HC (g)	CS	12	10	4
507a	Mixed HC (g)	CS	24	30	4
507b	Mixed HC (g)	CS	20	200	9

Appendix L: Utilities

L.1 Table of Cooling Water Utilities

L.2 Table of Electricity Utilities

L.3 Table of Refrigeration Utilities

L.1 Table of Cooling Water Utilities

Equipment #	Annual Duty	Units	Price	Units	Annual Cost
C-201	14,743,636	Kgal	0.43	\$/Kgal	6,339,763
T-101 (condenser)	2,243,855	Kgal	0.43	\$/Kgal	964,858
E-201	1,991,961	Kgal	0.43	\$/Kgal	856,543
C-200	1,460,000	Kgal	0.43	\$/Kgal	627,800
E-401	310,744	Kgal	0.43	\$/Kgal	133,620
E-300	257,689	Kgal	0.43	\$/Kgal	110,806
T-403 (reboiler)	102,464	Kgal	0.43	\$/Kgal	44,060
T-401 (reboiler)	79,730	Kgal	0.43	\$/Kgal	34,284
T-102 (reboiler)	57,528	Kgal	0.43	\$/Kgal	24,737
T-402 (reboiler)	51,579	Kgal	0.43	\$/Kgal	22,179
C-300	41,941	Kgal	0.43	\$/Kgal	18,035
C-101	33,913	Kgal	0.43	\$/Kgal	14,583
C-303	33,553	Kgal	0.43	\$/Kgal	14,428
E-400	23,432	Kgal	0.43	\$/Kgal	10,076
E-301	15,178	Kgal	0.43	\$/Kgal	6,527
C-302	8,288	Kgal	0.43	\$/Kgal	3,564
C-301	121	Kgal	0.43	\$/Kgal	52
Cooling Water Total					9,225,913

L.2 Table of Electricity Utilities

Equipment #	Annual Duty	Units	Price	Units	Annual Cost
C-201, EXP-200	1,242,000,821	kWh	0.057	\$/kWh	70,794,047
F-500	82,486,710	kWh	0.057	\$/kWh	4,701,742
C-200	68,000,000	kWh	0.057	\$/kWh	3,876,000
C-100	22,366,560	kWh	0.057	\$/kWh	1,274,894
C-101	16,164,960	kWh	0.057	\$/kWh	921,403
P-300	15,136,345	kWh	0.057	\$/kWh	862,772
C-500	4,684,571	kWh	0.057	\$/kWh	267,021
C-300	4,630,590	kWh	0.057	\$/kWh	263,944
C-303	3,704,472	kWh	0.057	\$/kWh	211,155
C-302	926,118	kWh	0.057	\$/kWh	52,789
P-100	270,259	kWh	0.057	\$/kWh	15,405
P-200	75,676	kWh	0.057	\$/kWh	4,314
P-500	45,648	kWh	0.057	\$/kWh	2,602
B-100	22,032	kWh	0.057	\$/kWh	1,256
C-301	13,313	kWh	0.057	\$/kWh	759
F-100	6,936	kWh	0.057	\$/kWh	395
Power Total					83,250,496

L.3 Table of Refrigeration Utilities

Equipment #	Utility	Annual Duty	Units	Price	Units	Annual Cost
T-102 (condenser)	-50 C	10624.32	GJ	60	\$/GJ	637,459
E-104	-20 C	1370.88	GJ	32	\$/GJ	43,868
E-104	-50 C	3672	GJ	60	\$/GJ	220,320
Refrigeration Total						901,647

Appendix M: Heat Integration

Since our entire cryogenic process is extremely energy-intensive, it is necessary to have good heat integration within the process to lower refrigeration and heating costs. For distillation columns systems, several strategies are practiced in industry to improve its energy performance:

1. Use of the divided-wall distillation column (also called the Petlyuk scheme)
2. Use of side stripper and side rectifiers. This reduces the need for additional full sized distillation columns.
3. Use of thermal couplings, where heat transfer is accomplished by contacting streams between other columns in the system. This is the method we are using in this project.

In general, the Petlyuk has been shown to be the most efficient in terms of heat integration and overall energy performance, followed by the use of side strippers and side rectifiers, then finally the use of thermal couplings. We decided to pick the third option because it is the most intuitive to understand and also used widely in industry.

A general method used in this project for heat integration design is listed below:

1. Determine flow rates and required rate of transfer.
2. Select type of heat exchanger with equipment specifications
3. Evaluate overall heat transfer coefficient and film coefficients (not necessary for this project)
4. Evaluate T profiles throughout the heat exchanger.
5. Determine the required area of the heat exchanger for sizing purposes
6. Analyze results including dimensions, pressure drop, and costing.

The primary aim of heat integration is to use process duties instead of utilities (i.e. steam, cooling water, etc.) to achieve desired cooling/heating. The following rules of thumb for heat integration were followed:

- Avoid large temperature differences across heat exchangers (< 100°C). Strategies include using a multiple-stage heat exchangers or pumparounds.
- Feed can be preheated with hot products.
- Condensers and reboiler of adjacent columns can be integrated.
- Use of insulation will eliminate external effects such as sunlight during the day and rainstorms.

There are currently two heat integration synthesis methodologies used to identify the best use of all hot and cold process streams: Pinch analysis (Linnhoff) and Mixed-Integer Non-Linear Programming (MINLP). Pinch analysis, also known as the Linnhoff method, uses heuristics, or shortcuts, to heat integrate processes. It gives valuable insight using the concept of pinch. We used the Linnhoff pinch analysis method to pair up appropriate streams. The final pairings for heat integration can be seen in our PFDs in Appendix N.

Appendix N: Process Flow Diagrams

N.1 Stage 1

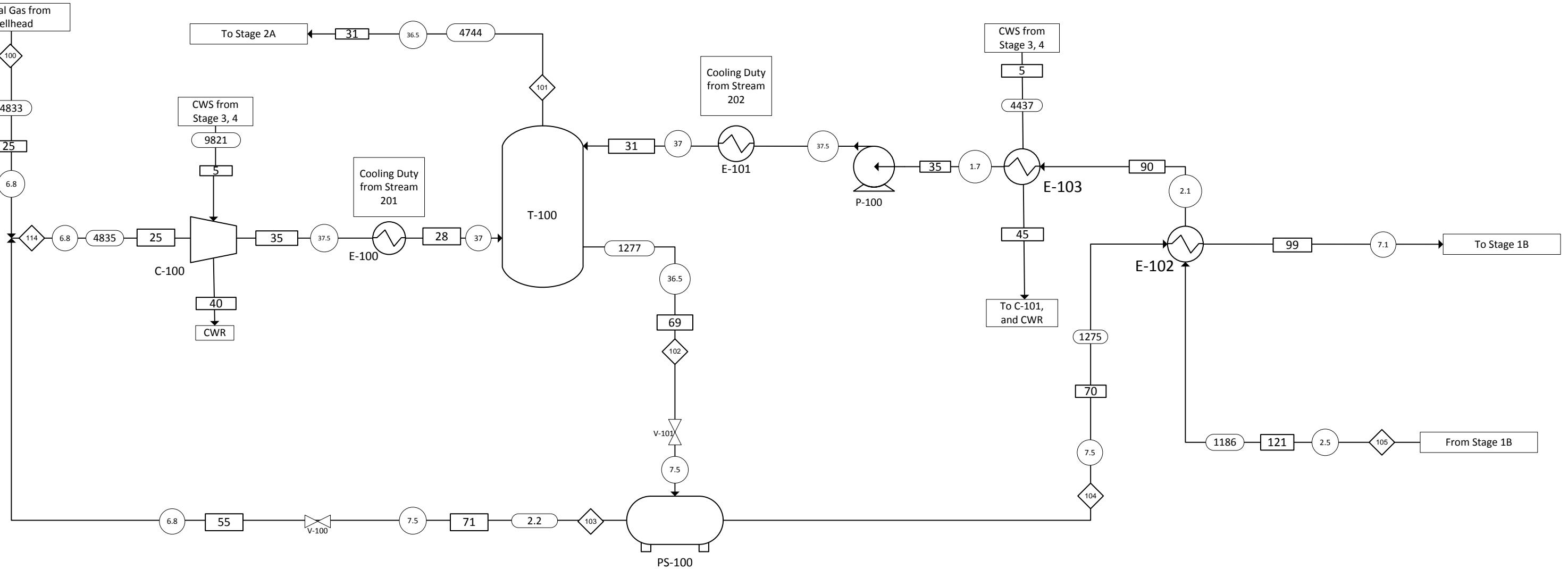
N.2 Stage 2a

N.3 Stage 2b

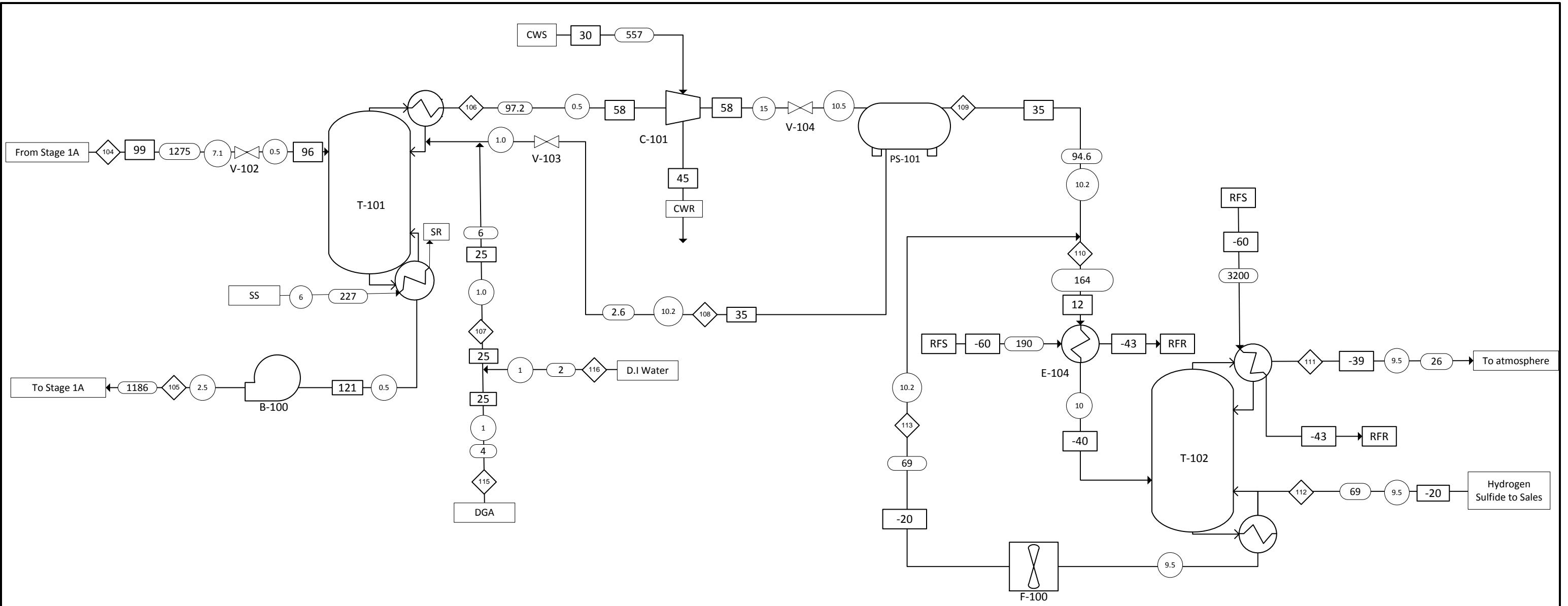
N.4 Stage 3

N.5 Stage 4

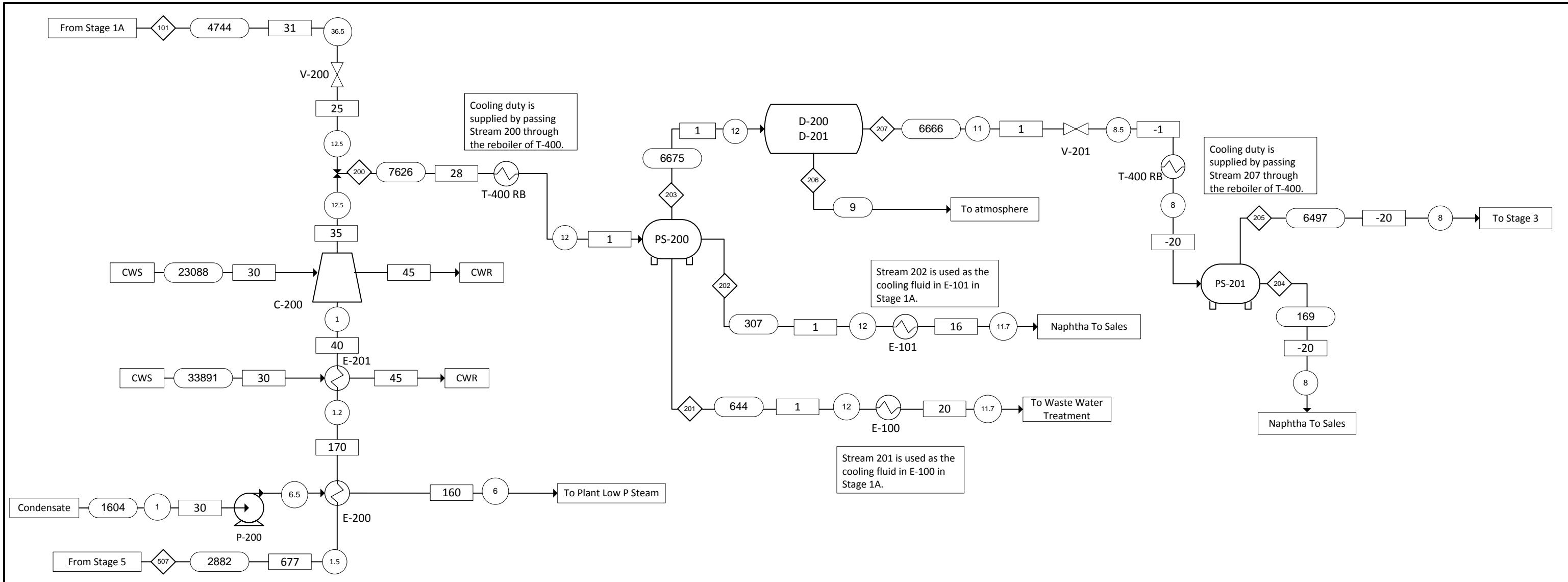
N.6 Stage 5



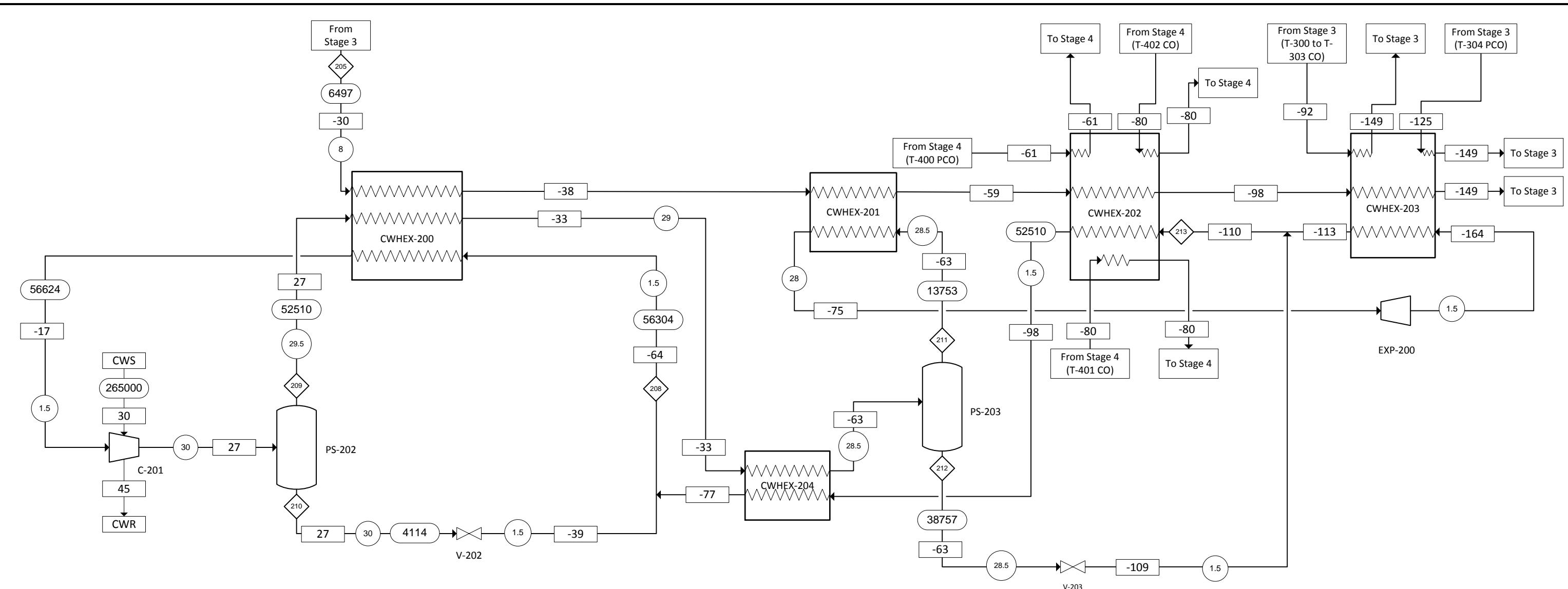
STREAM IDENTIFICATION NO.	100	101	102	103	104	105	106	107	108	109	110	111	112	113	114	115	116			NOTES: CWS = Cooling Water Supply CWR = Cooling Water Return RFS = Refrigerant Supply DGA = 60% DGA, 40% Water	TOWER		
STREAM DESCRIPTION																		PHASE SEPARATOR					
TOTAL MASS FLOW RATE (LB/MIN)	4833	4744	1277	2.2	1275	1186	97.2	6	2.6	94.6	164	26	69	69	4835	4	2						
COMPONENTS	FORMULA	Wt %	Wt %	Wt %	Wt %	Wt %	Wt %	Wt %	Wt %	Wt %	Wt %	Wt %	Wt %	Wt %	Wt %	Wt %	Wt %						
Methane	CH ₄	44.3	45.2	0.1	44.6	0	0	0	0	0	0	0	0	0	44.3	0	0				LEGEND		
Ethane	C ₂ H ₆	17.5	17.8	Trace	17.7	0	0	0	0	0	0	0	0	0	17.5	0	0				REVISIONS		
Propane	C ₃ H ₈	16.0	16.3	Trace	16.2	0	0	0	0	0	0	0	0	0	16.0	0	0						
Iso-Butane	C ₄ H ₁₀	2.2	2.3	Trace	2.2	0	0	0	0	0	0	0	0	0	2.2	0	0						
N-Butane	C ₄ H ₁₀	7.0	7.2	Trace	7.2	0	0	0	0	0	0	0	0	0	7.0	0	0						
Iso-Pentane	C ₅ H ₁₂	1.6	1.6	Trace	1.6	0	0	0	0	0	0	0	0	0	1.6	0	0						
N-Pentane	C ₅ H ₁₂	2.4	2.4	Trace	2.4	0	0	0	0	0	0	0	0	0	2.4	0	0						
Hexanes	C ₆ H ₁₄	1.3	1.4	Trace	1.4	0	0	0	0	0	0	0	0	0	1.3	0	0						
Heptanes plus	C ₇ +	1.3	1.3	Trace	1.3	0	0	0	0	0	0	0	0	0	1.3	0	0						
Nitrogen	N ₂	4.4	4.4	Trace	Trace	0	0	0	0	0	0	0	0	0	4.4	0	0						
Hydrogen Sulfide	H ₂ S	0.8	0	3.1	0	3.1	0	57.3	0	0.7	59	67.7	Trace	80	80	.8	0	0					
Carbon Dioxide	CO ₂	1.1	0	6.4	0	6.4	2.2	40	0	7.8	41	30	100	20	20	1.1	0	0					
Water	H ₂ O	0	0.1	36.1	5.4	36.2	39.3	0	100	91.4	0	2.6	0	0	0	40	100						
DGA	C ₄ H ₁₁ NO ₂	0	trace	54.3	0	54.4	58.5	2.6	0	0	0	0	0	0	0	60	0						

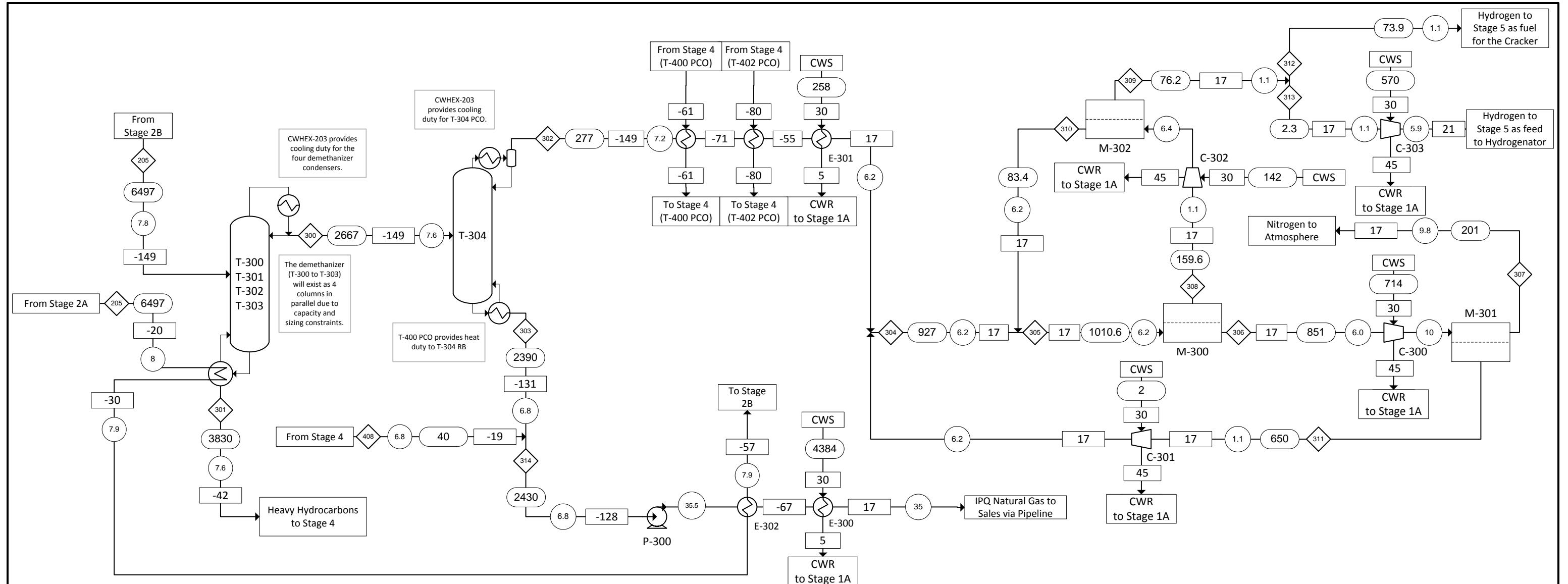


STREAM IDENTIFICATION NO.	100	101	102	103	104	105	106	107	108	109	110	111	112	113	114	115	116			NOTES: CWS = Cooling Water Supply CWR = Cooling Water Return RFS = Refrigerant Supply (Freon) RFR = Refrigerant Return DGA = 60% DGA, 40% Water SR= Steam Return SS=Steam Supply	T = Tower D = Flash Tank PS = Phase Separator B = Blower SS=Steam Supply		
STREAM DESCRIPTION																							
TOTAL MASS FLOW RATE (LB/MIN)	4833	4744	1277	2.2	1275	1186	97.2	6	2.6	94.6	164	26	69	69	4835	4	2						
COMPONENTS	FORMULA	Wt %	Wt %	Wt %	Wt %	Wt %	Wt %	Wt %	Wt %	Wt %	Wt %	Wt %	Wt %	Wt %	Wt %	Wt %	Wt %						
Methane	CH ₄	44.3	45.2	0.1	44.5	0	0	0	0	0	0	0	0	0	44.3	0	0	LEGEND					
Ethane	C ₂ H ₆	17.5	17.8	Trace	17.7	0	0	0	0	0	0	0	0	0	17.5	0	0	REVISIONS					
Propane	C ₃ H ₈	16.0	16.3	Trace	16.2	0	0	0	0	0	0	0	0	0	16.0	0	0	REV	DATE	DESCRIPTION			
Iso-Butane	C ₄ H ₁₀	2.2	2.3	Trace	2.2	0	0	0	0	0	0	0	0	0	2.2	0	0	1	3/10/2013	INITIAL DESIGN			
N-Butane	C ₄ H ₁₀	7.0	7.2	Trace	7.1	0	0	0	0	0	0	0	0	0	7.0	0	0	2	3/14/2013	Added recycle stream, phase separator			
Iso-Pentane	C ₅ H ₁₂	1.6	1.6	Trace	1.6	0	0	0	0	0	0	0	0	0	1.6	0	0	3	4/5/2013	Added cooling water from heat integration			
N-Pentane	C ₅ H ₁₂	2.4	2.4	Trace	2.4	0	0	0	0	0	0	0	0	0	2.4	0	0						
Hexanes	C ₆ H ₁₄	1.3	1.4	Trace	1.3	0	0	0	0	0	0	0	0	0	1.3	0	0						
Heptanes plus	C ₇ +	1.3	1.3	Trace	1.3	0	0	0	0	0	0	0	0	0	1.3	0	0						
Nitrogen	N ₂	4.4	4.4	Trace	0	0	0	0	0	0	0	0	0	0	4.4	0	0	University of Michigan DEPARTMENT OF CHEMICAL ENGINEERING					
Hydrogen Sulfide	H ₂ S	0.8	0	3.1	0	3.1	0	57.3	0	0.7	59	67.7	Trace	80	80	.8	0	0	COURSE NO. ChE 487	DRAWN BY MWM	DATE 4/3/2013		
Carbon Dioxide	CO ₂	1.1	0	6.4	0	6.4	2.2	40	0	7.8	41	30.0	100	20	20	1.1	0	0	GROUP NO. 5	PROCESS FLOW DIAGRAM (PFD)			
Water	H ₂ O	0	0.1	36.1	5.4	36.2	39.3	2.6	60	91.4	0	2.6	0	0	0	40	100		DRAWING TITLE				
DGA	C ₄ H ₁₁ NO ₂	0	0	54.3	0	54.4	58.5	0	40	0	0	0	0	0	0	60	0		REV.	3			

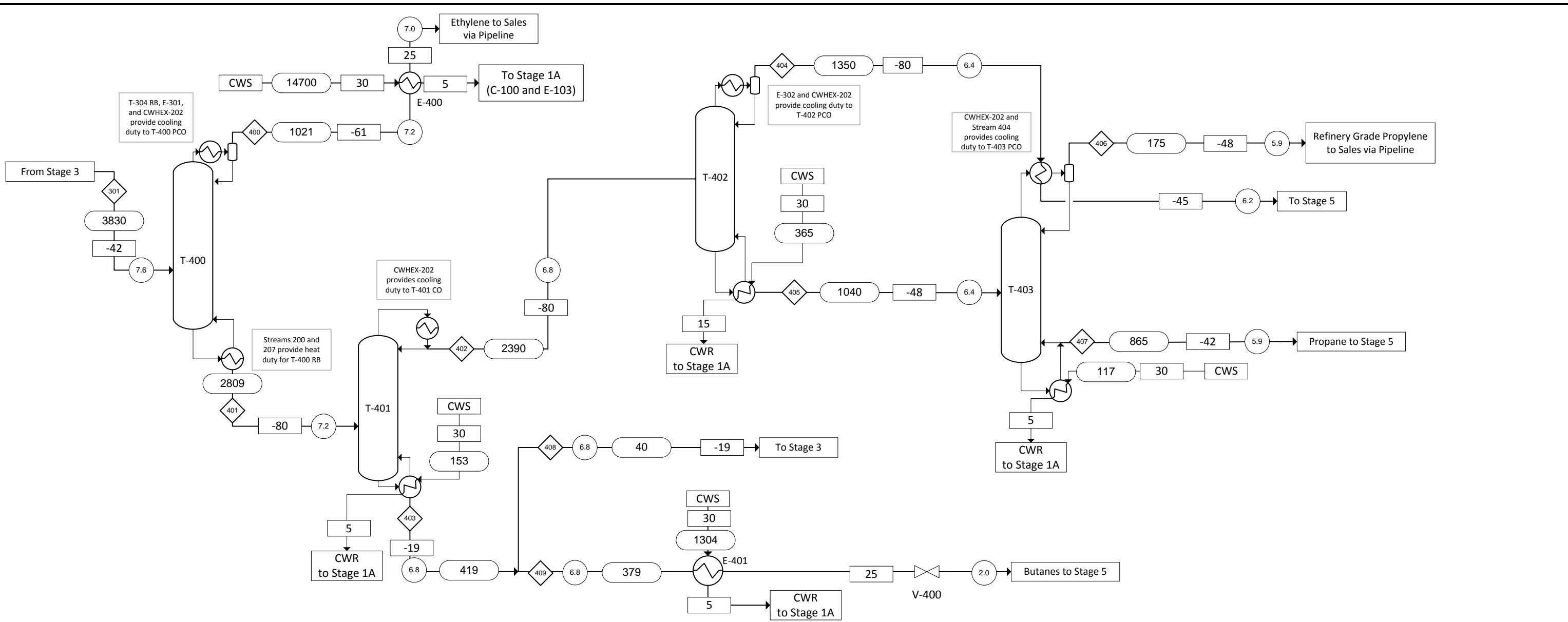


STREAM IDENTIFICATION NO.																	
STREAM DESCRIPTION																	
TOTAL MASS FLOW RATE (LB/MIN)	4744	2882	7626	644	307	6675	169	6497	9	6666							
COMPONENTS	FORMULA	Wt%	Wt%	Wt%	Wt%	Wt%	Wt%	Wt%	Wt%								
Hydrogen	H ₂	0	2.3	0.9	0	0	1.0	0	1.0	0	1.0						
Nitrogen	N ₂	4.4	trace	2.8	0	0	3.1	0	3.2	0	3.1						
Water	H ₂ O	0.1	22.5	8.5	100	0	0.1	0	0	100	0						
Methane	CH ₄	45.2	8.6	31.4	0	0	36.0	0	36.8	0	36.0						
Acetylene	C ₂ H ₂	0	0.3	0.1	0	0	0.2	0	0.2	0	0.2						
Ethylene	C ₂ H ₄	0	35.4	13.4	0	0	15.3	0	15.7	0	15.3						
Ethane	C ₂ H ₆	17.8	17.2	17.6	0	0	20.3	0	20.6	0	20.2						
Methylacetylene	C ₃ H ₄	0	0.2	0	0	0	0	0	0	0	0						
Propylene	C ₃ H ₆	0	6.1	2.3	0	0	2.6	0	2.7	0	2.7						
Propane	C ₃ H ₈	16.3	3.0	11.3	0	0	12.9	0	13.3	0	12.9						
Butadiene	C ₄ H ₆	0	2.0	0.6	0	2.7	0.7	4.9	0.7	0	0.7						
isoButane	C ₄ H ₁₀	2.3	trace	1.4	0	4.7	1.4	8.5	1.3	0	1.4						
nButane	C ₄ H ₁₀	7.2	trace	4.5	0	18.9	4.2	32.0	3.5	0	4.2						
Pentanes	C ₅ H ₁₂	4.0	0	2.5	0	25.1	1.7	32.8	0.9	0	1.8						
Hexanes	C ₆ H ₁₄	1.4	0	0.8	0	15.6	0.2	9.5	trace	0	0.2						
Heptanes Plus	C ₇ +	1.3	0	0.8	0	20.5	0.2	7.6	trace	0	0.3						
Aromatic Naphthas	C ₆ H ₆ , C ₇ H ₈	0	2.3	1.0	0	12.5	0.1	4.6	0	0	0						





STREAM IDENTIFICATION NO.	205	300	301	302	303	304	305	306	307	308	309	310	311	312	313	314	408		NOTES: CO = Condenser PCO = Partial Condenser RB = Reboiler TRB = Total Reboiler IPQ = Interstate Pipeline CWHEX = Coil-wound Heat Exchanger		
STREAM DESCRIPTION																					
TOTAL MASS FLOW RATE (LB/MIN)	6497	2667	3830	277	2390	927	1010.6	851	201	159.6	76.2	83.4	650	73.9	2.3	2430	40				
COMPONENTS	FORMULA	Wt%	Wt%	Wt%	Wt%	Wt%	Wt%	Wt%	Wt%	Wt%	Wt%	Wt%	Wt%	Wt%	Wt%	Wt%					
Hydrogen	H ₂	1.0	2.5	0	24.2	0	8.3	13.4	1.3	0.2	78.2	87.5	69.8	1.6	87.5	87.5	0	0			
Nitrogen	N ₂	3.2	7.9	0	75.8	0	91.7	86.6	98.7	98.8	21.8	12.5	30.2	98.4	12.5	12.5	0	0			
Methane	CH ₄	36.8	89.6	trace	trace	100	trace	0	0	0	0	0	0	0	0	0	98.4	0			
Acetylene	C ₂ H ₂	0.2	trace	0.3	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
Ethylene	C ₂ H ₄	15.7	0	26.7	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
Ethane	C ₂ H ₆	20.6	0	35.0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
Methylacetylene	C ₃ H ₄	0.1	0	0.1	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
Propylene	C ₃ H ₆	2.7	0	4.6	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
Propane	C ₃ H ₈	13.2	0	22.5	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
Vinylacetylene	C ₄ H ₄	trace	0	trace	0	0	0	0	0	0	0	0	0	0	0	0	trace	0.2			
Butadienes	C ₄ H ₆	0.5	0	0.9	0	0	0	0	0	0	0	0	0	0	0	0	0.1	8.4			
Butenes	C ₄ H ₈	0.1	0	0.2	0	0	0	0	0	0	0	0	0	0	0	0	trace	1.9			
isobutane	C ₅ H ₁₀	1.3	0	2.1	0	0	0	0	0	0	0	0	0	0	0	0.3	19.5				
n-butane	C ₆ H ₁₀	3.5	0	6.0	0	0	0	0	0	0	0	0	0	0	0	0	1.0	55.0			
isopentane	C ₅ H ₁₂	0.4	0	0.7	0	0	0	0	0	0	0	0	0	0	0	0.1	6.8				
n-pentane	C ₅ H ₁₂	0.5	0	0.9	0	0	0	0	0	0	0	0	0	0	0	0.1	8.1				

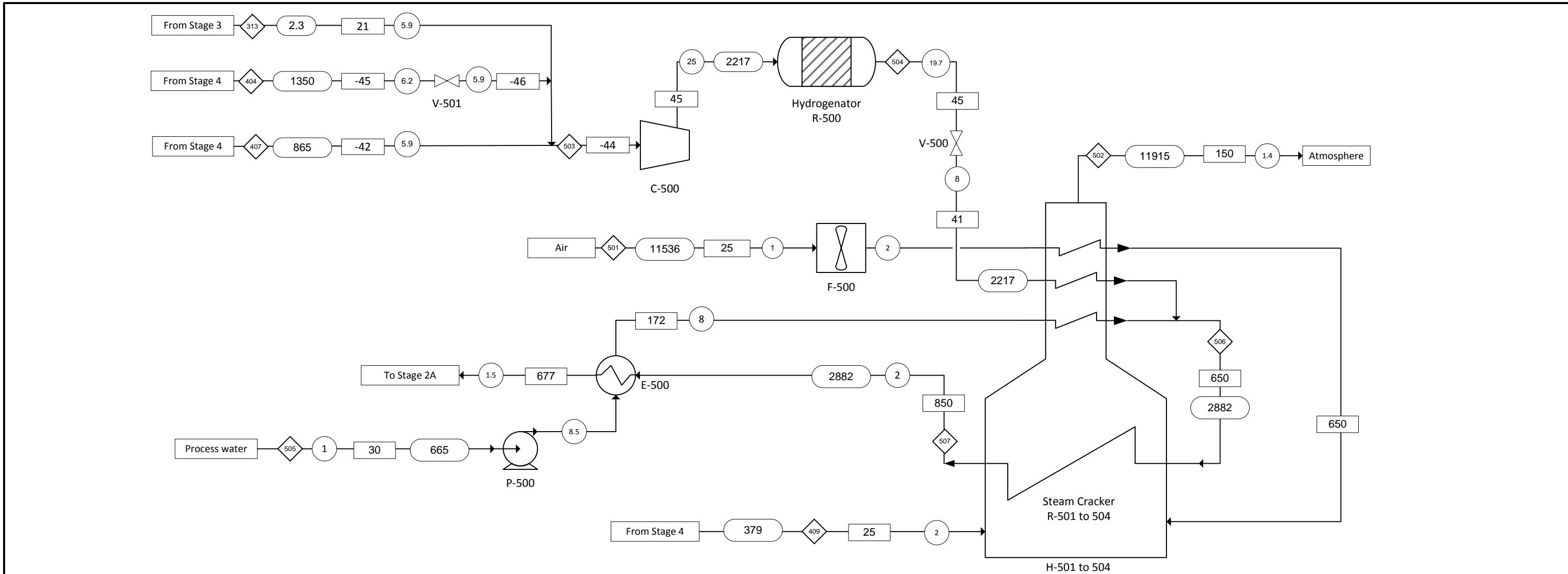


LEGEND		REVISIONS		
		REV	DATE	DESCRIPTION
	Stream Number	1	2/18/2013	INITIAL DESIGN
	Mass Flow (lb/min)	2	2/23/2013	FOR E AND S REVIEW
	Temperature (C)	3	3/14/2013	FOR DESIGN REPORT
	Pressure (atm)	4	4/4/2013	FOR DESIGN LOCK

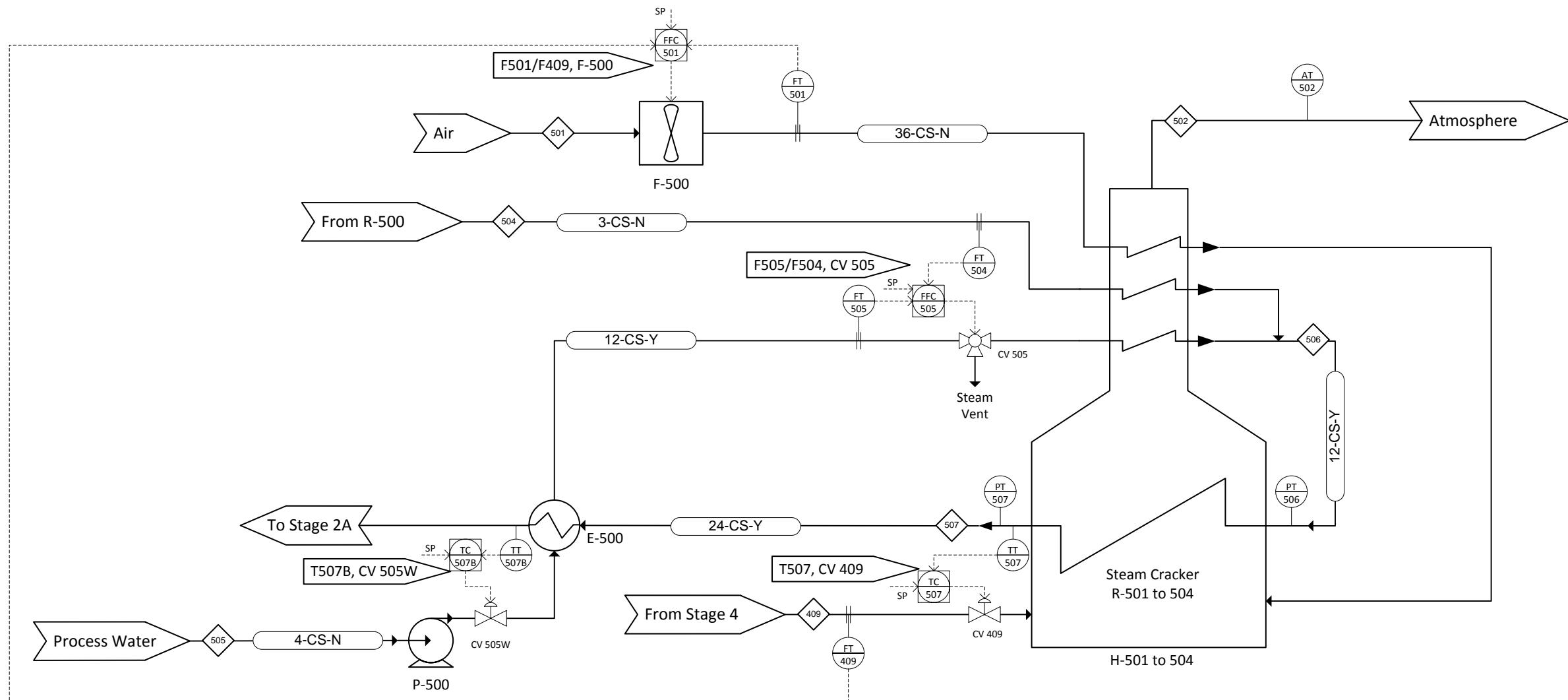
University of Michigan
DEPARTMENT OF
CHEMICAL ENGINEERING

COURSE NO.	DRAWN BY	DATE
ChE 487	AJS	4/4/2013
GROUP NO. 5	PROCESS FLOW DIAGRAM (PFD)	

DRAWING TITLE		
Heavy Component Separations – Stage 4	REV.	4



Appendix O: Piping and Instrumentation Diagram



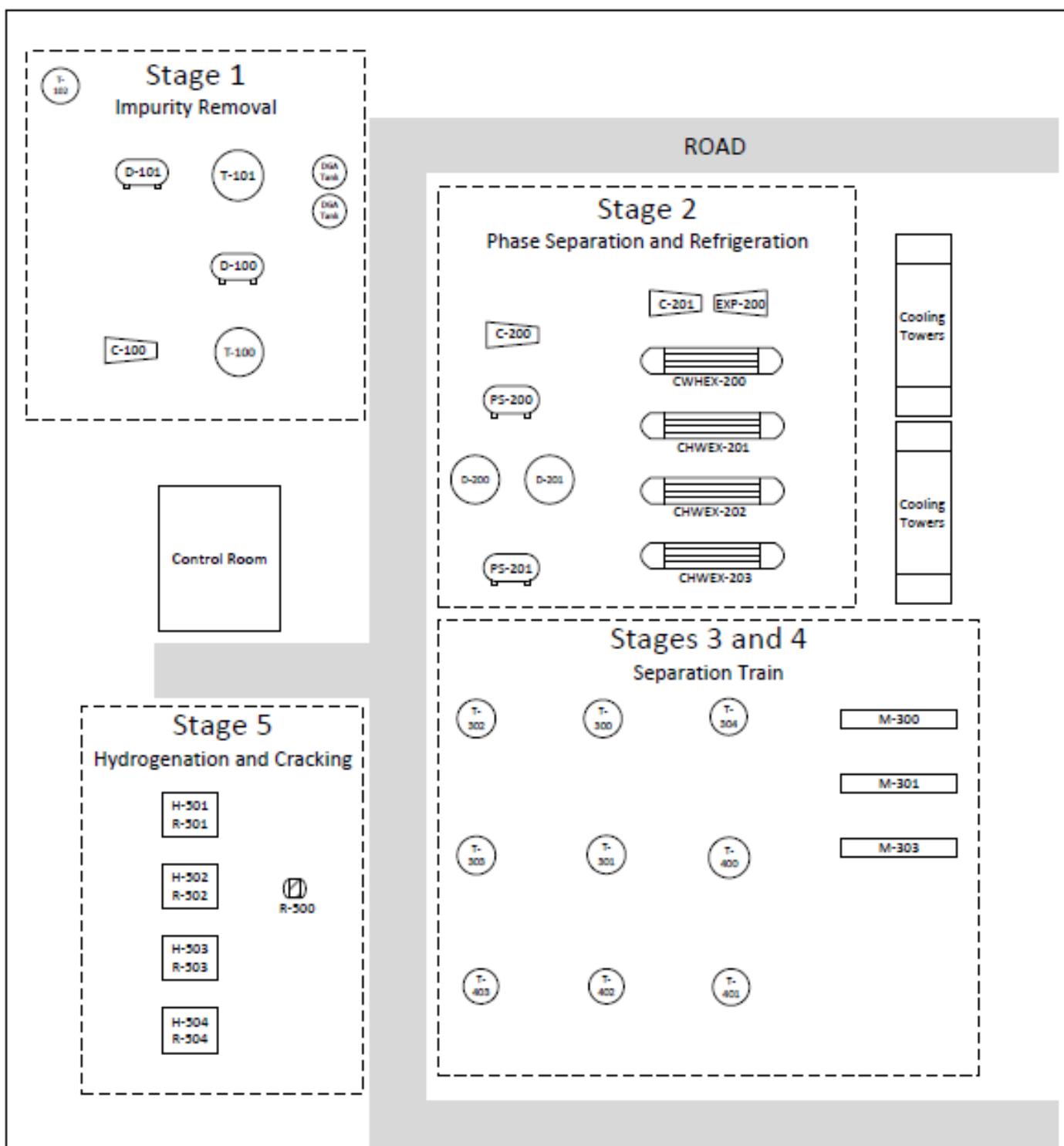
Appendix P: Plant Layout

The plant layout is one of the most important decisions of a process design team. The correct placement of equipment increases the inherent safety of the plant, decreases costs by minimizing pipe length and subsequently replacement and upkeep costs, and also is a great way to maximize heat integration by separating processes that operate at hot and cool temperatures to ensure efficiency. Our proposed plant layout is shown in Figure P-1.

Safety was the foremost concern in the plant layout diagram and can be seen by the distance between equipment, the accessibility of each major process unit, and the separation of the impurity removal (Stage 1) from the rest of the plant. Stage 1 contains hazardous chemicals such as DGA and hydrogen sulfide. Stage 1 is separated from the rest of the plant to minimize the risk for operator exposure to these chemicals.

To be safest, the equipment would be hundreds of yards of away from each other, but this is not economically feasible. Costs of piping and the maintenance it requires was minimized as much as possible by placing each stage in proximity to any connected stages. Suggested distances between equipment was adapted from An Engineer's Guide to Process-Plant Layout [55].

The heat integration of an ethylene cracking plant is paramount to its economic feasibility. The hottest stage (Stage 5) is separated by a road from the coldest stages (Stages 3 and 4). Stages 2, 3, and 4 are located near each other, which helps to minimize the costs of the extensive heat integration that occurs between them.



NOTES	REVISIONS			University of Michigan DEPARTMENT OF CHEMICAL ENGINEERING	COURSE NO. ChE 487	DRAWN BY AJS	DATE 4/10/13
	REV	DATE	DESCRIPTION				
C = Compressor EXP = Expander T = Tower PS = Phase Separator D = Dehydration Unit CWHEX = Coil-wound Heat Exchanger M = Membrane Separator H = Heat Box R = Reactor	1	3/10/2013	INITIAL DESIGN	DRAWING TITLE Ethylene from Natural Gas Plant Layout	GROUP NO. 5	Plant Layout	REV. 4
	2	3/15/2013	FOR DESIGN REPORT				
	3	4/10/2013	REMOVED CLUTTER				
	4	4/12/2013	FIXED SPACING				

Appendix Q: Supply Chain

This section will talk about the fate of our streams past the Lindgren Group's MichiSite chemical plant. It is necessary to determine the most economical supply option for our particular geographic location: Michigan.

Natural Gas

The supply chain for the natural gas industry is shown in Figure Q-1 below. Natural gas is first collected from the wellheads and sent to a separation unit where water is flashed out. This oil is then sent to a gas processing plant where products are purified. The natural gas product is sent to compressor stations which pipe the natural gas to the market where some are stored underground for times of great demand and others are sent to consumers including residential houses, industries, and cities.

MichiChem, Corp. has recently purchased natural gas wells and has asked the Lindgren Group, LLC to design a gas processing plant to produce natural gas for this market along with other valuable by products such as ethylene.

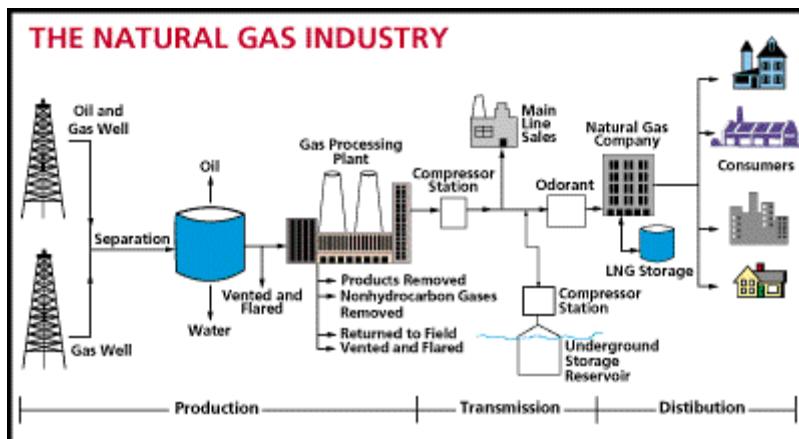


Figure Q-1: The natural gas value chain [56]

From our process, IPQ natural gas will be sent to a pipeline company that ultimately collects natural gas from other companies. To transport these gases effectively, it is necessary to reduce the amount of volume they take up by increasing the gas' density. Maron Raymon confirmed that channeling our IPQ natural gas stream at 35 atm and 17°C was an acceptable specification. [57] The pipeline company then sends the natural gas to a Local Distribution Company where the natural gas is channeled to its customer for residential, commercial, and industrial uses. [58]

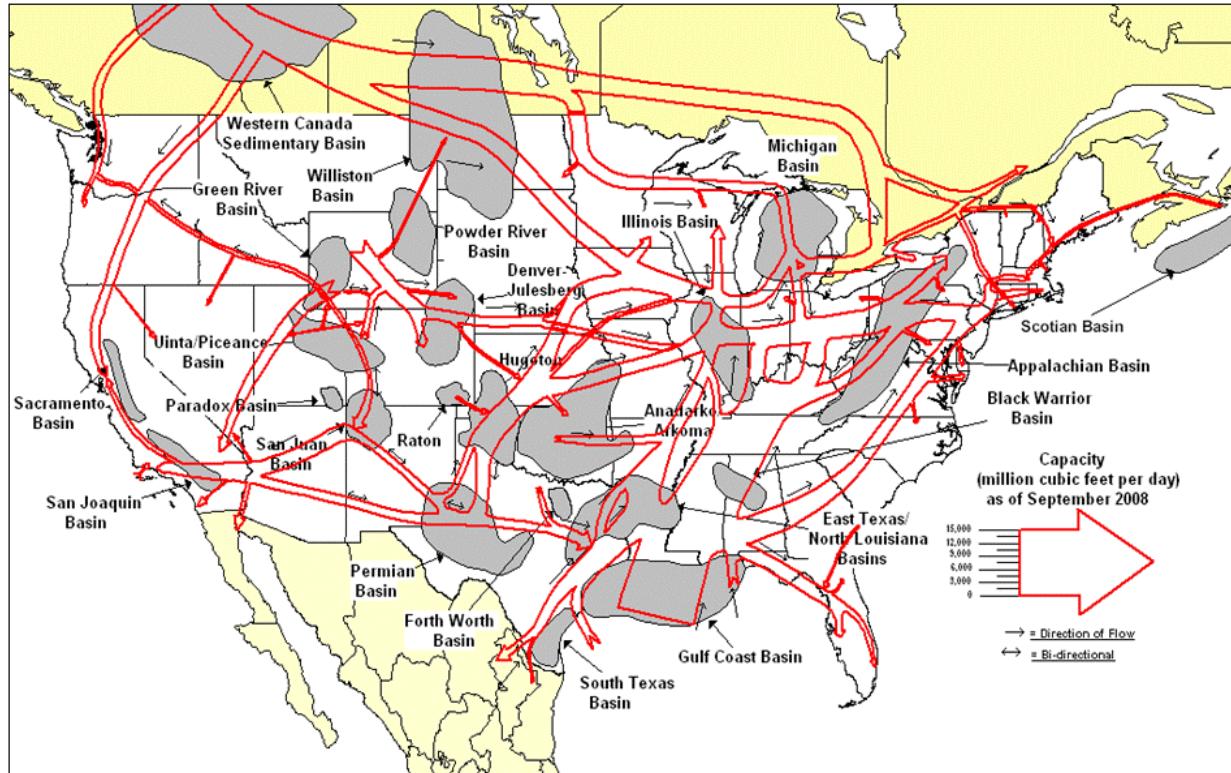


Figure Q-2: Structure of the US natural gas pipeline system [59]

Ethylene

Ethylene is an intermediate chemical that is useful in the production of various products such as polyethylene (plastic bags), ethylene glycol (antifreeze), and polyester (shirts), just to name a few. Chemical grade ethylene is produced and shipped out via pipeline to our customers who use ethylene to produce the products we mentioned earlier.

Other Byproducts

Other byproducts such as propylene, butanes, and hydrogen will all be pipelined out to sales for customers.

Appendix R: Economics Calculations

- R.1 Sample Calculation for Equipment Costing
- R.2 Capital Costs for Equipment
- R.3 Capital Costs for Piping
- R.3 Commentary on NPV Calculation

R.1 Sample Calculation for Equipment Costing

Below is the calculation used to find the capital cost of T-100.

$$D = 97 \text{ in} = 2.46 \text{ m}$$

$$P = 37 \text{ atm} = 543 \text{ psi}$$

Material = carbon steel shell, stainless steel trays

20 trays

Figure 15-15: \$7,500/tray \rightarrow \$150,000

$$F_{bm} = 4.16$$

$$F_d = 1$$

$F_m = 1$ (accounted for in graph)

$F_p = 2.7$ (linear interpolation between 150 psia and 725 psia from Figure 15-11)

$$I_{2013} = 1685.9$$

$$I_{2002} = 1104.2$$

$$F_{bm} = C_{fob} \left(\frac{I_{2013}}{I_{2002}} \right) [F_{bm} + (F_d F_p F_m - 1)]$$
$$F_{bm} = \$150,000 \left(\frac{1685.9}{1104.2} \right) [4.16 + (1 * 2.7 * 1 - 1)]$$
$$F_{bm} = \$1,342,063$$

R.2 Capital Costs for Equipment

Equipment #	Type	Capital
Towers		
T-100	Amine absorber	1,342,063
T-101	Regenerator	1,071,318
T-102	Distillation	64,375
T-300	Cryogenic	715,273
T-301	Cryogenic	715,273
T-302	Cryogenic	715,273
T-303	Cryogenic	715,273
T-304	Cryogenic	722,426
T-400	Cryogenic	3,825,319
T-401	Cryogenic	2,742,573
T-402	Cryogenic	1,785,530
T-403	Cryogenic	2,885,416
Tower total		17,300,112
Compressors/Pumps		
C-100	9 stages	12,214,454
C-101	3 stages	1,832,168
C-200	2 stages	7,634,034
C-201	5 stages	610,723
C-300	1 stage	45,804
C-301	1 stage	32,063
C-302	1 stage	15,268
C-303	1 stage	219
C-500	1 stage	152,681
B-100	Blower	45,804
F-100	Fan	4,580
F-500	Fan	22,902
P-100	Pump	7,329
P-200	Pump	3,817
P-300	Pump	10,688
P-500	Pump	13,741
EXP-200	Expander	137,413
Compressor total		22,783,688

Heat Exchangers

E-100	Shell and tube	78,680
E-101	Shell and tube	66,520
E-102	Shell and tube	85,833
E-103	Shell and tube	57,222
E-200	Shell and tube	15,268
E-201	Shell and tube	27,483
CWHEX-200	>2 streams	1,430,547
CWHEX-201	>2 streams	786,801
CWHEX-202	>2 streams	1,144,438
CWHEX-203	>2 streams	572,219
CWHEX-204	>2 streams	1,430,547
E-300	Shell and tube	85,833
E-301	Shell and tube	1,287,493
E-302	Shell and tube	572,219
E-400	Shell and tube	171,666
E-401	Shell and tube	1,573,602
E-500	Shell and tube	15,268
Heat Exchanger total		9,401,639

Reactors

R-500	Hydrogenator catalyst	41,063
R-501	Steam cracker	10,077
R-502	Steam cracker	10,077
R-503	Steam cracker	10,077
R-504	Steam cracker	10,077
Reactors total		81,371

Other tanks

D-100	Flash tank	197,721
D-101	Flash tank	9,161
PS-200	V/L/L phase separator	45,804
PS-201	V/L/L phase separator	45,804
D-200	Desiccant bed	491,000
D-201	Desiccant bed	491,000
M-300	Membrane separator	1,553,685
M-301	Membrane separator	1,360,149
M-302	Membrane separator	788,566
H-501	Furnace	1,526,807
H-502	Furnace	1,526,807
H-503	Furnace	1,526,807
H-504	Furnace	1,526,807
Other total		11,090,118
Equipment total		60,656,928

R.3 Capital Cost for Piping

Line #	Service	Material	Dia (in)	Length (ft)	Qty.	Cost (\$/ft)	Total cost
100	NG	SS	24	50	1	80	5,722
101	NG	CS	18	100	1	35	5,007
102	DGA/Water	SS	6	30	1	20	858
103	NG	SS	1	30	1	1.6	69
104	DGA/WATER	SS	6	45	1	20	1,287
105	DGA/WATER	CS	6	75	1	10	1,073
106	CO2 H2S	1075 CS	4	45	1	5	322
107	Water/DGA	CS	1	20	1	0.8	23
108	CO2 H2S/water	1075 CS	1	45	1	0.8	51
109	CO2 H2S	1075 CS	4	30	1	5	215
110	CO2 H2S	1075 CS	6	45	1	0.8	51
111	CO2 H2S	1075 CS	1	50	1	0.8	57
112	CO2 H2S	1075 CS	4	75	1	5	536
113	CO2 H2S	1075 CS	4	55	1	5	393
114	NG	SS	24	75	1	80	8,583
115	DGA	CS	1	15	1	0.8	17
116	Water	CS	1	15	1	0.8	17
200	Mixed HC (g)	CS	24	425	1	40	24,319
201	Water	CS	4	1000	1	5	7,153
202	Mixed HC (l)	CS	2	1000	1	2	2,861
203	Mixed HC (g)	CS	18	30	1	35	1,502
204	Mixed HC (l)	CS	2	1000	1	2	2,861
205	Mixed HC (g)	CS	24	140	1	40	8,011
207	Mixed HC (g)	CS	18	30	1	35	1,502
208	CH+N2	SS	17	60	3	70	18,025
209	CH+N2	SS	17	60	3	70	18,025
210	CH+N2	SS	8	60	1	24	2,060
211	CH+N2	SS	15	60	1	60	5,150
212	CH+N2	SS	18	60	2	70	12,017
213	CH+N2	SS	7	60	4	18	6,180
300	CH4,H2,N2	SS	20	50	5	70	25,035
301	C2+	SS	15	50	1	60	4,292
302	H2/N2	SS	17	50	3	70	15,021
303	CH4	SS	19	1000	3	70	300,415
304	H2/N2	Copper	19	20	2	42	2,403
305	H2/N2	Copper	20	20	2	42	2,403
306	H2/N2	Copper	20	20	2	42	2,403
307	N2	Copper	13	20	1	36	1,030
308	H2/N1	Copper	11	20	1	31.2	893
309	H2/N2	Copper	8	20	1	14.4	412

Line #	Service	Material	Dia (in)	Length (ft)	Qty.	Cost (\$/ft)	Total cost
310	H2/N2	Copper	8	20	1	14.4	412
311	H2/N2	Copper	16	20	2	37.2	2,129
312	H2	Copper	8	1000	1	14.4	20,600
313	H2/N2	Copper	2	20	1	2.4	69
400	Ethylene	SS	20	1000	1	70	100,138
401	C2+	SS	19	20	5	70	10,014
402	C2-C4	SS	19	20	4	70	8,011
403	C4+	SS	16	20	1	64	1,831
404	C2	SS	16	20	2	64	3,662
405	C3	SS	18	100	2	70	20,028
406	C3	SS	18	1000	1	70	100,138
407	C3	SS	18	100	1	70	10,014
408	C4+	CS	9	1000	1	14	20,028
409	C4+	CS	12	100	1	30	4,292
501	Air	CS	18	30	16	35	24,033
503	Mixed HC (g)	CS	6	100	1	10	1,431
504	Mixed HC (g)	CS	3	30	4	4	687
505-liq	Water	CS	4	1000	1	5	7,153
505-gas	Steam	CS	12	45	4	30	7,725
506	Mixed HC (g)	CS	12	10	4	30	1,717
507a	Mixed HC (g)	CS	24	30	4	40	6,867
507b	Mixed HC (g)	CS	20	200	9	35	90,124
Piping Total							905,073

R.4 Commentary on NPV Calculation

The proposed ethylene plant is constructed over two years. Half of the capital is spent in the first year. The other half is spent at the end of the second year of construction. This is also when the working capital and startup costs are incurred. In these first two years, no profit is made, and so no taxes are due. Therefore, the cumulative cash flow increases in the negative direction.

In the first year of operation, the depreciation allowance begins. MichiChem uses the 7-year MACRS schedule shown below. The depreciation is calculated as the allowance percentage multiplied by the equipment capital.

Year	Depreciation Allowance Percentage
1	14.29 %
2	24.49 %
3	17.49 %
4	12.49 %
5	8.93 %
6	8.92 %
7	8.93 %
8	4.46 %

Additionally, in the first year of production, the plant runs at half capacity. Because of this, sales are only half of what they should be. Even at half capacity, however, all production costs are incurred. This follows under the assumption that the plant runs the whole time, but many adjustments have to be made and only half of the product is of saleable quality. In this year, the costs exceed the sales, so the gross revenue is negative. Since no profit is made, no taxes are due.

In the second year of production and for every subsequent year, the plant runs at full capacity. This is the first year that depreciation makes a difference. First, the gross revenue is calculated.

$$\text{Gross revenue} = \text{Sales} - \text{Costs}$$

Second, the amount taxable is found.

$$\text{Taxable} = \text{Gross revenue} - \text{Depreciation}$$

$$\text{Tax due} = 0.52 * \text{Taxable}$$

Taxes due is based on the state and federal tax rates. 4% of the taxable income goes to the state government and 48% is allotted to the federal government. From this, the cash flow is determined.

$$\text{Cash Flow} = \text{Gross revenue} - \text{Tax due}$$

To account for the future value of money, this cash flow must be discounted. As per the MichiChem standards, the MARR is 11%.

$$Discounted = \frac{Undiscounted}{(1 + MARR)^{project\ year}}$$

The project year begins when construction begins, so the first year of plant operating is the second project year. One would expect it to be the third project year, except the first project year is considered to be year 0.

At this point, the NPV is calculated.

$$NPV = \sum \text{Discounted Cash Flow}$$