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# Process Design for the Production of Ethylene from Ethanol

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# Process Design for the Production of Ethylene from Ethanol

## **Abstract**

This project considers using ethanol dehydration as a means to mass-produce ethylene. 2.3MM tonnes of a 95% ethanol / 5% water feed will be converted into 1MM tonnes of 99.96% pure ethylene per year using a series of adiabatic, fixed-bed catalytic reactors operating at 750°F and 600psi. The catalyst is gamma-alumina in the form of 1cm diameter spherical pellets. After the dehydration process, the product will be purified using two flash separation units, an adsorption unit with zeolite 13X sorbent, and finally a cryogenic distillation unit. The plant will be located in São Paulo, Brazil. Because ethanol production in Brazil is seasonal, the plant will operate only 280 days per year at a very high capacity. This includes 30 days worth of on-site feed storage. After conducting an analysis of the sensitivity of the plant's Net Present Value and Internal Rate of Return to ethylene and ethanol prices, it was determined that while profitability is not attainable in the current market (which prices ethanol at \$0.34/lb and ethylene at \$0.60/lb), profitability is attainable should ethylene prices rise to \$0.64/lb and ethanol prices fall to \$0.305/lb.

## **Disciplines**

Biochemical and Biomolecular Engineering

# **Process Design for the Production of Ethylene from Ethanol**

Design Project By:

Gregory Cameron

Linda Le

Julie Levine

Nathan Nagulapalli

Presented To:

Professor Leonard Fabiano

Dr. Raymond Gorte

April 10, 2012

Department of Chemical and Biomolecular Engineering

University of Pennsylvania

School of Engineering and Applied Science



April 10, 2012  
Professor Leonard Fabiano  
Dr. Raymond Gorte  
University of Pennsylvania  
School of Engineering and Applied Science  
Department of Chemical and Biomolecular Engineering

Dear Professor Fabiano and Dr. Gorte,

We would like to present our solution to the *Ethylene from Ethanol* design project suggested by Mr. Bruce Vrana. We have designed a plant, to be located in São Paulo, Brazil, which will produce one million tonnes of polymer-grade ethylene (99.96% pure) per year from a 95% ethanol feed. The ethanol will be dehydrated using fixed-bed, adiabatic reactors filled with gamma-alumina catalyst. The products of the dehydration will then be separated using flash distillation, adsorption over a zeolite packing, and cryogenic distillation. This method of ethylene production presents an alternative to the popular hydrocarbon cracking technique that is presently widely used.

This report contains a detailed description of the plant process equipment and operating conditions. Our plant is expected to be complete in 2015 and has an anticipated life of 20 years. It will require an annual ethanol feed of 2,300,000 tonnes of 95% purity ethanol. Because we will be operating in Brazil (where ethanol is only produced nine months out of the year), we expect to operate 280 days per year (including 30 days of operating from on site storage). This design is expected to meet the required one million tonnes of 99.96% purity ethylene per year.

Additionally, this report discusses our decision to locate the plant in São Paulo and the technical and economic implications of operating in Brazil. We will present a comparison of the details of operating in the United States and Brazil which led us to make this choice. Additionally, we will discuss the economics of building and running the plant and its potential profitability. As it stands, current ethylene and ethanol prices do not allow this plant to be profitable. However, prices for which this plant can be successful are not far off.

Sincerely,

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Gregory Cameron

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Linda Le

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Julie Levine

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Nathan Nagulapalli



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# **Section I**

## **Abstract**

This project considers using ethanol dehydration as a means to mass-produce ethylene. 2.3MM tonnes of a 95% ethanol / 5% water feed will be converted into 1MM tonnes of 99.96% pure ethylene per year using a series of adiabatic, fixed-bed catalytic reactors operating at 750°F and 600psi. The catalyst is gamma-alumina in the form of 1cm diameter spherical pellets. After the dehydration process, the product will be purified using two flash separation units, an adsorption unit with zeolite 13X sorbent, and finally a cryogenic distillation unit. The plant will be located in São Paulo, Brazil. Because ethanol production in Brazil is seasonal, the plant will operate only 280 days per year at a very high capacity. This includes 30 days worth of on-site feed storage. After conducting an analysis of the sensitivity of the plant's Net Present Value and Internal Rate of Return to ethylene and ethanol prices, it was determined that while profitability is not attainable in the current market (which prices ethanol at \$0.34/lb and ethylene at \$0.60/lb), profitability is attainable should ethylene prices rise to \$0.64/lb and ethanol prices fall to \$0.305/lb.

# **Section II**

## **Introduction**

## **Background**

The purpose of this project is to design a plant that efficiently converts liquid ethanol into high purity ethylene gas using an alumina catalyst. Ethylene is currently the most consumed intermediate product in the world. In 2009 it was estimated that the world demand for ethylene was over 140 million tons per year, with an approximate yearly increase of 3.5%. One of the most important uses of ethylene is the production of polyvinyl chloride (PVC). PVC currently serves over 70% of the construction market. This includes plastics, dominating pipe and fittings, windows, siding, decking and fencing. In addition, PVC serves 60% of the wire and cable plastics market and 25% of the coatings market.

Ethylene was first obtained from ethanol in the 18<sup>th</sup> century, when ethanol was passed over a heated catalyst. The plastics industry gave rise to several ethanol dehydration units which operated from the 1930s up until the 1960s. The advent of naphtha (liquefied petroleum gas) cracking rendered these dehydration units defunct. Naphtha cracking involves a liquid feed of saturated hydrocarbons diluted with steam and heated to extreme temperatures in the absence of oxygen. The functionality of this process reversed industrial trends, turning ethylene into a raw material for ethanol, as opposed to a derivative of it.

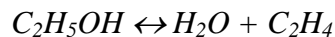
However, with increasing global demand for hydrocarbons and increasingly stricter environmental regulations, this process for ethylene production has proven to become very costly. Therefore, a cheaper process of creating ethylene is highly sought in today's economy, and the original production method of ethanol dehydration is being reconsidered.

## **Process Goals**

This project focuses on using the dehydration of ethanol as an alternative to cracking for producing ethylene. This report details a plant that produces 1MM tonnes of 99.96% pure ethylene per year from approximately 2.19MM tonnes of 95% ethanol, along with a thorough economic analysis. US Patent 4,396,789 has been used as the basis for the plant design, with several modifications and optimized design decisions put in place.

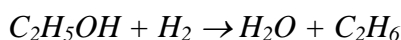
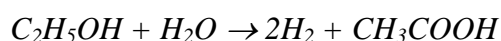
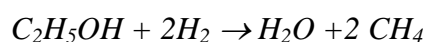
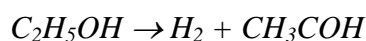
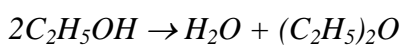
## Reaction

The dehydration reaction of ethanol to yield ethylene is shown below.



This reaction is zero-order and endothermic, having a standard heat of reaction ( $\Delta H_{RXN}$ ) of approximately 401BTU/lb. In addition, the reaction does not progress to completion under standard temperature and pressure (298K and 1atm) and exhibits an equilibrium that favors ethanol formation.

A high temperature reactor operating at 750°F is needed in order to shift the equilibrium toward product formation and efficiently produce ethylene with a high conversion. Additionally, the reaction over  $\gamma$ -Alumina yields a number of byproducts that must be removed through the separations train. The side reactions that produce these byproducts are listed in approximate order of decreasing prevalence.



Due to the high purity of ethylene product required (99.96 %), nearly all of the byproducts must be removed from the final product stream. These two factors form the basis of this plant design: a high temperature reactor and an intricately designed separations train with product purity as the main goal.

## **Plant Location**

In the United States, ethanol is produced from corn, which is grown year-round. In Brazil, ethanol is produced from sugar cane, which is only available nine months per year. However, the cheaper Brazilian ethanol prices and greater costal access for shipping purposes allow for a more cost-effective process. Therefore, a plant situated in and around the Sao Paulo area is the most fiscally sensible plan. For a more detailed discussion regarding the choice to locate in Brazil, please refer to Section 8)

## **Safety**

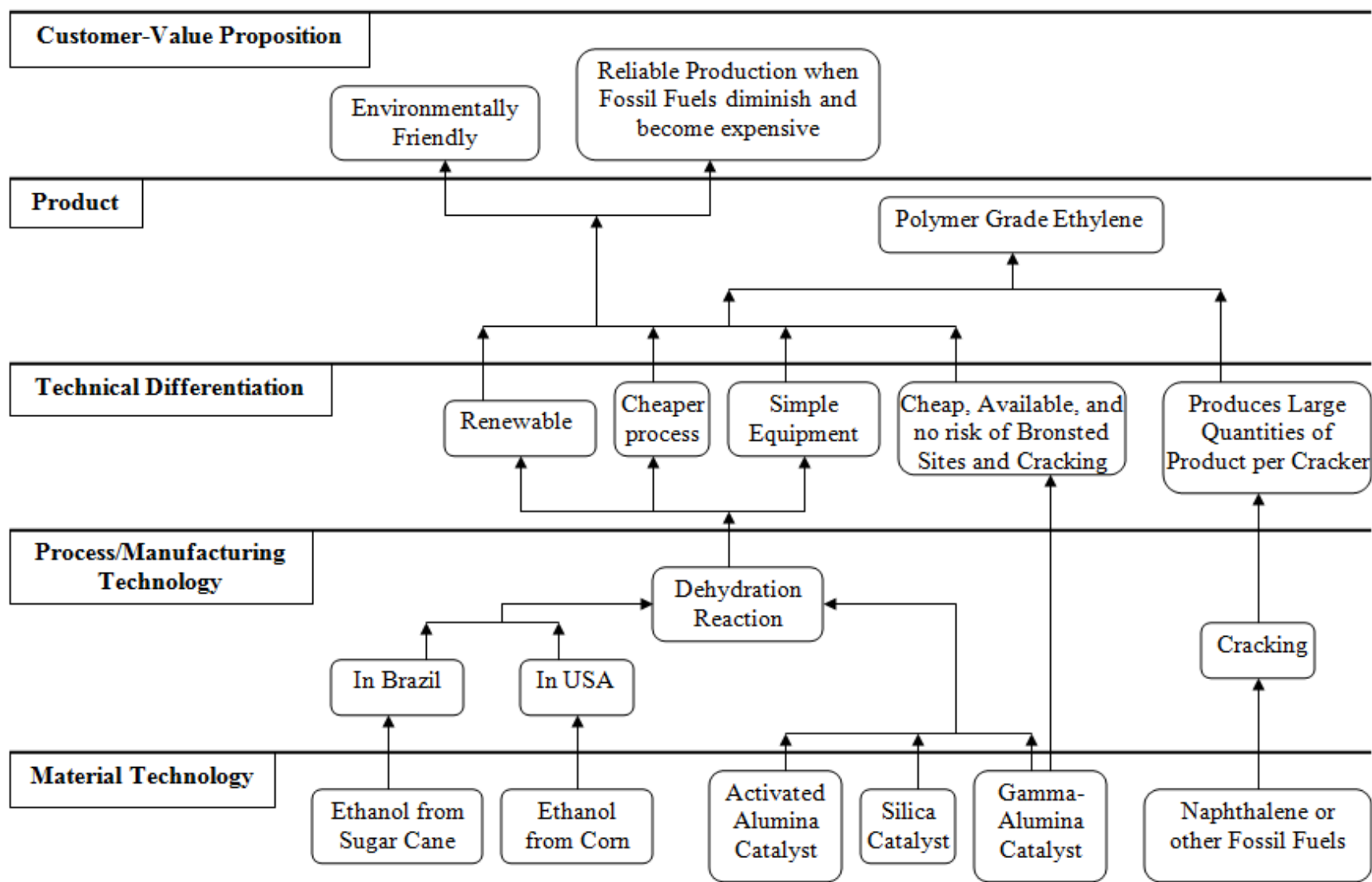
Both ethanol and ethylene are potentially dangerous materials if handled incorrectly. Section 9 contains a detailed discussion of safety considerations. Additionally, MSDS reports for all materials handled in this process are supplied in the appendix.

# **Section III**

## **Customer Requirements**

Figure 3.1

## Innovation Map





**Voice of the Customer**

The main customers for this plant are plastic companies that require ethylene for polymerization into products such as high-density polyethylene (HDPE), low-density polyethylene (LDPE), polystyrene, ethylene glycol, or polyvinyl chloride (PVC). Ethylene demand is generally demand and classified as fitness-to-standard, based upon the existing characteristics of ethylene produced by cracking of fossil fuels. Figure 3.1 shows an innovation map, which illustrates the relationship between customer values and the two main ethylene production processes (ethanol dehydration and hydrocarbon cracking). Most customers require their ethylene to be polymer-grade, or 99.96% pure. In general, an environmentally friendly process with low carbon emissions and waste is desired. It has been projected that by 2030, the demand for ethylene in the United States alone will be about 5MM tonnes /year. Most industrializing countries, such as Brazil, have a growing market for plastics, and resultantly, an increasing demand for ethylene.



# **Section IV**

## **Process Flow Diagram and Material Balances**

Figure 4.1: Reactor Section 100

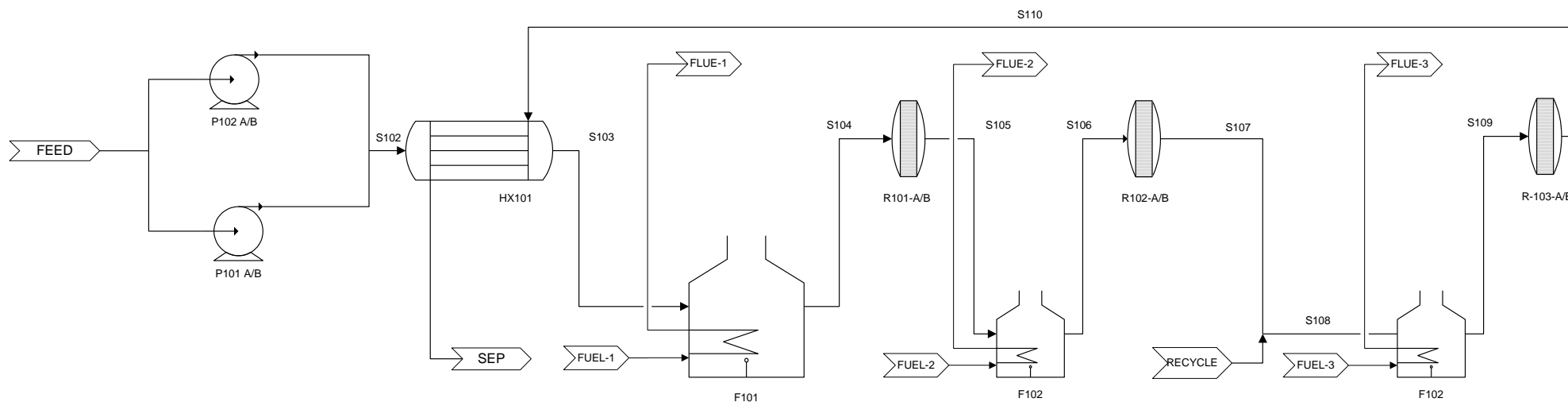


Table 4.1

Stream Table for Reactor Section 100								
Stream ID	FEED	S102	S103	S104	S105	S106	S107	RECYCLE
Temperature (°F)	77.0	78.8	572.0	752.0	590.0	752.0	590.0	96.9
Pressure (psi)	14.7	602.5	595.4	618.0	584.2	580.2	582.7	2.0
Vapor Fraction	0.00	0.00	1.00	1.00	1.00	1.00	1.00	1.00
Volume Flow (ft <sup>3</sup> /h)	11,485	11,502	209,159	256,490	394,244	471,246	445,761	208
Enthalpy (BTU/h)	-1.621E+09	-1.620E+09	-1.259E+09	-1.196E+09	-1.080E+09	-1.025E+09	-1.029E+09	-3.846E+07
Mass Flow (lb/hr)								
Ethanol	5.499E+05	5.499E+05	5.499E+05	5.499E+05	1.615E+05	1.615E+05	4.382E+04	9.998E+03
Water	2.894E+04	2.894E+04	2.894E+04	2.894E+04	1.800E+05	1.800E+05	2.257E+05	3.155E+03
Ethylene	0.000E+00	0.000E+00	0.000E+00	0.000E+00	2.344E+05	2.344E+05	3.052E+05	8.562E+02
Diethyl-Ether	0.000E+00	0.000E+00	0.000E+00	0.000E+00	2.212E+03	2.212E+03	3.187E+03	4.395E+02
Methane	0.000E+00	0.000E+00	0.000E+00	0.000E+00	3.830E+01	3.830E+01	7.205E+01	8.831E-02
Acetaldehyde	0.000E+00	0.000E+00	0.000E+00	0.000E+00	4.207E+02	4.207E+02	5.288E+02	1.169E+03
Ethane	0.000E+00	0.000E+00	0.000E+00	0.000E+00	3.589E+01	3.589E+01	4.644E+01	5.715E+01
Acetic Acid	0.000E+00	0.000E+00	0.000E+00	0.000E+00	1.792E+02	1.792E+02	2.108E+02	6.111E-02
Hydrogen	0.000E+00	0.000E+00	0.000E+00	0.000E+00	2.406E+01	2.406E+01	2.618E+01	2.309E-02
Total Mass Flow (lb/h)	5.788E+05	5.788E+05	5.788E+05	5.788E+05	5.788E+05	5.788E+05	5.788E+05	1.568E+04

Table 4.2

Section 100 Cont.				
Stream ID	S108	S109	S110	SEP
Temperature (°F)	591.1	752.0	590.0	179.3
Pressure (psi)	582.7	577.3	581.2	577.3
Vapor Fraction	1.00	1.00	1.00	0.47
Volume Flow (ft <sup>3</sup> /h)	454,243	541,479	473,540	127,545
Enthalpy (BTU/h)	-1.067E+09	-1.011E+09	-1.049E+09	-1.409E+09
Mass Flow (lb/hr)				
Ethanol	5.383E+04	5.383E+04	1.027E+04	1.027E+04
Water	2.289E+05	2.289E+05	2.458E+05	2.458E+05
Ethylene	3.061E+05	3.061E+05	3.323E+05	3.323E+05
Diethyl-Ether	3.627E+03	3.627E+03	3.952E+03	3.952E+03
Methane	7.214E+01	7.214E+01	9.276E+01	9.276E+01
Acetaldehyde	1.701E+03	1.701E+03	1.747E+03	1.747E+03
Ethane	1.037E+02	1.037E+02	1.107E+02	1.107E+02
Acetic Acid	2.108E+02	2.108E+02	2.214E+02	2.214E+02
Hydrogen	2.621E+01	2.621E+01	2.597E+01	2.597E+01
Total Mass Flow (lb/h)	5.945E+05	5.945E+05	5.945E+05	5.945E+05

Table 4.3

Utilities Table for Reactor Section 100			
Stream ID	FUEL-1	FUEL-2	FUEL-3
Type	Natural Gas	Natural Gas	Natural Gas
Temperature (°F)	70	70	70
Pressure (psi)	14.7	14.7	14.7
Volume Flow (SCF/h)	60,106	52,908	53,734
Duty (BTU/h)	6.311E+07	5.555E+07	5.642E+07

Figure 4.2: Flash Separation 200

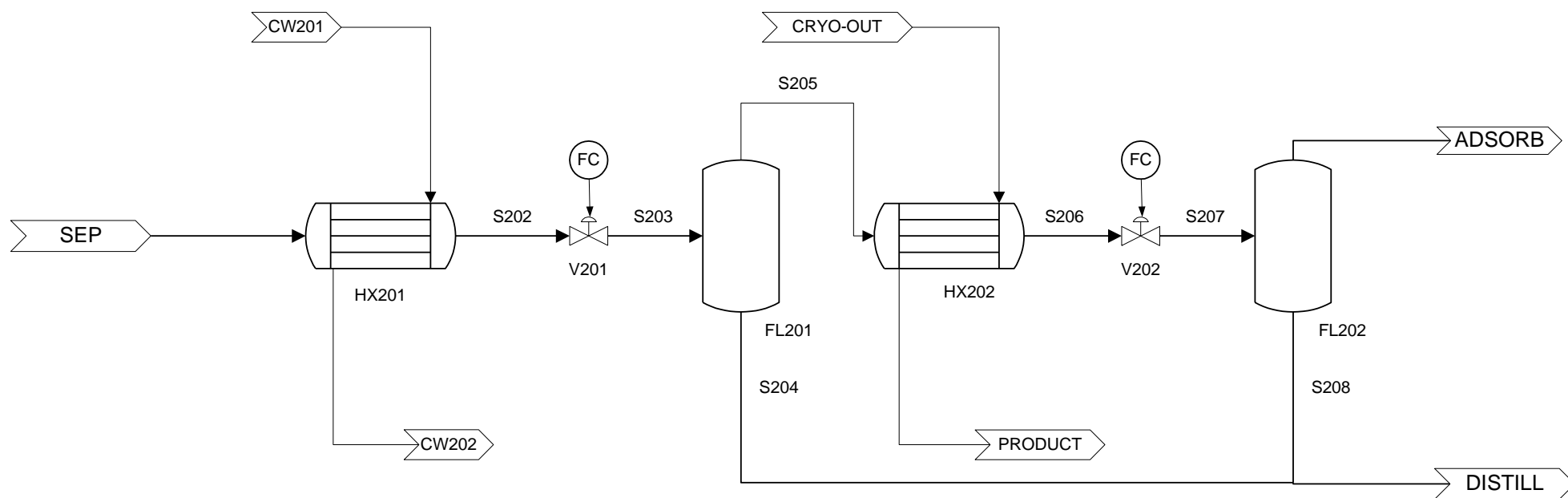


Table 4.4

Stream Table for Flash Section 200								
Stream ID	SEP	S202	S203	S204	S205	S206	S207	S208
Temperature (°F)	179.3	122	122	122	122	57	39	39
Pressure (psi)	577.3	574.3	573.1	573.1	573.1	569.3	455.6	455.6
Vapor Fraction	0.47	0.46		0.00	1.00	1.00	1.00	0.00
Enthalpy (BTU/h)	1.275E+05	-1.436E+09	-1.686E+09	-1.686E+09	2.498E+08	2.371E+08	-7.662E+06	-7.662E+06
Volume Flow (ft <sup>3</sup> /h)	-1.409E+09	107,996	108,259	4,306	103,952	78,294	141,740	24
Mass Flow (lb/h)								
Ethanol	1.027E+04	1.024E+04	1.024E+04	9.654E+03	5.907E+02	5.907E+02	5.907E+02	3.452E+02
Water	2.458E+05	2.453E+05	2.453E+05	2.443E+05	1.044E+03	1.044E+03	1.044E+03	9.563E+02
Ethylene	3.323E+05	3.316E+05	3.316E+05	8.357E+02	3.308E+05	3.308E+05	3.308E+05	2.046E+01
Diethyl-Ether	3.952E+03	3.943E+03	3.943E+03	4.090E+02	3.534E+03	3.534E+03	3.534E+03	3.050E+01
Methane	9.276E+01	9.256E+01	9.256E+01	8.640E-02	9.248E+01	3.534E+03	9.248E+01	1.911E-03
Acetaldehyde	1.747E+03	1.743E+03	1.743E+03	1.104E+03	6.391E+02	3.534E+03	6.391E+02	6.516E+01
Ethane	1.107E+02	1.105E+02	1.105E+02	5.673E+01	5.377E+01	3.534E+03	5.377E+01	4.149E-01
Acetic Acid	2.214E+02	2.209E+02	2.209E+02	2.200E+02	9.218E-01	3.534E+03	9.218E-01	8.441E-01
Hydrogen	2.597E+01	2.592E+01	2.592E+01	2.285E-02	2.589E+01	3.534E+03	2.589E+01	2.367E-04
Total Mass Flow (lb/h)	5.945E+05	5.933E+05	5.933E+05	2.565E+05	3.368E+05	3.368E+05	3.368E+05	1.419E+03

Table 4.5

Section 200 cont.				
Stream ID	CRYO-OUT	PRODUCT	ADSORB	DISTILL
Temperature (°F)	-35	52	39	122
Pressure (psi)	275.6	275.6	455.6	455.6
Vapor Fraction	1.00	1.00	1.00	0.00
Enthalpy (BTU/h)	2.452E+08	2.578E+08	2.448E+08	-1.694E+09
Volume Flow (ft <sup>3</sup> /h)	141,716	202,904	100,528	4,391
Mass Flow (lb/h)				
Ethanol	7.443E-11	7.443E-11	7.320E-04	3.876E-02
Water	8.816E-19	8.816E-19	2.606E-04	9.506E-01
Ethylene	9.996E-01	9.996E-01	9.863E-01	3.319E-03
Diethyl-Ether	1.219E-07	1.219E-07	1.045E-02	1.704E-03
Methane	2.804E-04	2.804E-04	2.758E-04	3.424E-07
Acetaldehyde	4.917E-08	4.917E-08	1.711E-03	4.533E-03
Ethane	8.322E-05	8.322E-05	1.591E-04	2.215E-04
Acetic Acid	7.519E-18	7.519E-18	2.315E-07	8.561E-04
Hydrogen	7.852E-05	7.852E-05	7.721E-05	8.951E-08
Total Mass Flow (lb/h)	3.298E+05	3.298E+05	3.353E+05	2.580E+05

Table 4.6

Utilities Table for Flash Section 200		
Stream ID	CW201	CW202
Type	Cooling Water	Cooling Water
Temperature (°F)	100	120
Pressure (psi)	14.7	14.7
Mass Flow (lb/h)	903,320	903,320
Duty (BTU/h)	-1.436E+09	

Figure 4.3: Distillation 300

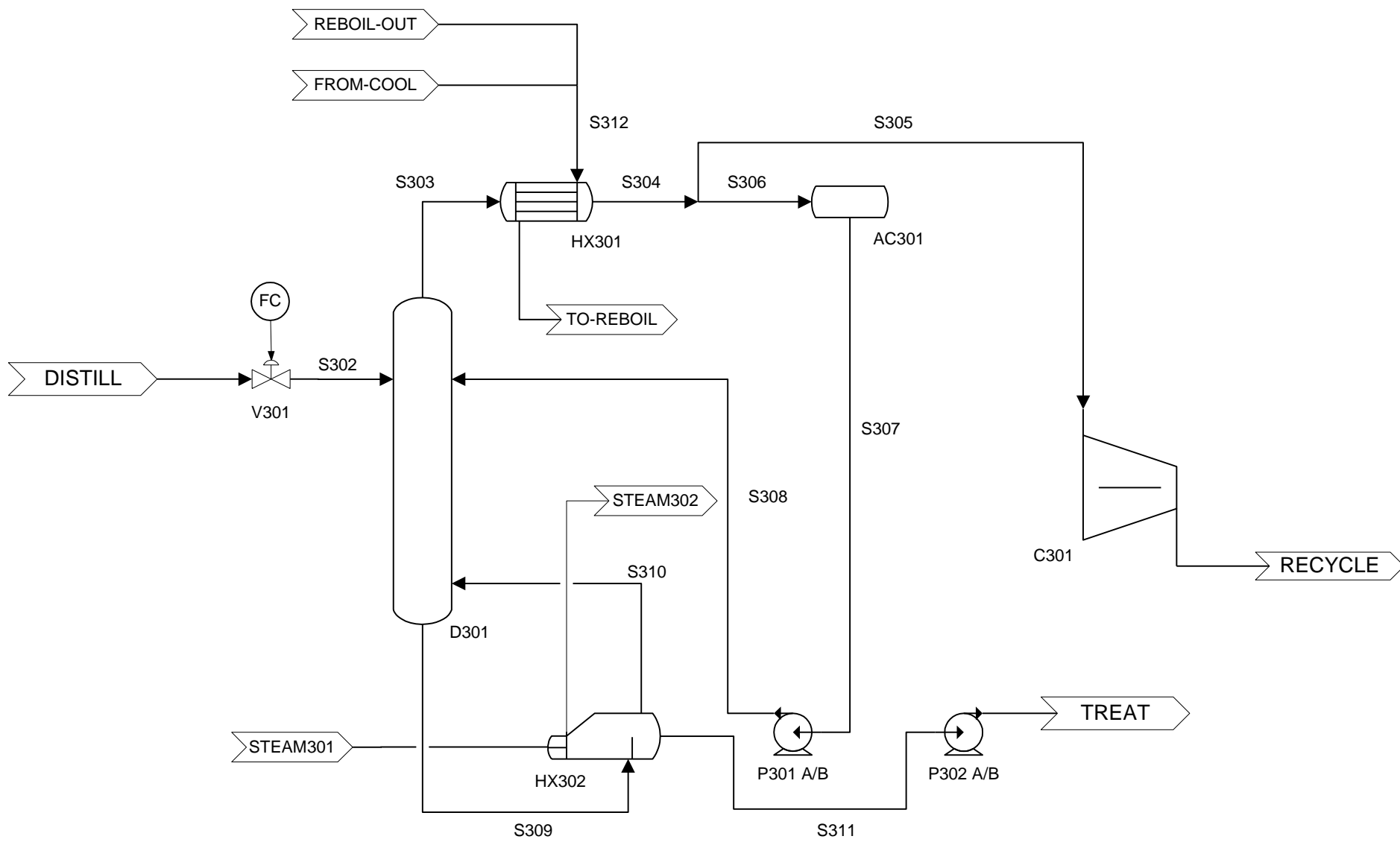




Table 4.7

Stream Table for Distillation Section 300								
Stream ID	DISTILL	S302	S303	S304	S305	S306	S307	S308
Temperature (°F)	121.7	122.1	221.7	206.4	206.4	206.4	206.4	206.4
Pressure (psi)	455.6	30.9	29.5	29.4	29.4	29.4	28.0	29.4
Vapor Fraction	0.00	0.00	1.00	0.54	1.00	0.00	0.00	0.00
Volume Flow (ft <sup>3</sup> /h)	4,391	10,794	-	-	109,081	-	-	-
Enthalpy (BTU/h)	-1.694E+09	-1.694E+09	-9.379E+08	-1.029E+08	-4.139E+07	-6.153E+07	-6.153E+07	-6.153E+07
Mass Flow (lb/h)								
Ethanol	1.002E+04	1.002E+04	1.633E+04	1.633E+04	1.002E+04	6.307E+03	6.307E+03	6.307E+03
Water	2.457E+05	2.457E+05	9.922E+03	9.922E+03	3.161E+03	6.760E+03	6.760E+03	6.760E+03
Ethylene	8.580E+02	8.580E+02	8.588E+02	8.588E+02	8.580E+02	8.367E-01	8.367E-01	8.367E-01
Diethyl-Ether	4.404E+02	4.404E+02	4.475E+02	4.475E+02	4.404E+02	7.088E+00	7.088E+00	7.088E+00
Methane	8.850E-02	8.850E-02	8.852E-02	8.853E-02	8.850E-02	2.541E-05	2.541E-05	2.541E-05
Acetaldehyde	1.172E+03	1.172E+03	1.444E+03	1.444E+03	1.172E+03	2.718E+02	2.718E+02	2.718E+02
Ethane	5.727E+01	5.727E+01	6.201E+01	6.201E+01	5.727E+01	4.743E+00	4.743E+00	4.743E+00
Acetic Acid	2.213E+02	2.213E+02	4.650E-01	4.650E-01	6.124E-02	4.037E-01	4.037E-01	4.037E-01
Hydrogen	2.314E-02	2.314E-02	2.314E-02	2.314E-02	2.314E-02	4.290E-06	4.290E-06	4.290E-06
Total Mass Flow (lb/h)	2.585E+05	2.585E+05	2.906E+04	2.906E+04	1.571E+04	1.335E+04	1.335E+04	1.335E+04

Table 4.8

Section 300 cont.					
Stream ID	S309	S310	S311	TREAT	RECYCLE
Temperature (°F)	252.4	252.6	252.6	252.6	634.4
Pressure (psi)	31.1	31.2	31.1554114	45.9	599.6
Vapor Fraction	0.00	1.00	0.00	0.00	1.00
Volume Flow (ft <sup>3</sup> /h)	-	-	4350.76317	4,351	8,028
Enthalpy (BTU/h)	-1.958E+09	-2.970E+08	-1.612E+09	-1.612E+09	-4.139E+07
Mass Flow (lb/h)					
Ethanol	5.459E+00	3.996E+00	1.486E+00	1.486E+00	1.002E+04
Water	2.947E+05	5.244E+04	2.426E+05	2.426E+05	3.161E+03
Ethylene	1.953E-42	1.964E-42	6.070E-46	6.070E-46	8.580E+02
Diethyl-Ether	8.149E-25	8.148E-25	4.791E-27	4.791E-27	4.404E+02
Methane	7.363E-52	7.404E-52	9.732E-56	9.732E-56	8.850E-02
Acetaldehyde	8.445E-05	7.106E-05	1.380E-05	1.380E-05	1.172E+03
Ethane	4.494E-06	3.744E-06	7.715E-07	7.715E-07	5.727E+01
Acetic Acid	2.473E+02	2.619E+01	2.212E+02	2.212E+02	6.124E-02
Hydrogen	3.883E-52	3.905E-52	5.683E-56	5.683E-56	2.314E-02
Total Mass Flow (lb/h)	2.950E+05	5.247E+04	2.428E+05	2.428E+05	1.571E+04

Table 4.9

Utilities Table for Distillation Section 300					
Stream ID	REBOIL-OUT	FROM-COOL	TO-REBOIL	STEAM301	STEAM302
Type	Cooling Water	Cooling Water	Cooling Water	Steam	Steam
Temperature (°F)	100	100	120	298	298
Pressure (psi)	14.7	14.7	14.7	50	50
Mass Flow (lb/h)	49,342	209,162	258,504	54,267	54,267
Duty (BTU/h)	9.063E+06			49,469,600	

Figure 4.4: Adsorption Sequence 400

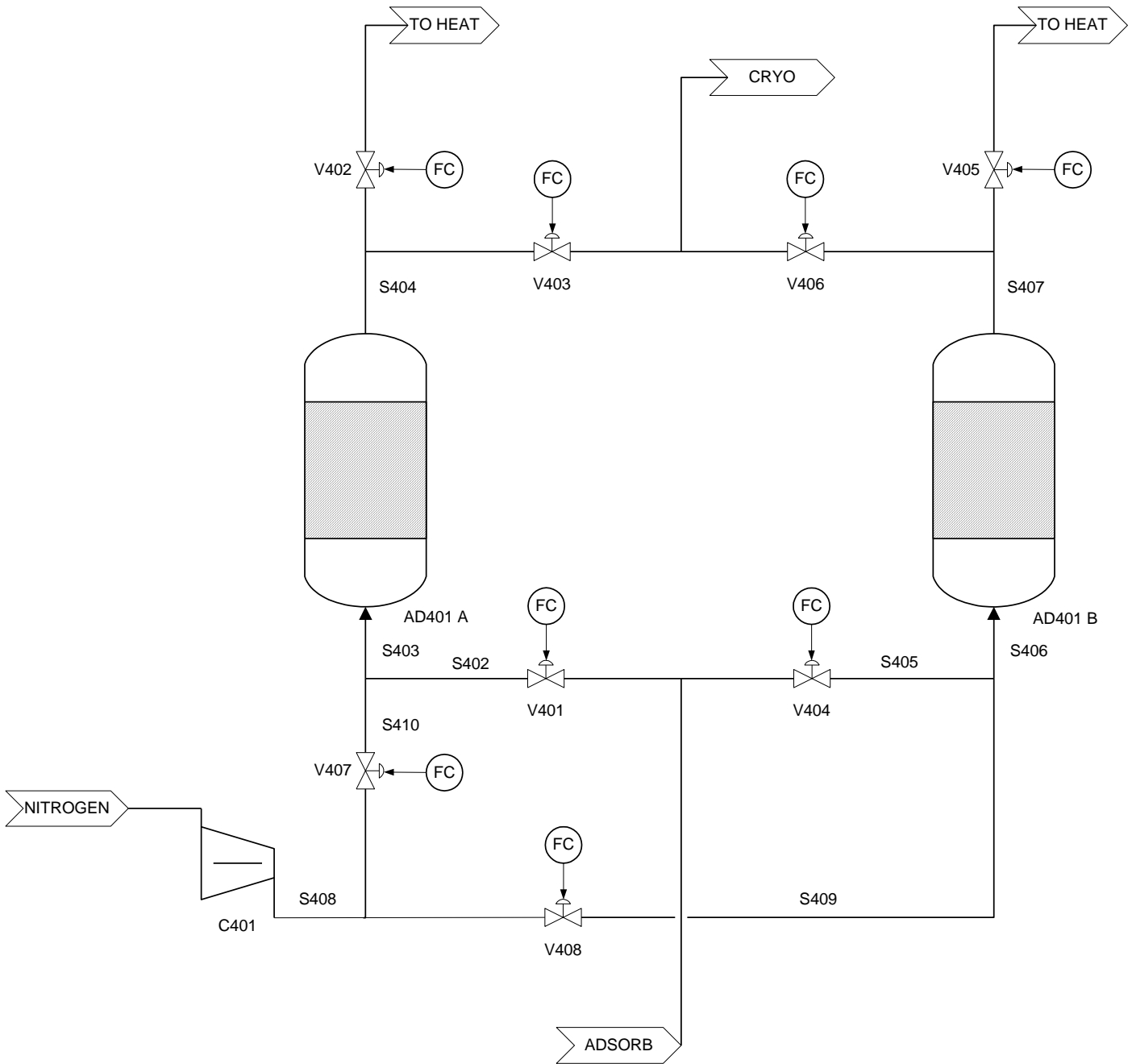


Table 4.10

Stream Table for Adsorption Section 400					
Stream ID	ADSORB	CRYO	NITROGEN	S408	TO HEAT
Temperature (°F)	39.0	39.6	80.0	350.0	352.0
Pressure (psi)	455.6	441.0	15	41	26.3
Vapor Fraction	1.00	1.00	1	1	1.00
Enthalpy (BTU/hr)	2.448E+08	2.459E+08	2.632E+03	2.603E+05	2.608E+05
Volume Flow (ft <sup>3</sup> /h)	100,525	100,854	67,506.0000	36,171.0000	38,210
Mass Flow (lb/hr)					
Ethanol	3.315E+05	3.315E+05	0.000E+00	0.000E+00	0.000E+00
Water	2.460E+02	0.000E+00	0.000E+00	0.000E+00	0.000E+00
Ethylene	6.770E+01	0.000E+00	0.000E+00	0.000E+00	0.000E+00
Diethyl-Ether	3.511E+03	3.511E+03	0.000E+00	0.000E+00	0.000E+00
Methane	4.204E+01	4.204E+01	0.000E+00	0.000E+00	0.000E+00
Acetaldehyde	2.609E+02	2.609E+02	0.000E+00	0.000E+00	0.000E+00
Ethane	1.180E+01	1.180E+01	0.000E+00	0.000E+00	0.000E+00
Acetic Acid	3.500E-02	3.500E-02	0.000E+00	0.000E+00	0.000E+00
Hydrogen	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
Nitrogen	0.000E+00	0.000E+00	4.070E+03	4.070E+03	4.070E+03
Total Mass Flow (lb/h)	3.353E+05	3.350E+05	4.070E+03	4.070E+03	4.070E+03

\*Note: The 400 section is designed such that at a given time the only active streams are ADSORB and CRYO, which are run through one column. The other streams are used for hot Nitrogen purge gas, which cleans the sorbent.

Figure 4.4: Cryogenic Distillation 500

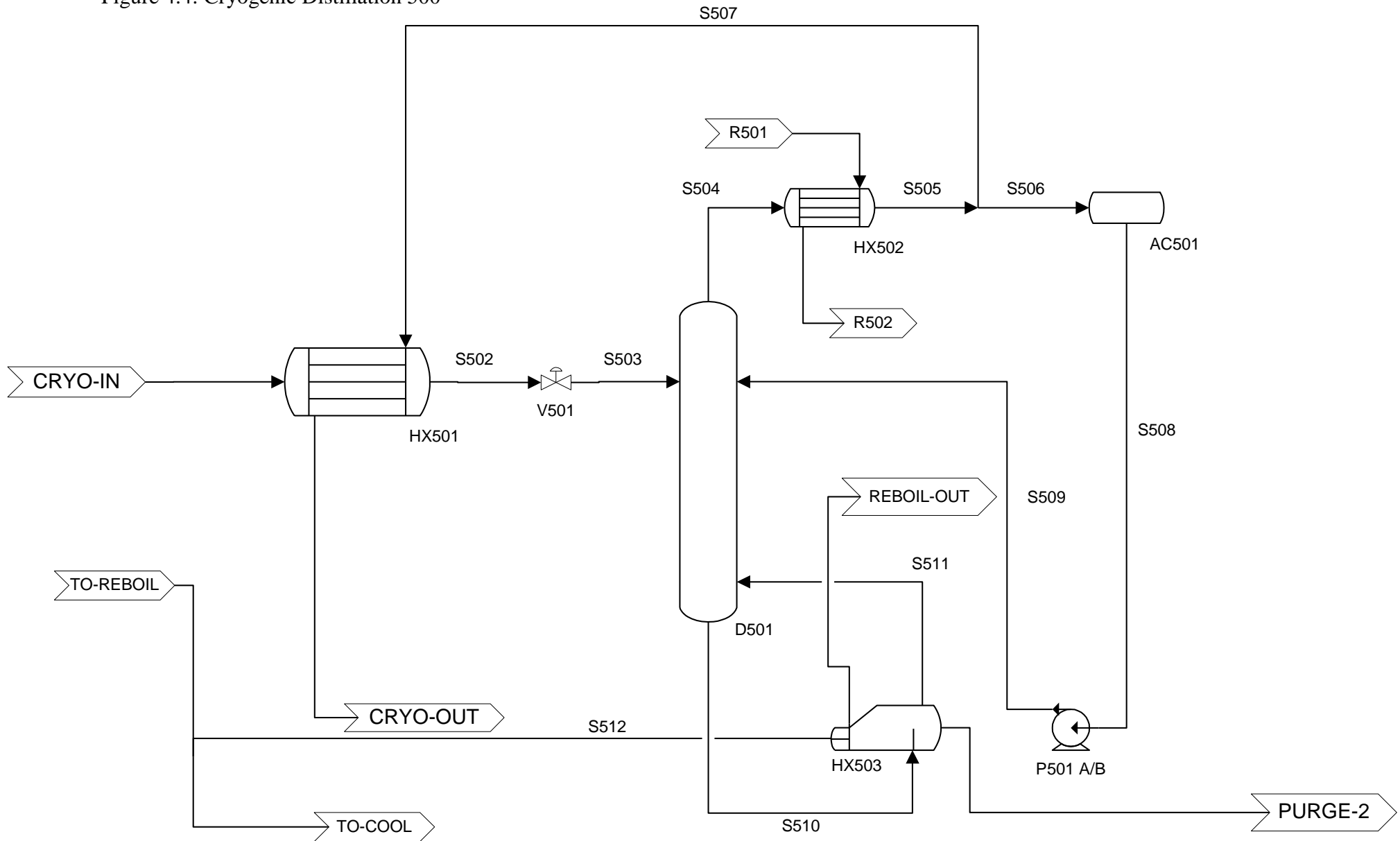


Table 4.11

Stream Table for Cryogenic Distillation Section 500									
Stream ID	CRYO-IN	S502	S503	S504	S505	S506	S507	S508	S509
Temperature (°F)	39.61	6.80	-35.11	-67.15	-67.54	-67.54	-67.54	-67.54	-67.54
Pressure (psi)	455.6	452.5	279.2	279.3	279.2	279.2	279.2	238.2	279.2
Vapor Fraction	1.00	1.00	1.00	1.00	0.57	0.00	1.00	0.00	0.00
Volume Flow (ft <sup>3</sup> /h)	100,864	80,797	139,354	-	-	-	102,938	-	-
Enthalpy (BTU/h)	2.460E+08	2.394E+08	2.394E+08	4.177E+08	3.613E+08	1.228E+08	2.386E+08	2.386E+08	2.386E+08
Mass Flow (lb/h)									
Ethanol	8.716E-07	8.716E-07	8.716E-07	2.460E-05	2.460E-05	3.090E-26	2.460E-05	3.090E-26	3.090E-26
Water	3.103E-07	3.103E-07	3.103E-07	7.312E-10	2.009E-06	2.009E-06	2.913E-13	2.009E-06	2.009E-06
Ethylene	1.174E+04	1.174E+04	1.174E+04	5.781E+05	5.739E+05	2.436E+05	3.303E+05	2.436E+05	2.436E+05
Diethyl-Ether	1.244E+02	1.244E+02	1.244E+02	1.600E+01	3.544E+03	3.544E+03	4.028E-02	3.544E+03	3.544E+03
Methane	3.284E+00	3.284E+00	3.284E+00	1.038E+02	9.970E+01	7.035E+00	9.267E+01	7.035E+00	7.035E+00
Acetaldehyde	2.038E+01	2.038E+01	2.038E+01	4.261E+00	6.204E+02	6.204E+02	1.625E-02	6.204E+02	6.204E+02
Ethane	1.894E+00	1.894E+00	1.894E+00	8.621E+01	1.311E+02	1.036E+02	2.750E+01	1.036E+02	1.036E+02
Acetic Acid	2.757E-03	2.757E-03	2.757E-03	1.532E-07	5.665E-03	5.665E-03	2.485E-12	5.665E-03	5.665E-03
Hydrogen	9.194E-01	9.194E-01	9.194E-01	2.616E+01	2.607E+01	1.205E-01	2.595E+01	1.205E-01	1.205E-01
Total Mass Flow (lb/h)	1.190E+04	1.190E+04	1.190E+04	5.783E+05	5.783E+05	2.479E+05	3.305E+05	2.479E+05	2.479E+05

Table 4.12

Section 500 cont.				
Stream ID	S510	S511	PURGE-2	CRYO-OUT
Temperature (°F)	-66.59	-21.20	-21.15	-35.44
Pressure (psi)	280.0	272.0	279.8	275.6
Vapor Fraction	0.00	1.00	0.00	1.00
Volume Flow (ft <sup>3</sup> /h)	-	-	122	141,716
Enthalpy (BTU/h)	8.236E+07	1.379E+08	-6.496E+06	2.386E+08
Mass Flow (lb/h)				
Ethanol	5.156E-67	7.499E-69	5.081E-67	2.460E-05
Water	8.935E-06	1.792E-07	8.756E-06	2.914E-13
Ethylene	1.918E+05	1.907E+05	1.124E+03	3.303E+05
Diethyl-Ether	5.209E+03	1.697E+03	3.511E+03	4.028E-02
Methane	2.378E-02	2.374E-02	4.273E-05	9.267E+01
Acetaldehyde	1.133E+03	5.583E+02	5.751E+02	1.625E-02
Ethane	1.131E+03	1.105E+03	2.596E+01	2.750E+01
Acetic Acid	7.816E-02	3.482E-04	7.781E-02	2.485E-12
Hydrogen	1.292E-07	1.292E-07	2.089E-11	2.595E+01
Total Mass Flow (lb/h)	1.993E+05	1.940E+05	5.237E+03	3.305E+05

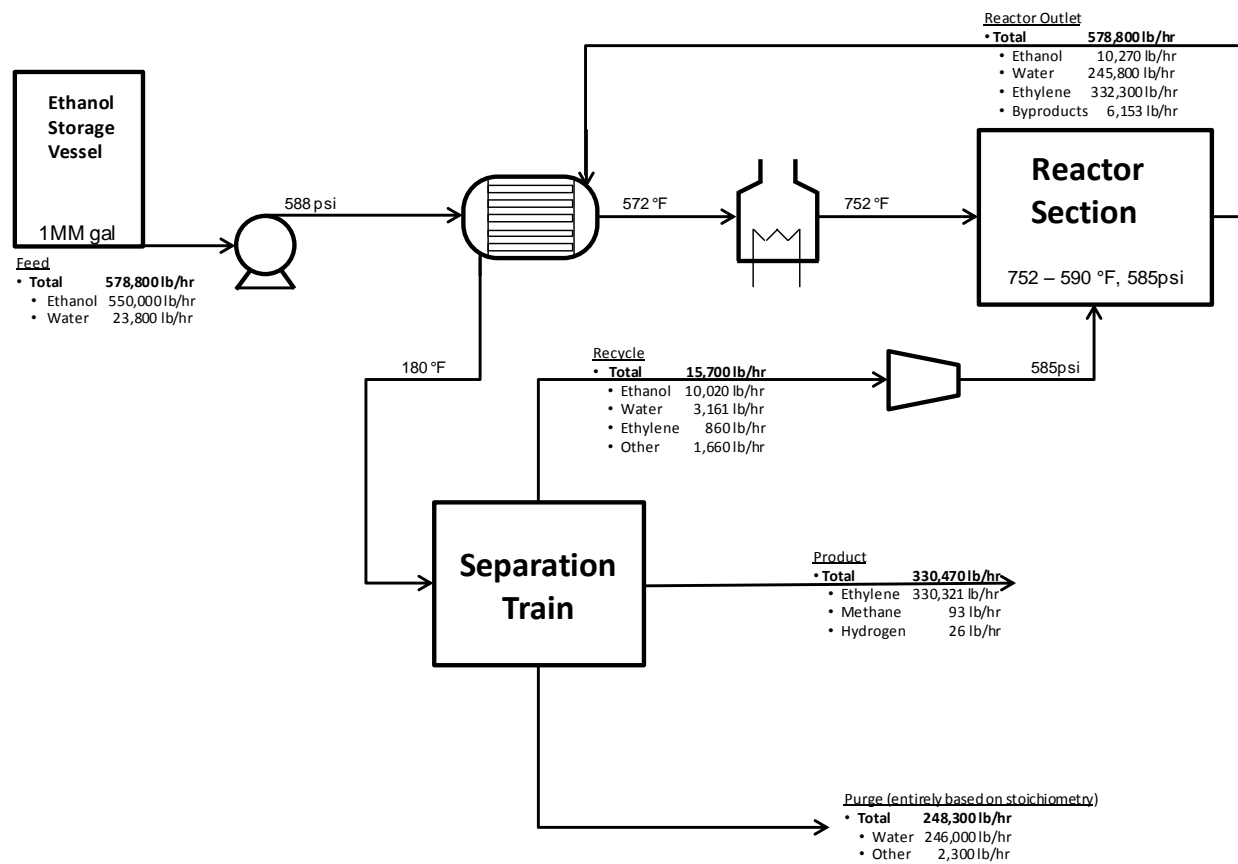
Table 4.13

Utilities Table for Distillation Section 500					
Stream ID	TO-REBOIL	TO-COOL	REBOIL-OUT	R501	R502
Type	Water	Water	Water	Propylene	Propylene
Temperature (°F)	100	100	120	-78	-78
Pressure (psi)	14.7	14.7	14.7	-	-
Mass Flow (lb/h)	258,504	49,342	49342	420000	420000
Duty (BTU/h)	N/A	4.904E+07		-5.637E+07	

# **Section V**

## **Process Description**

Figure 6.1



## Overview

The above illustration (Figure 6.1) provides a brief introduction to the specifics of the process. Each item mentioned will be described in more detail in the sections immediately following. In addition, the exact specifications for each process unit are provided in Section X. The process begins with a 1MM gallon feed storage tank. A tank of this size can hold a one month supply of ethanol. The feed is then pumped to a high pressure, vaporized, and passed through a series of three adiabatic reactors. Just after leaving the second reactor, it is combined with a recycle stream. The reaction products are sent through a separation train designed to purify the ethylene product to a polymer-grade level of 99.96%. The ethylene product stream is sent directly into the customer's barge or, if necessary, into one of the two on-site spherical storage tanks available. A plant operating at this capacity is capable of filling a 3000 ton barge in 18 hours. The separation train also produces a waste stream of mostly water, which is sent directly to an off-site waste treatment facility.



## **Feed Storage**

A 95% solution of ethanol (5% water) feed is stored at atmospheric pressure and temperature in a 1MM gallon, floating-roof storage tank. This volume is large enough to hold a one month supply of ethanol and will be replenished by the ethanol plants located conveniently in the area. The large volume of storage allows the plant to continue operation for one month into the rainy season when Brazilian ethanol plants cease production and the price of ethanol increases. In addition, it provides flexibility in scheduling feed replenishment and helps ensure consistent production. In the future, it might be of value to install a direct piping route from one of those plants; however, for now it is assumed that all feed ethanol arrives via railcars and barges and is pumped directly into the storage tank.

## **Reactor Section**

The reactor section of this process is shown in Figure 4.1 and details regarding the conditions and contents of the streams in this section are included in Tables 4.1, 4.2, and 4.3. Two, three-staged pumps in parallel (P101 A/B and P102 A/B) are used to increase the pressure of the feed stream to 603 psi. This very high pressure is used to obviate subsequent compression that would be needed in the separation train. At the high flow rates at which this plant operates, the economic difference between pumping here and compressing later is on the order of \$12MM/year.

The stream is then passed through a shell and tube heat exchanger (HX101) which is used to preheat the feed to 572°F. HX101 uses the heated reactor effluent stream (S110) to reduce the energy required to raise the feed to temperatures. A furnace (F101) is necessary to heat the feed stream the rest of the way to the desired reactor inlet temperature of 752°F. Furnace F101 will require about 60,000SCF/h of natural gas to supply enough energy and impart this temperature increase.

A series of three adiabatic, fixed-bed reactors follows (R101, R102, and R103) in which the overall reaction of ethanol to water, ethylene, diethyl-ether, methane and the other byproducts takes place. The reactors are sized progressively to accommodate the increasing volume of fluid and ensure adequate overall conversion of ethanol. R101 is 224 ft<sup>3</sup>, R102 is 256 ft<sup>3</sup>, and R103 is

310 ft<sup>3</sup>. The large increase in volume between R102 and R103 is due to the addition of the ethanol recycle stream (RECYCLE). The high pressure and temperature conditions at which these reactors operate result in an overall ethanol conversion of 98% and an ethylene yield of 98%.

The three reactors are filled to capacity with  $\gamma$ -alumina catalyst in the form of 1cm diameter spherical pellets. The total weight of catalyst required is 126,260lb. Every 90 days it is necessary to discard and replace all of the catalyst. Regeneration is not feasible because the loss of catalytic activity is due directly to irreversible damage caused by constant exposure to the high temperature and pressure conditions in the reactors. It was deemed economical to have a separate, identical reactor train running in parallel. For a 1% (~\$600,000) increase in the total permanent investment (Table 7.2), the cost of 3 additional reactors (Table 7.1), the plant can run consistently and not have to shut down every 90 days. This investment pays for itself in under 3 years. If it takes 2 days to replace the catalyst, the plant would lose approximately \$250,000 in net revenue without the spare reactors.

Between each reactor is a furnace (F102 and F103) that heats the stream from 590°F back to the desired 752°F. The intermittent heating steps serve to negate the temperature reduction caused by the endothermic dehydration reaction and maintain the driving force toward ethylene production. These furnaces require about 53,000SCF/hr of natural gas.

Upon leaving the reactor, the products enter HX101 which lowers their temperature to 179° F. It is desirable to remove as much heat as possible from this stream since the separation train requires low temperatures. In addition, the stream that is being heated requires additional heating after this step. Thus, this heat exchanger was designed to transfer as much heat as possible by specifying the temperature of the stream going into the reactors (S103 above) at the maximum it can possibly reach without violating a minimum approach temperature of 40°F. Having a minimum approach temperature helps to increase heat exchanger efficiency and keeps the necessary surface area for transfer from growing out of control. The reactor effluent stream then enters the separation train.

## **Separation Train**

After the reactor effluent stream (S110) passes through HX101 and is cooled by the feed stream, it enters the separation phase of the process. The separations section is designed to bring the ethylene product to a 99.96% purity using as little equipment and as few utilities as possible. It can roughly be broken into 4 sections as shown in the flow diagrams above: a flash section that removes the high boiling components (Figure 4.2), a distillation section (Figure 4.3) that removes most of the water from the process so that the unreacted ethanol can be recycled without causing reactor volume to grow too large, a drying section (Figure 4.4) in which adsorption is used to remove any remaining water and ethanol, and a cryogenic distillation section (Figure 4.5) in which very low temperatures are used to finally achieve the needed purity of ethylene. A more detailed run down of each step follows.

Upon passing through HX101, the stream goes through a cooler, HX201, to further reduce the temperature. This cooler is designed so that it can use cooling water as its utility. It requires approximately 903,000 lb/h of cooling water (Table 4.4) to achieve the necessary heat transfer. Next, the stream is throttled to the desired pressure of 558.4psi and fed into a flash drum, FL201.

This first of two flash vessels (FL201, FL202) serves to remove the bulk of the water and unreacted ethanol and to lighten the duty of the intermediate heat exchanger (HX202). The bottom stream (S204) is sent to a distillation tower (D301) and the top stream (S205) is sent to the intermediate cooler (HX202).

The top stream (S205) is cooled to 57°F, throttled to 455psi, and fed into the second flash drum (FL202). The vapor product is then passed through an adsorption unit (AD401A) and the liquid product is fed along with the previous product into the distillation tower (D301). This vessel was designed with the purity of the top stream in mind rather than the flow rate of ethylene. It was deemed more important to remove as much water and ethanol as possible from this stream, even though some ethylene must be sent to the distillation tower (D301) to do so. If the flash specifications are modified so that 50% of the ethylene that exits through the bottom stream now exits through the top, it takes about 2646lb/h of water and ethanol with it (this is likely due to solubility). This is a 400% increase from what the design currently specified and results in a roughly \$3.5MM increase in capital cost to cover the much larger adsorption column

dimensions. In contrast, increasing the ethylene flow rate into the distillation tower does not change capital costs appreciably and has hardly any effect at all on annual utilities.

The combined liquid streams from the flash vessels are then fed into a 26 stage distillation column (D301). The main purpose of this column is to strip away most of the water so that a more concentrated ethanol stream can be returned to the reactors. The detailed specifications of the column are included in Section X.

Care was taken to ensure that almost no ethanol was purged. The partial condenser utilizes cooling water and requires approximately 260,000 lb/hr to achieve the necessary heat transfer. The reboiler uses 50psi steam and requires approximately 54,000 lb/hr. The distillate stream (S305) is fed into a compressor (C301) where it is returned to roughly 600psi and recycled into the reactors. The bottoms (TREAT) is purged and pumped to an off-site waste treatment facility.

When designing this column, additional consideration was paid to finding the best pressure at which to operate. It was determined from economic analysis that throttling the feed all the way down to 14.7 psig and then compressing the reflux back to 600psi reduces annual costs considerably. This is because the utility costs for the reboiler greatly diminish as the column pressure decreases. If the column is operated at the column feed stream's pressure of 455 psi, the temperature of the bottoms stream is 440°F. This high temperature requires 450psi steam and accounts for roughly \$6.2MM/yr in operating costs. When compared to the cost of the reboiler, the \$33,000 annual cost of compression disappears in the rounding. Throttling to 14.7psig reduces the reboiler temperature to 256°F which can easily be achieved with only 50psi steam. While the cost of compression does skyrocket all the way to \$360,000 /yr, the reboiler cost decreases to only \$1.4M/yr for a net 73% utilities cost.

The vapor stream from the second flash vessel (ADSORB) then enters stage 4 of the separation train: the drying stage. In this stage, the vapor is fed through an adsorption column (AD401A) packed with zeolite 13X particles. This step is critical in ensuring that absolutely no water or ethanol remains in the stream that will next be fed into the cryogenic distillation tower. If any of either of those two components remains, the cryogenic conditions could cause them to freeze and damage the column.

In order to have a continuous process, it is necessary to run two units in parallel, with one unit processing the stream while the other unit is undergoing regeneration of the sorbent. It was recommended that our design incorporate a daily cycle where each column is active for a day, then regenerated for a day with that cycle repeating. This recommendation proved to give reasonable column sizes and capital costs.

The dried stream (CRYO) passes through a heat exchanger (HX501) where the stream is cooled to 6.8°F by exchanging with the final product stream (S507). Then it is throttled one last time. This step reduces the temperature all the way to -35°F by dropping the pressure to 279psi, a suitable temperature to perform cryogenic distillation.

The ethylene-rich stream is then fed into the cryogenic distillation unit (D501). D501 has 8 sieve trays and operates with a condenser pressure of 279.2psi. The partial condenser (HX502) operates at -67.54°F and requires  $5.637 \times 10^7$  BTU/hr of refrigeration to achieve the necessary reflux ratio of 0.75. For temperatures in this range, propylene was selected as an appropriate refrigerant and it was determined that 420,000 lb/hr are required to achieve this degree of refrigeration.

The reboiler (HX503) operates at -35°F and therefore only requires cooling water to heat. 49,342 lb/hr of cooling water are needed to achieve the required heat transfer of  $4.904 \times 10^7$  BTU/hr. The cooling water used for this heat exchanger is piped directly from that used to cool the condenser in the recycling distillation section (HX301). Following the path of the cooling water (stream S312 in Figure 4.3), first it enters HX301 at 90°F. It exchanges with the top stream of D301 and exits at 120°F (stream TO-REBOIL). From there (moving to Figure 4.5), it splits into two fractions (S512 and TO-COOL). TO-COOL is sent directly to the cooling tower and recycled to the process. Stream S512 is sent to the reboiler of the cryogenic column (HX503). The split fraction was set so that the amount of cooling water that flows through HX503 allows for a temperature change from 120°F to 90°F. In this way, 49.342 lb/h of cooling water is both heated and cooled within the process and can be considered a close to free utility.

Distillation column (D501) removes ethane and the other heavy impurities to the bottom (S510) and leaves the 99.96% pure ethylene product in the top (S504). This stream is then passed through two heat exchangers in series (HX501 then HX202) to fully utilize its cooling ability. First it pre-cools the feed to D501 by exchanging with CRYO-IN. Then it exchanges with S205

to cool the feed to the second flash vessel (FL202). After exiting these two exchangers, the ethylene product stream (PRODUCT) is at a temperature of 52°F.

The 1MM tonnes of ethylene product coming from HX202 is fed directly into the customers' barges for transportation to plastic plants around the world. Anticipating a maximum barge capacity of 3000 tons, our plant will require barges to cycle every 18 hours. To maintain reliable production and hopefully be able to run continuously throughout the dry season, 2MM gallon tanks are included in the design to store approximately 3 hours worth of ethylene in case of unforeseen delays in the transportation. Any more than that results in simply too great of a capital and land strain.

# **Section VI**

## **Energy Balance and Utility Requirements**

The major heating requirements of the ethanol processing plant lie mainly in the three fired heaters (F101, F102, and F103) intermittently placed between the three adiabatic reactors. Together these three furnaces account for 175,000,000 BTU/hr. The various pumps and compressors necessary to move the liquid/vapor streams through the process contribute relatively little to overall energy requirements of the process. The other major heating/cooling requirements lie in the heat exchangers. HX301 and HX302 function as the condenser and reboiler of distillation column D301, respectively. HX502 functions as the condenser of the cryogenic distillation column D501. Meanwhile, HX203 is the only standalone heat exchanger that contributes a heat duty to the process, utilizing cooling water to achieve the remaining cooling of the reactor effluent.

Additionally, various other heat exchangers are present throughout the process, such as HX202, HX501, and HX503, which do not contribute a heat duty to overall process. This is a result of efficient stream matching, coupling necessary hot and cold streams within the process with each other to achieve the desired result. HX202 and HX501 each utilize the distillate stream, S507, of D501 to respectively cool the vapor product of the flash vessel FL201 and the input to D501. HX503 similarly uses the exit cooling water of HX301 to reboil the bottoms stream of D501.

Table 6.2 shows a complete list of all utilities that are necessary. Cooling water, low pressure steam (50 psig), natural gas, and propylene are needed to achieve the proper heating and cooling within the process. Also shown in Table 6.2 are the electrical power requirements of each piece of equipment.



Table 6.1

<b>ENERGY REQUIREMENTS OF PROCESS</b>			
<u>Equipment</u>	<u>Description</u>	<u>Duty</u> (BTU/hr)	<u>Source</u>
<u>Section 100</u>			
<b>F101</b>	Fired Heater	63,111,000	Natural Gas
<b>F102</b>	Fired Heater	55,553,221	Natural Gas
<b>F103</b>	Fired Heater	56,420,329	Natural Gas
<b>P101 AB</b>	Pump	839,261	Electricity
<b>P102 AB</b>	Pump	839,261	Electricity
		<b><u>176,763,072</u></b>	<i>Net Section 100</i>
<u>Section 200</u>			
	Heat		Cooling
<b>HX201</b>	Exchanger	-27,014,000	Water
		<b><u>-27014000</u></b>	<i>Net Section 200</i>
<u>Section 300</u>			
<b>P301</b>	Pump	1,356	Electricity
	Heat		Cooling
<b>HX301</b>	Exchanger	-39,976,822	Water
	Heat		Steam (50
<b>HX302</b>	Exchanger	49,469,600	psig)
<b>P302</b>	Pump	16,426	Electricity
<b>C301</b>	Compressor	2,936,625	Electricity
		<b><u>12,447,185</u></b>	<i>Net Section 300</i>
<u>Section 400</u>			
<b>C401</b>	Compressor	295,482	Electricity
	Adsorbtion		
<b>AD401</b>	Column	113,400	Electricity
		<b><u>408,882</u></b>	<i>Net Section 400</i>
<u>Section 500</u>			
<b>P501</b>	Pump	36,566	Electricity
	Heat		
<b>HX502</b>	Exchanger	-56,357,300	Propylene
		<b><u>-56,320,734</u></b>	<i>Net Section 500</i>
<b>Required</b>		<b><u>106,284,405 BTU/HR</u></b>	

Table 6.2

<b>UTILITIES REQUIREMENT OF PROCESS</b>			
<b>Electricity</b>		<b>kW</b>	
<u>Equipment List</u>	<u>Description</u>	<u>Usage</u>	<u>Cost (\$)</u>
P101AB		230	129,367
P102AB		230	129,367
P301		0.4	160
P302		4.81	1,941
C301		860	452,562
C401		86.6	45,457
AD401		33.2	10,000
P501		10.7	4,321
<b>Cooling Water</b>		<b>lb/hr</b>	
<u>Equipment List</u>	<u>Description</u>	<u>Usage</u>	<u>Cost (\$)</u>
HX201		901,425	55,068
HX301		253,085	24,100
<b>Steam (50 psig)</b>		<b>lb/hr</b>	
<u>Equipment List</u>	<u>Description</u>	<u>Usage</u>	<u>Cost (\$)</u>
HX302		54,266	1,091,736
<b>Natural Gas</b>		<b>SCF/hr</b>	
<u>Equipment List</u>	<u>Description</u>	<u>Usage</u>	<u>Cost (\$)</u>
F101		60,106	2,176,170
F102		52,908	1,915,565
F103		53,734	1,945,465
<b>Refrigeration</b>		<b>lb/hr</b>	
<u>Equipment List</u>	<u>Description</u>	<u>Usage</u>	<u>Cost (\$)</u>
HX502	Propylene	420,000	5,368,643
<b>Cleaning</b>		<b>lb/hr</b>	<b>Cost (\$)</b>
<u>Equipment List</u>	<u>Description</u>	<u>Usage</u>	
C401	Nitrogen		91,800

# **Section VII**

## **Economic Discussion and Market Analysis**

One major difficulty with this project is that the selling price of ethylene relative to ethanol is too low for the plant to be profitable, given 1.73lb ethanol are required to produce 1lb ethylene. An evaluation of current markets (discussed later) suggests that the selling price of ethylene in 2014 should be around \$0.60/lb, while the price of ethanol is expected to fall around \$0.34/lb. With these values, sales of ethylene will not cover operating and raw material costs, and the Net Present Value of the venture will become increasingly negative over time. However, a sensitivity analysis of the response of NPV and Internal Rate of Return to ethanol and ethylene prices does provide some hope; should the prices of these commodities fall around \$0.64/lb ethylene and \$0.305/lb ethanol, the plant will become profitable.

Additionally, in an attempt to cut costs, the same analyses were conducted under the condition that Research and Development (a variable cost previously equal to 4.8% of sales) was shut down completely. With this change, the potential profitability of the plant increases considerably. Realistically, it is unwise to entirely scrap all R&D; however it is interesting to consider the potential value of shrinking the department.

The following section details the various costs of the plant, and shows the aforementioned sensitivity analysis. Additionally, there is a discussion of other important economic considerations.

**Summary of Costs**

The following cost analysis is based on selling prices of \$0.60/lb ethylene and \$0.34/lb ethanol. It was determined that the total equipment cost for the plant will be \$40MM (Figure 7.1). The Direct Permanent Investment will be \$49MM and the Total Permanent Investment will be \$65MM. The Total Depreciable Capital will be \$58MM (Figure 7.2). The plant's total capital investment will be around \$78MM (Figure 7.5). At the current market prices for ethylene and ethanol, the Internal Rate of Return for the project will be negative (Figure 7.7), which is obviously undesirable. Later in this section, the conditions for a positive IRR and Net Present Value are discussed in more detail.

Figure 7.1

<u>Equipment Description</u>		<u>Bare Module Cost</u>
P101 A/B	Process Machinery	\$129,000
P102 A/B	Process Machinery	\$129,000
HX101	Fabricated Equipment	\$860,000
F101	Fabricated Equipment	\$4,022,000
R101-A/B	Fabricated Equipment	\$192,000
F102	Fabricated Equipment	\$1,916,000
R102-A/B	Fabricated Equipment	\$250,000
F103	Fabricated Equipment	\$1,945,000
R1023-A/B	Fabricated Equipment	\$250,000
HX201	Fabricated Equipment	\$253,000
FL201	Fabricated Equipment	\$252,000
HX202	Fabricated Equipment	\$149,000
FL202	Fabricated Equipment	\$179,000
D301	Fabricated Equipment	\$809,000
HX301	Fabricated Equipment	\$84,000
AC301	Fabricated Equipment	\$32,000
P301 A/B	Process Machinery	\$16,000
P302 A/B	Process Machinery	\$27,000
C301	Fabricated Equipment	\$4,634,000
HX302	Fabricated Equipment	\$380,000
C401	Fabricated Equipment	\$290,000
AD401	Fabricated Equipment	\$729,000
AD402	Fabricated Equipment	\$729,000
HX501	Fabricated Equipment	\$157,000
D501	Fabricated Equipment	\$720,000
HX502	Fabricated Equipment	\$9,464,000
AC501	Fabricated Equipment	\$268,000
P501 A/B	Process Machinery	\$33,000
HX503	Fabricated Equipment	\$225,000
FEED TANK	Fabricated Equipment	\$1,820,000
PRODUCT TANK	Fabricated Equipment	\$4,257,000
PRODUCT TANK	Fabricated Equipment	\$4,257,000
P101 A/B	Fabricated Equipment	\$129,000
P102 A/B	Fabricated Equipment	\$129,000
R102-A/B	Fabricated Equipment	\$16,000
		\$27,000
		\$33,000
		\$192,000
		\$250,000
<b>Total</b>		<b><u>\$40,233,000</u></b>

Figure 7.2

<b><u>Investment Summary</u></b>		
<b><u>Bare Module Costs</u></b>		
Fabricated Equipment	\$	43,956,199
Process Machinery	\$	334,964
Spares	\$	-
Storage	\$	558,300
Other Equipment	\$	-
Catalysts	\$	-
Computers, Software, Etc.	\$	-
<b><u>Total Bare Module Costs:</u></b>		<b><u>\$ 44,849,463</u></b>
<b><u>Direct Permanent Investment</u></b>		
Cost of Site Preparations:	\$	2,242,473
Cost of Service Facilities:	\$	2,242,473
Allocated Costs for utility plants and related facilit	\$	-
<b><u>Direct Permanent Investment</u></b>		<b><u>\$ 49,334,409</u></b>
<b><u>Total Depreciable Capital</u></b>		
Cost of Contingencies & Contractor Fees	\$	8,880,194
<b><u>Total Depreciable Capital</u></b>		<b><u>\$ 58,214,603</u></b>
<b><u>Total Permanent Investment</u></b>		
Cost of Land:	\$	1,164,292
Cost of Royalties:	\$	-
Cost of Plant Start-Up:	\$	5,821,460
<b>Total Permanent Investment - Unadjusted</b>		<b>\$ 65,200,355</b>
Site Factor		1.00
<b><u>Total Permanent Investment</u></b>		<b><u>\$ 65,200,355</u></b>

Figure 7.3

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**Fixed Cost Summary**


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**Operations**

Direct Wages and Benefits	\$	364,000
Direct Salaries and Benefits	\$	54,600
Operating Supplies and Services	\$	21,840
Technical Assistance to Manufacturing	\$	-
Control Laboratory	\$	-
<b>Total Operations</b>	<b>\$</b>	<b>440,440</b>

**Maintenance**

Wages and Benefits	\$	2,619,657
Salaries and Benefits	\$	654,914
Materials and Services	\$	2,619,657
Maintenance Overhead	\$	130,983
<b>Total Maintenance</b>	<b>\$</b>	<b>6,025,211</b>

**Operating Overhead**

General Plant Overhead:	\$	262,215
Mechanical Department Services:	\$	88,636
Employee Relations Department:	\$	217,897
Business Services:	\$	273,295
<b>Total Operating Overhead</b>	<b>\$</b>	<b>842,043</b>

**Property Taxes and Insurance**

Property Taxes and Insurance:	\$	1,164,292
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**Other Annual Expenses**

Rental Fees (Office and Laboratory Space):	\$	-
Licensing Fees:	\$	-
Miscellaneous:	\$	-
<b>Total Other Annual Expenses</b>	<b>\$</b>	<b>-</b>

<b><u>Total Fixed Costs</u></b>	<b>\$</b>	<b><u>8,471,987</u></b>
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Figure 7.4

<b>Variable Cost Summary</b>		
<b><u>Variable Costs at 100% Capacity:</u></b>		
<b><u>General Expenses</u></b>		
Selling / Transfer Expenses:		\$ 39,872,544
Direct Research:		\$ 63,796,071
Allocated Research:		\$ 6,645,424
Administrative Expense:		\$ 26,581,696
Management Incentive Compensation:		\$ 16,613,560
<b>Total General Expenses</b>		<b>\$ 153,509,295</b>
<b><u>Raw Materials</u></b>	\$0.595680 per lb of Ethylene	\$1,319,515,398
<b><u>Byproducts</u></b>	\$0.000000 per lb of Ethylene	\$0
<b><u>Utilities</u></b>	\$0.006222 per lb of Ethylene	\$13,783,367
<b><u>Total Variable Costs</u></b>		<b><u>\$ 1,486,808,060</u></b>

Figure 7.5

<b>Working Capital</b>			
	<b><u>2015</u></b>	<b><u>2016</u></b>	<b><u>2017</u></b>
Accounts Receivable	\$ 49,157,931	\$ 24,578,966	\$ 24,578,966
Cash Reserves	\$ 823,143	\$ 411,572	\$ 411,572
Accounts Payable	\$ (49,313,790)	\$ (24,656,895)	\$ (24,656,895)
Ethylene Inventory	\$ 6,554,391	\$ 3,277,195	\$ 3,277,195
Raw Materials	\$ 3,253,600	\$ 1,626,800	\$ 1,626,800
<b>Total</b>	<b>\$ 10,475,275</b>	<b>\$ 5,237,637</b>	<b>\$ 5,237,637</b>
<i>Present Value at 15%</i>	\$ 6,887,663	\$ 2,994,636	\$ 2,604,032
<b><u>Total Capital Investment</u></b>		<b><u>\$ 77,686,686</u></b>	

Figure 7.6

Cash Flow Summary															
Year	Percent Capacity	Product Unit Price	Sales	Sales	Capital Costs	Working Capital	Var Costs	Fixed Costs	Depreciation	Taxible Income	Taxible Income	Taxes	Net Earnings	Cash Flow	NPV
2012	0%		-	-	-	-	-	-	-	-	-	-	-	-	-
2013	0%		-	-	(65,200,400)	-	-	-	-	-	-	-	-	(65,200,400)	(56,696,000)
2014	0%		-	-	-	-	-	-	-	-	-	-	-	-	(56,696,000)
2015	0%		-	-	-	(10,475,300)	-	-	-	-	-	-	-	(10,475,300)	(63,583,600)
2016	45%	\$0.60	598,088,164	598,088,200	-	(5,237,600)	(669,063,600)	(8,472,000)	(11,642,900)	(91,090,370)	(91,090,400)	33,703,400	(57,386,900)	(50,981,700)	(92,732,500)
2017	68%	\$0.60	897,132,246	897,132,200	-	(5,237,600)	(1,003,595,400)	(8,472,000)	(18,628,700)	(133,563,854)	(133,563,900)	49,418,600	(84,145,200)	(70,754,200)	(127,909,900)
2018	90%	\$0.60	1,196,176,327	1,196,176,300	-	-	(1,338,127,300)	(8,472,000)	(11,177,200)	(161,600,117)	(161,600,100)	59,792,000	(101,808,100)	(90,630,900)	(167,092,100)
2019	90%	\$0.60	1,196,176,327	1,196,176,300	-	-	(1,338,127,300)	(8,472,000)	(6,706,300)	(157,129,235)	(157,129,200)	58,137,800	(98,991,400)	(92,285,100)	(201,785,500)
2020	90%	\$0.60	1,196,176,327	1,196,176,300	-	-	(1,338,127,300)	(8,472,000)	(6,706,300)	(157,129,235)	(157,129,200)	58,137,800	(98,991,400)	(92,285,100)	(231,953,700)
2021	90%	\$0.60	1,196,176,327	1,196,176,300	-	-	(1,338,127,300)	(8,472,000)	(3,353,200)	(153,776,074)	(153,776,100)	56,897,100	(96,878,900)	(93,525,800)	(258,539,500)
2022	90%	\$0.60	1,196,176,327	1,196,176,300	-	-	(1,338,127,300)	(8,472,000)	-	(150,422,913)	(150,422,900)	55,656,500	(94,766,400)	(94,766,400)	(281,964,300)
2023	90%	\$0.60	1,196,176,327	1,196,176,300	-	-	(1,338,127,300)	(8,472,000)	-	(150,422,913)	(150,422,900)	55,656,500	(94,766,400)	(94,766,400)	(302,333,700)
2024	90%	\$0.60	1,196,176,327	1,196,176,300	-	-	(1,338,127,300)	(8,472,000)	-	(150,422,913)	(150,422,900)	55,656,500	(94,766,400)	(94,766,400)	(320,046,300)
2025	90%	\$0.60	1,196,176,327	1,196,176,300	-	-	(1,338,127,300)	(8,472,000)	-	(150,422,913)	(150,422,900)	55,656,500	(94,766,400)	(94,766,400)	(335,448,500)
2026	90%	\$0.60	1,196,176,327	1,196,176,300	-	-	(1,338,127,300)	(8,472,000)	-	(150,422,913)	(150,422,900)	55,656,500	(94,766,400)	(94,766,400)	(348,841,700)
2027	90%	\$0.60	1,196,176,327	1,196,176,300	-	-	(1,338,127,300)	(8,472,000)	-	(150,422,913)	(150,422,900)	55,656,500	(94,766,400)	(94,766,400)	(360,487,900)
2028	90%	\$0.60	1,196,176,327	1,196,176,300	-	-	(1,338,127,300)	(8,472,000)	-	(150,422,913)	(150,422,900)	55,656,500	(94,766,400)	(94,766,400)	(370,615,100)
2029	90%	\$0.60	1,196,176,327	1,196,176,300	-	-	(1,338,127,300)	(8,472,000)	-	(150,422,913)	(150,422,900)	55,656,500	(94,766,400)	(94,766,400)	(379,421,400)
2030	90%	\$0.60	1,196,176,327	1,196,176,300	-	-	(1,338,127,300)	(8,472,000)	-	(150,422,913)	(150,422,900)	55,656,500	(94,766,400)	(94,766,400)	(387,079,000)
2031	90%	\$0.60	1,196,176,327	1,196,176,300	-	20,950,500	(1,338,127,300)	(8,472,000)	-	(150,422,913)	(150,422,900)	55,656,500	(94,766,400)	(73,815,900)	(392,265,700)

Figure 7.7

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**Profitability Measures**

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<b>The Internal Rate of Return (IRR) for this project is</b>	Negative IRR
<b>The Net Present Value (NPV) of this project in 2012 is</b>	\$ (392,265,700)

**ROI Analysis (Third Production Year)**

<b>Annual Sales</b>	<b>1,196,176,327</b>
<b>Annual Costs</b>	<b>(1,346,599,240)</b>
<b>Depreciation</b>	<b>(5,216,028)</b>
<b>Income Tax</b>	<b>57,586,408</b>
<b>Net Earnings</b>	<b>(98,052,533)</b>
<b>Total Capital Investment</b>	<b>86,150,905</b>
<b>ROI</b>	<b>-113.81%</b>

### Ethylene/Ethanol Price Sensitivity (With Research and Development)

The following figures (Figure 7.8, 7.9) show how the NPV and IRR vary with the prices of ethylene and ethanol. Notice that the plant will only be profitable with relatively high ethylene prices (\$0.63/lb) and low ethanol prices (\$0.32/lb).

Figure 7.8

#### Net Present Value for Varied Ethanol and Ethylene Prices

		ETHYLENE \$/LB					
		\$0.62	\$0.63	\$0.64	\$0.65	\$0.66	\$0.67
E T H A N O L \$/LB	\$0.360	(505,735,700)	(429,816,500)	(391,857,000)	(353,897,400)	(315,937,800)	(277,978,300)
	\$0.355	(467,878,300)	(391,959,200)	(353,999,600)	(316,040,000)	(278,080,500)	(240,120,900)
	\$0.350	(430,020,900)	(354,101,800)	(316,142,200)	(278,182,600)	(240,223,100)	(202,263,500)
	\$0.345	(392,163,500)	(316,244,400)	(278,284,800)	(240,325,300)	(202,365,700)	(164,406,100)
	\$0.340	(354,306,100)	(278,387,000)	(240,427,400)	(202,467,900)	(164,508,300)	(126,548,800)
	\$0.335	(467,878,300)	(240,529,600)	(202,570,100)	(164,610,500)	(126,650,900)	(88,691,400)
	\$0.330	(278,591,400)	(202,672,200)	(164,712,700)	(126,753,100)	(88,793,600)	(50,834,000)
	\$0.325	(240,734,000)	(164,814,900)	(126,855,300)	(88,895,700)	(50,936,200)	(12,976,600)
	\$0.320	(202,876,600)	(126,957,500)	(88,997,900)	(51,038,400)	(13,078,800)	24,880,800
	\$0.315	(165,019,200)	(89,100,100)	(51,140,500)	(13,181,000)	24,778,600	62,738,100
	\$0.310	(127,161,900)	(51,242,700)	(13,283,200)	24,676,400	62,636,000	100,595,500
	\$0.305	(89,304,500)	(13,385,300)	24,574,200	62,533,800	100,493,300	138,452,900
\$0.300	(51,447,100)	24,472,000	62,431,600	100,391,200	138,350,700	176,310,300	

Figure 7.9

#### Internal Rate of Return for Varied Ethanol and Ethylene Prices

		ETHYLENE \$/LB					
		\$0.62	\$0.63	\$0.64	\$0.65	\$0.66	\$0.67
E T H A N O L \$/LB	\$0.360	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
	\$0.355	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
	\$0.350	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
	\$0.345	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
	\$0.340	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
	\$0.335	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
	\$0.330	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	2%
	\$0.325	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	12%
	\$0.320	Negative IRR	Negative IRR	Negative IRR	Negative IRR	12%	19%
	\$0.315	Negative IRR	Negative IRR	Negative IRR	12%	19%	25%
	\$0.310	Negative IRR	Negative IRR	12%	19%	25%	30%
	\$0.305	2%	12%	19%	25%	30%	34%
\$0.300	12%	19%	25%	30%	34%	38%	

**Ethylene/Ethanol Price Sensitivity (Without Research and Development)**

The following figures (Figure 7.10, 7.11) show the same analysis except with no expenses for research and development. Notice that the plant becomes profitable at lower prices of ethylene and higher prices of ethanol. Since prices of ethylene over \$0.62 are unlikely, this option for cutting costs is recommended. Realistically, it is prudent to only downsize R&D spending, rather than cutting it altogether. This analysis merely illustrates the sensitivity of profitability to R&D spending.

Figure 7.10

		ETHYLENE \$/LB					
		\$0.62	\$0.63	\$0.64	\$0.65	\$0.66	\$0.67
E T H A N O L \$/LB	\$0.360	(\$323,125,700)	(\$282,833,100)	(\$242,540,400)	(\$202,247,800)	(\$161,955,100)	(\$121,662,500)
	\$0.355	(\$285,268,300)	(\$244,975,700)	(\$204,683,000)	(\$164,390,400)	(\$124,097,800)	(\$83,805,100)
	\$0.350	(\$247,410,900)	(\$207,118,300)	(\$166,825,700)	(\$126,533,000)	(\$86,240,400)	(\$45,947,800)
	\$0.345	(\$209,553,500)	(\$169,260,900)	(\$128,968,300)	(\$88,675,600)	(\$48,383,000)	(\$8,090,400)
	\$0.340	(\$171,696,200)	(\$131,403,500)	(\$91,110,900)	(\$50,818,300)	(\$10,525,600)	\$29,767,000
	\$0.335	(\$133,838,800)	(\$93,546,100)	(\$53,253,500)	(\$12,960,900)	\$27,331,800	\$67,624,400
	\$0.330	(\$95,981,400)	(\$55,688,800)	(\$15,396,100)	\$24,896,500	\$65,189,100	\$105,481,800
	\$0.325	(\$58,124,000)	(\$17,831,400)	\$22,461,300	\$62,753,900	\$103,046,500	\$143,339,200
	\$0.320	(\$20,266,600)	\$20,026,000	\$60,318,600	\$100,611,300	\$140,903,900	\$181,196,500
	\$0.315	\$17,590,700	\$57,883,400	\$98,176,000	\$138,468,600	\$178,761,300	\$219,053,900
	\$0.310	\$55,448,100	\$95,740,800	\$136,033,400	\$176,326,000	\$216,618,700	\$256,911,300
	\$0.305	\$93,305,500	\$133,598,100	\$173,890,800	\$214,183,400	\$254,476,000	\$294,768,700
	\$0.300	\$131,162,900	\$171,455,500	\$211,748,200	\$252,040,800	\$292,333,400	\$332,626,100

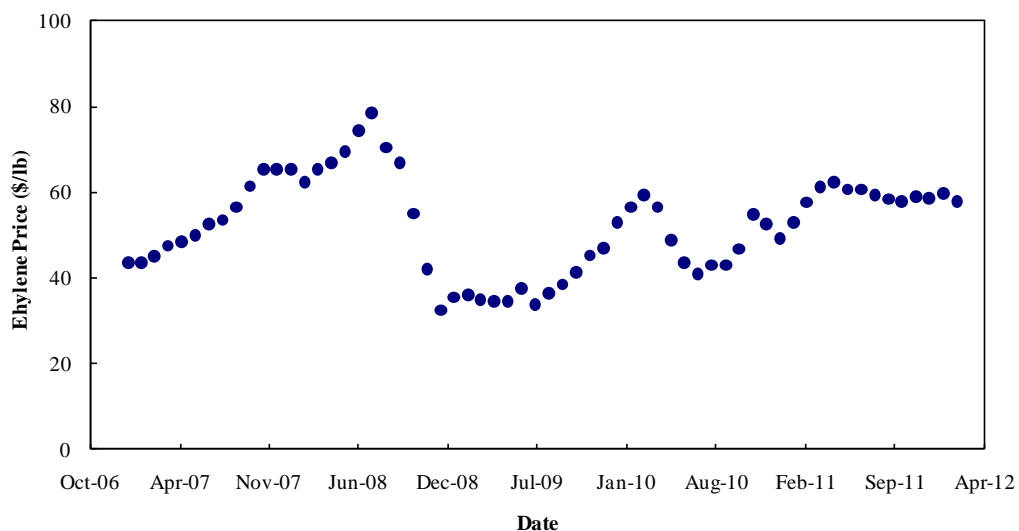
Figure 7.11

### Internal Rate of Return for Varied Ethanol and Ethylene Prices Without R&D

		ETHYLENE \$/LB					
		\$0.62	\$0.63	\$0.64	\$0.65	\$0.66	\$0.67
E T H A N O L \$/LB	\$0.360	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
	\$0.355	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
	\$0.350	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR	Negative IRR
	\$0.345	Negative IRR	Negative IRR	Negative IRR	Negative IRR	2%	13%
	\$0.340	Negative IRR	Negative IRR	Negative IRR	Negative IRR	13%	20%
	\$0.335	Negative IRR	Negative IRR	Negative IRR	12%	20%	26%
	\$0.330	Negative IRR	Negative IRR	12%	20%	26%	31%
	\$0.325	Negative IRR	11%	19%	25%	30%	35%
	\$0.320	10%	19%	25%	30%	35%	39%
	\$0.315	18%	25%	30%	34%	38%	42%
	\$0.310	24%	30%	34%	38%	42%	45%
	\$0.305	29%	34%	38%	42%	45%	48%
	\$0.300	34%	38%	41%	45%	48%	51%

### Historical Ethylene Prices

Figure 7.12



As it is clearly seen in figure 7.12, the price of ethylene is hardly stable. This in mind, it is not unreasonable to assume that prices may rise adequately to make this plant profitable.

## **Market Considerations**

Ethylene is a high demand product because it is an essential raw material in the production of plastics, in particular low and high density polyethylenes and PVC. In the US alone, the yearly demand is approximately 5MM tonnes of ethylene. Traditionally, ethylene is produced by cracking of heavy hydrocarbons from fossil fuels. In fact, in the 1960's this process was so profitable that ethylene was used to produce ethanol in the reverse of the process used by this plant. However, a worldwide oil crisis in 1973 raised petroleum prices making cracking a much less economically reasonable method of ethanol production. Since plastics remain in high demand, ethylene production via ethanol is being explored again.

The major benefit of using ethanol as the raw material for ethylene production instead of fossil fuels is that ethanol is renewable; it can be produced from fermentation of feedstocks such as corn or sugar cane. If the demand for ethylene remains high while the supply of fossil fuels is diminished, the selling price of ethylene may be driven up, making this process profitable. Additionally, as environmental awareness becomes more socially prevalent, governments are encouraging companies to move away from fossil fuels because they are non-renewable and have high carbon emissions. Government support of this "greener," renewable process may further impact ethylene costs and also investment and operating costs for the plant.

## **Comparison to Traditional Ethylene Plants**

According to Seider, Seader, Lewin, and Widago, the typical total depreciable capital associated with a traditional ethylene plant (naphthalene cracking) is \$681MM. The total depreciable capital for this plant is \$58MM (Figure 7.5) which is far less. The total permanent investment for a traditional cracking plant is \$855MM, while the total permanent investment for this plant is \$65MM (Figure 7.2), again far less.

The values were generated with the following assumptions: Land cost is typically 2% of the  $C_{TDC}$ . The cost of plant start-up is typically 10% of the  $C_{TDC}$ . However, since the process is well-known, the figure can be estimated around 9%. The total permanent investment can be estimated as 8% of the  $C_{TDC}$ , and is corrected to a site factor which is now 1.0 for Brazil.

## **Additional Economic Considerations**

### *Transportation of Materials*

Transportation of the ethylene product is generally the responsibility of the buyers, who may use barges docked near the plant. Ethylene can thus be piped directly from the plant onto the barges at minimal cost. Because there are many ethanol vendors near the plant location, it may be possible to pipe ethanol directly to the plant at minimal cost. If not it can be transported cheaply by rail.

With efforts by the Brazilian government to reduce transportation costs in Brazil, it is safe to assume a low price for shipping the ethylene product to a nearby port, such as Rio de Janeiro, so that buyers do not have to come to São Paulo to pick up the ethylene.

### *Cyclic Ethanol Availability*

Since the sugar cane ethanol price increases dramatically during the winter months (because sugar cane growth is seasonal), it was decided that the plant will only operate 280 days per year. This was determined because storage tanks for three months worth of ethanol (which would cover the off-season) would require almost 21.5MM cubic feet of volume, which comes at an astronomical cost.

### *Environmental Awareness*

One major advantage of this process over hydrocarbon cracking is that ethanol dehydration is relatively “green” because it has very low carbon emissions. This in mind, it is reasonable to expect government support, possibly in the form of subsidies.



# **Section VIII**

## **Location**

A major factor regarding the profitability of the project is the location of the plant. Based on the supply of ethanol and demand for ethylene, it was necessary to choose between building in either the United States or Brazil. Different sites may affect the economics of the plant due to differences in the site factors, supply of ethanol, price of ethanol, price of ethylene, ability to transport goods, and environmental regulations. The considerations and explanation of the final decision to locate in São Paulo, Brazil are discussed here.

### **Site Factor**

Site factors help companies compare the cost of building a plant in various locations based on the availability of labor, efficiency of the workforce, local rules and customs, and union status among other considerations. Overall, Brazil has a site factor of 1.0 compared to the United States Gulf Coast, so these factors do not affect the choice of location. In the past, Brazil's site factor was 0.90 due to lower exchange rates and labor costs. More recently, it has been the largest and fastest growing economy in South America, so its construction costs have increased. Also, because the United States has been the center of industry for such a long time, it has grown more competitive, developing a more low-cost manufacturing economy with decreasing construction costs despite providing better benefits for laborers.

### **Ethanol Price**

The price of our ethanol feed plays a large factor in the profitability of the project. It is crucial to find inexpensive ethanol that is near the plant to decrease transportation costs as much as possible. Corn ethanol, which is largely produced in the United States, is \$0.30/L whereas Brazilian sugar cane ethanol is only \$0.22/L. Additionally, since there are many sugar cane fields near São Paulo, transportation costs will be competitive with those in the US, if not lower. Consequently, locating in Brazil is more economical from an ethanol standpoint.

### **Ethanol Supply**

Differences in the supply of ethanol feed for the plant are enormous. In the United States, ethanol is largely made from corn while Brazil generally produces ethanol using sugar cane. The presence of plants to produce the needed quantity of ethanol is essential to the survival of this project. Corn ethanol is widely available in the Midwest of the United States. Meanwhile,

Brazil is a large producer of sugar cane ethanol with the exception of the cold, rainy season which eliminates the sugar cane supply for ethanol from June-September. To compensate, either a storage tank of ethanol for those months must be built, or the plant must be operated at higher capacity for the rest of the year. A storage tank would need to hold 481,000 tonnes of ethanol to support the plant's production. This would consist of many tanks with a total volume of 21.5MM ft<sup>3</sup>, which would cost roughly \$87MM. Because the economics of the project are so tight and space is a big issue, it would be most beneficial to not use a storage tank. Therefore, it is recommended to operate the plant at a higher capacity for the rest of the year to make up for the nonproduction during the 3 months. Due to the already incredibly high capacity of this plant, scaling up is not an issue at all.

### **Ethylene Price**

The price of ethylene gives insight on the market where the product will be introduced. As discussed in the Economics Section of this report, the price of ethylene worldwide has shown dramatic fluctuation over the past decade; however, if the price stabilizes around its current value it is reasonable to estimate a selling price of \$0.65/lb in 2014 when the plant is expected to be complete. This number accounts for the decrease in availability of natural fuels, like naphthalene, for cracking into ethylene. Since the price for ethylene is the same in both the Brazilian and American markets, the major concern with the profitability of ethanol becomes the cost of shipping.

### **Transportation**

A plant is only operable if there is a suitable means of transportation to and from it. This is necessary because in order for the plant to be built, materials must be shipped to the site. Additionally, in order for it to run, raw materials, products, and employees must be brought to and from the site. Good roads, a railway infrastructure, and access to ports and waterways are a large factor in determining the location of the plant. Locating the plant in Brazil allows for easy access to both a feed of ethanol from a nearby plant (there are several near São Paulo) and a port to ship the ethylene product. All of the ethanol plants in the United States are landlocked, so transportation would have to be by railcar. This limits the shipping quantity of both ethanol and

ethylene and also the buyer of ethylene. Access to ports allows for easier access to international markets than railcars from the central United States.

There are additional benefits to specifically locating in São Paulo. It is a large city with a good road and rail infrastructure, which means that it can easily supply a sizable workforce. Also, it is only 220 miles from the major economic center Rio de Janeiro. Sao Paulo also boasts the availability of freight transportation to Ports Santos and Sepetiba. Finally, it is promising to note that the Brazilian government is sponsoring projects for improving transportation to and from Sao Paulo.

# **Section IX**

## **Safety and Other Important Considerations**

## **Safety**

Ethanol and ethylene are both very flammable, and as such careful attention must be paid to their transportation to and from and storage at the facility. Ethanol spontaneously combusts at about 790°F. Since the reactors operate near this limit (750°F), it is very important to invest in accurate and careful controllers to ensure that the temperatures in the furnaces and compressor outlet stream never reach this level. The plant is at no risk of ethylene accidentally autoigniting as ethylene's ignition temperature is 914°F and it spends most of the process under cryogenic conditions. In addition, none of the byproducts are at serious risk.

While spontaneous combustion of ethylene is not a serious concern, it is still a highly volatile and flammable hydrocarbon. Even while being treated in the cryogenic column at temperatures as low as -67°F, it is still well above its flash point (-218°F). Measures should be taken to ensure that minute leaks in process equipment, particularly the separation units which handle highly concentrated ethylene, can be quickly detected and isolated. In addition, it is advisable to invest a greater amount in the piping and transport equipment to lower the risk of leaks. If an ethylene leak is left undetected, immediate surroundings will rapidly reach the lower flammability limit of ethylene in air (about 3%) and put the plant, the operators, and the surroundings at serious risk.

Ethanol is not nearly as volatile as ethylene and is thus less likely to cause an explosion. However, as it is heated to a vapor, ethanol does become quite flammable and a greater risk to the plant. Similar treatment should be given to the highly concentrated ethanol reactor feed stream to ensure quick detection of potential leaks.

Another possible concern is the spontaneous free radical polymerization of ethylene. Such reactions are often used to generate polyethylene on industrial scales. This is not a huge operational risk in this plant, as free radical polymerization requires astronomically high pressures (on the order of 1000atm) to occur. However, to prevent runaway in the unlikely event that a free radical initiator is introduced in the concentrated ethylene streams (particularly stream S510 and PURGE on Figure 7.5 which carry liquid ethylene), pipes with periodic pinches should be used. The pinches help prevent the polymerization from spreading throughout the entire plant and ruining an entire ethylene stock.

For feed storage, a floating roof tank is being used. Some pure nitrogen will be available to ensure that no air contacts the stored ethanol and jeopardizes the feed.

### **Kinetic Considerations**

The reaction kinetic data used in this design was obtained from Fikry Ebeid's work. The data published specifically applies to high-temperature reactions, though there is no mention of the operating pressure in the paper. As such, it was assumed that the high operating pressures of this plant would not have a significant impact on the kinetics. It was also necessary to make the assumption that the rate constant followed the Arrhenius equation with no additional temperature correction factor. In order to verify that the kinetics are sufficiently independent of pressure, it would be necessary to conduct a small scale experiment in a laboratory setting.

### **Additional Considerations**

All of the chemicals reacting involved in this plant are well understood. In addition, dehydration reactions over alumina-based catalysts are also common. Thus there were few additional assumptions that had to be made.

One assumption was the composition of the byproducts. It was difficult to obtain side-reaction data, but based on the available material it was assumed that diethyl-ether and acetaldehyde are the main byproducts formed. Additionally, it was assumed that some quantity of methane would be formed, potentially posing a problem.

Methane is notoriously difficult to remove. After simulating the cryogenic distillation column for a host of different operating and inlet conditions, it was determined that using the property selection model NRTL-RK, it is impossible to purify an ethylene/methane stream to more than 99.92% pure ethylene using distillation. There are two explanations for this behavior. Ethylene and methane may form an azeotrope at these extremely non-ideal conditions (low temperature, high pressure). This explanation seems unlikely as both are light hydrocarbons having zero dipole moments. The second possible explanation is that methane can dissolve in ethylene to that extent.

If the side reactions were adjusted such that more methane was produced, this process may become infeasible. Since this reaction is so important, the reactor should be modeled to measure the extent of methane formation before this plant is designed.



# **Section X**

## **Equipment List and Unit Descriptions**

Table 7.1

PUMPS		PRESSURE VESSELS	
Equipment ID	Type	Equipment ID	Type
P101 A/B	Multistage Centrifugal Pump	R101 A/B	Fixed Bed Catalytic Reactor
P102 A/B	Multistage Centrifugal Pump	R102 A/B	Fixed Bed Catalytic Reactor
P301 A/B	Centrifugal Pump	R103 A/B	Fixed Bed Catalytic Reactor
P302 A/B	Centrifugal Pump	FL201	Flash Vessel
P501 A/B	Centrifugal Pump	FL202	Flash Vessel
P101 A/B	Centrifugal Pump		
P102 A/B	Centrifugal Pump		
HEAT EXCHANGERS		TOWERS	
Equipment ID	Type	Equipment ID	Type
HX101	Shell and Tube Heat Exchanger	D301	Distillation Tower
HX201	Shell and Tube Heat Exchanger	D501	Distillation Tower
HX202	Shell and Tube Heat Exchanger	AD401 A/B	Packed Tower
HX301	Shell and Tube Partial Condenser		
HX302	U Tube Kettle Reboiler		
HX501	Shell and Tube Heat Exchanger		
HX502	Shell and Tube Partial Condenser		
HX503	U Tube Kettle Reboiler		
F101	Furnace		
F102	Furnace		
F103	Furnace		
TANKS		COMPRESSORS	
Equipment ID	Type	Equipment ID	Type
FEED TANK	Floating Cylinder Tank	C301	Multistage Compressor
PRODUCT TANK	Spherical Tank	C401	Multistage Compressor
PRODUCT TANK	Spherical Tank		
AC301	Reflux Accumulator		
AC501	Reflux Accumulator		

## **Unit Descriptions**

### **100\_Reactors Section**

#### **Reaction Vessels**

R101 is a horizontal adiabatic reactor, made of carbon steel, with a length of 8.46 feet and a diameter of 5.81 feet. The wall thickness is 1.84 inches, with a total reactor volume for 224 cubic feet. 36,111lb of one cm  $\Gamma$ -Alumina diameter pellets are used as catalyst to convert ethanol to ethylene. The 578,839 lb/hr inlet flow enters at 752°F and 618psi and leaves at 590°F and 616psi.

R102 is a horizontal adiabatic reactor, made of carbon steel, with a length of 8.07 meters and a diameter of 6.36 feet. The wall thickness is 2.01 inches, with a total reactor volume for 256 cubic feet. It requires 41,227lb of catalyst. The 578,839 lb/hr inlet flow enters at 752°F and 608psi and leaves at 590°F and 600psi.

R103 is a horizontal adiabatic reactor, made of carbon steel, with a length of 7.78 feet and a diameter of 7.12 feet. The wall thickness is 2.24 inches, with a total reactor volume for 310 cubic feet. It requires 49,872lb of catalyst. The 578,839 lb/hr inlet flow enters at 752°F and 600psi and leaves at 590°C and 597psi.

Each reactor has an identical spare available in case of repair and catalyst regeneration. The catalyst is replaced every 90 days.

The choice of using three reactors is to ensure a proper conversion of ethanol to ethylene, achieving a required conversion of 98%. Due to the endothermic nature of the ethanol dehydration reaction, temperature is a clear factor in the reaction kinetics. The ability to reheat the reactants before running the catalyzed reactants ensures a high rate of reaction before an equilibrium state is reached. Additionally, the recycle stream is fed before the final reactor in order to reduce the heat duty of the furnaces for the two previous reactors. Finally, the choice of using three adiabatic reactors instead of using isothermal reactors is due to the tremendous amount of energy necessary to run an isothermal reactor at the necessary temperature. Due to

the endothermic nature of the reaction, sustaining an isothermal reactor is incredibly cumbersome; adiabatic reactors coupled with re-heating furnaces are more efficient.

### **Heat Exchanger**

HX101 is a shell and tube heat exchanger is used to simultaneously cool S110 (reactor effluent) while heating S102 (reactor inlet). The heat exchanger is made of carbon steel with a heat transfer area of 30,000 ft<sup>2</sup>. The total heat duty used is 361MM BTU/h.

### **Furnaces**

F101 is a fired heater used to heat stream S103 from an inlet temperature of 572°F to the desired temperature of 752°F before entering R101. Due to the fact that the feed is essentially at room temperature, a relatively large amount of heat must be used in order to reach the aforementioned reactor feed temperature. The heater supplies 63MM BTU/hr of heat, while utilizing 60,000 SCF/h of natural gas as fuel. Chromium-Molybdenum Steel is used as a construction material in order to withstand the high heating temperatures. A total mass of 580,000 lb/hr enters and exits the heater, consisting mainly of ethanol and water.

F102 is a fired heater used to heat stream S105 from an inlet temperature of 590°F to the desired temperature of 752°F before entering R102. The heater supplies 55.5MM BTU/hr of heat, while utilizing 53,000 SCF/h of natural gas as fuel. Chromium-Molybdenum Steel is used as a construction material in order to withstand the high heating temperatures. A total mass of 580,000 lb/hr enters and exits the heater.

F103 is a fired heater used to heat stream S107 from an inlet temperature of 572°F to the desired temperature of 752°F before entering R103. The heater supplies 56.4MM BTU/hr of heat, while utilizing 53,000 SCF/h of natural gas as fuel. Chromium-Molybdenum Steel is used as a construction material in order to withstand the high heating temperatures. A total mass of 580,000 lb/hr enters and exits the heater.

F101, F102, and F103 all emit flue streams that are released to the atmosphere.

## **Pumps**

P101 and P102 are identical cast iron three stage pumps. Each pump provides a pressure increase of 588 psi. Because of the considerable mass of the feed, it was necessary to use two pumps in parallel to raise its pressure; just one large pump would have had to be unreasonably large.

## **200\_Flash Distillation Section**

### **Flash Distillation**

FL201 is a flash distiller used to remove water and ethanol from the product stream. Stream S203, the product of the reactor section at a temperature and pressure of 122°F and 574 psi, is fed into the distiller. This stream is about 55.6% ethylene, with significant amounts of water and ethanol, as well as trace amounts of ether, ethane, acetaldehyde, methane, and acetic acid. After separation, the top product, stream S205, consists of 98.2% ethylene by weight along with trace amounts of the other components. The bottoms, stream S204, contains 3.8% ethanol and 95.2% water along with other impurities.

FL202 also serves to remove more water and ethanol from the product stream coming from the top of the previous flash distiller (FL201). Stream S207, the cooled and throttled top product of FL201, is fed into this distiller to achieve a more thorough separation of water and ethanol. The stream is at 569 psi and 57.2°F, and the resulting top stream is 98.6% ethylene by weight. The bottoms product contains 346 lb/hr ethanol (24.3% by weight). This stream will be recycled later.

### **Heat Exchangers**

HX201 is used to cool the reactor product using cooling water introduced in stream CW201. The reactor product, stream S110, was cooled to 180°F from a previous exchanger, and is now further cooled to 122°F before entering the flash distiller. This temperature is required to achieve an effective separation of ethanol and water from the ethylene product. The 182 tubes with 2 shell and 2 tube passes has a total transfer area is 7,630 ft<sup>2</sup> with an overall transfer coefficient of 80 BTU/hr\*ft<sup>2</sup>\*R and a heat duty of -27,014,000 BTU/hr.

HX202 is used to cool the ethylene rich stream from the 1<sup>st</sup> flash vessel using the product stream which exits the top of the cryogenic distiller, stream CRYO-OUT. This cold ethylene product stream at -35.4°F cools the flash feed stream from 122°F to 57.2°F so that the water and ethanol can be further separated from other impurities. HX202 also warms the cold product to 52.4°F, bringing it somewhat closer to the environmental temperature so that there is less expansion as the ethylene warms during shipment. The 250 tubes with 1 shell and 2 tube passes has a total transfer area is 2,629 ft<sup>2</sup> with an overall transfer coefficient of 60 BTU/hr\*ft<sup>2</sup>\*R and a heat duty of 12,630,433 BTU/hr.

### **Valves**

V201 is a throttle which decreases the pressure of the reactor product to 569 psi. This allows the stream to be at a pressure suitable for feeding into the flash distiller to achieve an efficient separation. This throttle also conveniently lowers the temperature to 122°F.

V202 brings the stream exiting FL201 from 569 to 441 psi for the 2<sup>nd</sup>, more thorough ethanol and water separation which takes place in FL202. The lowered pressure also helps to decrease the temperature of the stream to 36.6°F from the 57.2°F stream which was heat exchanged with the cryogenic distiller overhead.

## **300\_Distillation Column Section**

### **Distillation Column**

D301 is the distillation column responsible for the recycle stream. Its purpose is to take the bottoms products from both flash distillers, stream S302, and separate the ethanol from the water and other components. The tower is made of carbon steel and stands 64 feet tall with 26 trays spaced 2 feet apart and a diameter of 6 feet. It is operated at 122°F and 30.9 psi, resulting in an ethanol-rich stream as the top product. The distillate, S303, passes through a partial condenser which operates at 29.4 psi and 206°F while the bottoms, S309, pass through a reboiler operating at 31.2 psi and 252°F. The tower's reflux ratio given by the reflux accumulator, AC301, is 0.85. The distillate, a 10,044 lb/hr ethanol stream, is later recycled into the 3<sup>rd</sup> reactor. The distiller is very efficient with only 2 lb/hr of ethanol being lost to the bottoms stream.

## **Heat Exchanger**

HX301 is a carbon steel shell and tube heat exchanger that makes up the partial condenser section of the distillation tower. Using cooling water, it partially condenses the vapor stream exiting the top of the column so that it can enter the reflux accumulator (AC301). The condenser contains 122 tubes with one shell pass and one tube pass. The total transfer area is 642 ft<sup>2</sup> with an overall transfer coefficient of 180 BTU/hr\*ft<sup>2</sup>\*R. This condenser has a heat duty of 9,063,300 BTU/hr.

HX302 is carbon steel U-tube kettle reboiler which uses steam at 50 psi to vaporize the bottoms product (S309) which is then put back into the column. The kettle reboiler's total transfer area is 5,684 ft<sup>2</sup> and the overall transfer coefficient is 80 BTU/hr\*ft<sup>2</sup>\*R with a heat duty of 49,469,600 BTU/hr.

## **Reflux Accumulator**

AC301 accumulates the partially condensed reflux from D301 to send back to the column. It is 5 ft high with a 3 ft diameter and a storage volume of 264 gallons and is made of carbon steel. The accumulator operates at 206.4°F and 28 psi.

## **Multistage Compressor**

C301 is responsible for compressing the distillation column's distillate stream (S305) by 570 psi. The resulting stream is at 600 psi, which is the appropriate pressure for combining with the 3<sup>rd</sup> reactor feed, S107. Without the compressor, there cannot be a stream to recycle the 10,044 lb/hr ethanol.

## **Centrifugal Pumps**

P301 A/B is a centrifugal pump responsible for pumping the reflux from the accumulator back into the top of the column after it is condensed. It operates on electricity, is made of cast iron, and pumps 44 gallons per minute of the condensed vapor from stream S307 back into the column. The pump efficiency is 0.7 and consumes 1,356 BTU/hr. The discharge pressure will be 29.4 psi with a pressure head of 76 feet.

P302 A/B is the centrifugal pump which forces the bottoms product, S311, of the distillation tower away from the process to undergo waste treatment for disposal. The pump is also made of cast iron and consumes 16,426 BTU/hr of electricity to pump 597 gallons per minute of the purge (S311) which consists mainly of water and a little bit of ethanol and acetic acid.

### **Valve**

V301 is the valve which decreases the pressure of the feed into the distillation tower. The combined flash distiller bottoms (S209) is at 455.6 psi and must be reduced to 30.9 psi to achieve a good separation of ethanol from water. The valve is the piece of equipment which allows us to achieve this pressure drop.

## **400\_Adsorption Tower Section**

### **Adsorption Towers**

AD401 is an adsorption column which is fed with the ethylene-rich top product stream of the series of flash distillators (S210). It contains a 13X, 3mm spherical zeolite filling whose purpose is to absorb the rest of the water and ethanol as well as all other condensables that would clog the cryogenic distiller. The column is made of carbon steel and requires 772 ft<sup>3</sup> of zeolite filling. The eluent is 4,800 lb/hr of 350°F nitrogen. The ethylene stream feed enters at 335,339 lb/hr with residence time of 22 sec and a breakthrough time of 24 hr. It experiences a pressure drop of 15 psi and the column's heat of adsorption is 113,400 BTU/hr. The exit, stream S404 is now an ethylene stream along with various light key impurities that will not freeze at cryogenic temperatures.

AD402 is an identical adsorption tower to AD401 but alternates in productivity so that the plant can continue to run while one adsorption tower is being maintained. Maintenance of the tower occurs after one day of productivity and consists of cleaning the zeolite filling using a compressed nitrogen purge stream. The zeolite also needs to be replaced every 3 years.



## **Multistage Compressor**

C401 is a multistage compressor that sends the nitrogen into the adsorption column that is not in operation as a purge used to clean that tower. The nitrogen needs to be condensed to raise the temperature for optimal cleaning. Therefore, this carbon steel, one-stage compressor consumes 295,482 BTU/hr of electricity to condense the nitrogen stream by 26 psi, causing a temperature rise of 247°F. The compressor condenses 67,506 ft<sup>3</sup>/hr of nitrogen to 36,171ft<sup>3</sup>/hr for cleaning purposes.

## **Valves**

V401 and V404 decide which adsorption tower to send the future product stream (S210) to. This depends on which one is cleaned and ready for use while the other one is undergoing maintenance.

V403 and V406 open the pipe that contains the ethylene-rich stream exit (S404 or S407) from whichever adsorption tower is used. It is then sent to be further treated before being fed into the cryogenic distiller.

V407 and V408 determine the route of the nitrogen purge stream (S408), sending it to the unused adsorption tower that is to be cleaned.

V402 and V405 release the cleaning nitrogen purge stream. This condensed nitrogen is later sent through a heat exchanger to warm the cold cryogenic ethylene product stream.

## **500\_Cryogenic Distillation Section**

### **Cryogenic Distiller**

D501 is a cryogenic distiller which operates at the cold temperature of about -35°F to effectively separate ethylene from other light impurities such as ether, ethane, and methane. The impurities exit out the bottom as stream S511 which is burned and purged. The tower distillate (S507) contains 330,473 kg/hr of the final 99.96% pure ethylene product at -68°F. The cryogenic distiller is made of stainless steel because carbon steel is brittle at such low temperatures. The feed stream, S503, enters on the 3<sup>rd</sup> of 8 stages with 2 foot spacing. The tower is 24 feet with a

diameter of 10.5 feet. The tray efficiency is 0.75. With the cryogenic distiller, enough impurities are removed to achieve the 99.96% ethylene purity required to qualify as polymer grade.

### **Heat Exchangers**

HX501 cools the stream entering the cryogenic column by running it through this stainless steel shell and tube heat exchanger against the cold product stream exiting the cryogenic distiller. The exchanger consists of 144 tubes with a total transfer area of 2,951 ft<sup>2</sup> with an overall heat transfer coefficient of 30 BTU/hr\*ft<sup>2</sup>\*R and a heat duty of 6,591,610 BTU/hr. The -68°F ethylene product is warmed to -35°F while the cryogenic feed is cooled from 40°F to 7°F to reduce the necessary refrigeration in the cryogenic distillation column.

HX502 is a floating head shell and tube partial condenser which uses 420,000 lb/hr propylene introduced in stream R501 at -90°F to condense the 420,000 lb/hr vapor overhead of the cryogenic distiller so that it can be accumulated and reintroduced into the column for a more thorough separation. The condensed exit stream is partially sent to the HX501 exchanger and the other part is sent to the reflux accumulator. It is made of stainless steel and has 1,122 tubes with 8 tube and 2 shell passes, having a total transfer area of 188,500 ft<sup>2</sup> with an overall transfer coefficient of 50 BTU/hr\*ft<sup>2</sup>\*R and a heat duty of 56,357,300 BTU/hr. Exiting HX502 is the cold but purified product stream of 99.96% ethylene.

HX503 is a U-tube kettle reboiler for vaporizing the bottoms product (S510) using steam to reintroduce into the column again. 199,282 lb/hr of steam is used to partially vaporize 49,342 lb/hr of the eventual purge. It is made of stainless steel and has a total transfer area of 2,105 ft<sup>2</sup> with an overall transfer coefficient of 45 BTU/hr\*ft<sup>2</sup>\*R and a heat duty of 49,039,968 BTU/hr.

### **Valve**

V501 decreases the pressure of the feed into the cryogenic distillation tower from 452.5 psi to 279.2 psi. The decrease in pressure also causes a convenient temperature decrease from 6.8°F to -35.1°F which improves the separation in the cryogenic distiller. Without the valve, S503 would not be at an optimal temperature and pressure for removing the light keys from the ethylene product.

**Reflux Accumulator**

AC501 accumulates the partially condensed reflux from D501 to send back to the column. It is 20 ft high with a 7 ft diameter and a storage volume of 4,965 gallons. The accumulator operates at -68°F and 238 psi. Reflux accumulators for cryogenic distillers are made of stainless steel to withstand cold temperatures.

**Pumps**

P501 A/B is the centrifugal pump which works to send the reflux of condensed overhead (S508) back into the cryogenic distiller. This pump is made of stainless steel to withstand the low temperatures. It pumps 791 gallons per minute back into the column and causes a pressure rise of 41 psi and a pressure head of 107 feet. It consists of one stage with an efficiency of 0.70 and uses 36,566 BTU/hr of electricity. The result is stream S509 which is sent back into the column.



# **Section XI**

## **Specification Sheets**

## Reactor Section

Feed Storage Tank	
<b>Block Type:</b>	Floating Roof Storage Tank
<b>Function:</b>	Stores 1 month supply of feed
<b>Materials:</b>	
Mass Fraction:	
Ethanol	0.95
Water	0.05
<b>Operating Conditions:</b>	
Pressure (psi)	14.7
Temperature (°F)	80
<b>Design Data:</b>	
Construction Material	Carbon Steel
Volume (gal)	1,110,000
Diameter (ft)	350.000
Height (ft)	270
<b>Purchase Cost:</b>	\$574,000
<b>Bare Module Cost:</b>	\$1,819,580
<b>Annual Operating Cost:</b>	\$0

P101 A/B		
<b>Block Type:</b>	Multistage Centrifugal Pump	
<b>Function:</b>	Raise the FEED pressure	
<b>Materials:</b>	<i>Inlet</i>	<i>Outlet</i>
Stream	FEED	S102
<b>Operating Conditions:</b>		
Pressure Increase (psi)	587.8	
Pressure Head (ft)	1680	
Flow Rate (GPM)	788	
<b>Design Data:</b>		
Construction Material	Cast Iron	
Number of Stages	3	
Pump Efficiency	1	
Consumed Power (BTU/h)	839,261	
Power Source	Electricity	
<b>Purchase Cost:</b>	\$32,780	
<b>Bare Module Cost:</b>	\$103,913	
<b>Annual Operating Cost:</b>	\$129,367	

P102 A/B		
<b>Block Type:</b>	Multistage Centrifugal Pump	
<b>Function:</b>	Raise the FEED pressure	
<b>Materials:</b>	<i>Inlet</i>	<i>Outlet</i>
Stream	FEED	S102
<b>Operating Conditions:</b>		
Pressure Increase (psi)	587.8	
Pressure Head (ft)	1680	
Flow Rate (GPM)	788	
<b>Design Data:</b>		
Construction Material	Cast Iron	
Number of Stages	3	
Pump Efficiency	1	
Consumed Power (BTU/h)	839,261	
Power Source	Electricity	
<b>Purchase Cost:</b>	\$32,780	
<b>Bare Module Cost:</b>	\$103,913	
<b>Annual Operating Cost:</b>	\$129,367	



HX101			
<b>Block Type:</b>		U-Tube Shell and Tube Heat Exchange	
<b>Function:</b>		Heat FEED ethanol and cool S110	
<b>Tube:</b>		<i>Inlet</i>	<i>Outlet</i>
	Stream	S102	S103
	Temperature (°F)	79	572
	Pressure (psi)	602.5	595.4
<b>Shell:</b>		S110	SEP
	Stream	S110	SEP
	Temperature (°F)	590	179
	Pressure (psi)	581.2	577.3
<b>Operating Conditions:</b>			
Tube Flow Rate (lb/h)	578,839		
Shell Flow Rate (lb/h)	594,547		
<b>Design Data:</b>			
Construction Material	Carbon Steel		
Flow Direction	Countercurrent		
Number of Tubes	367		
Number of Tube Passes	4		
Number of Shell Passes	2		
Transfer Area (ft <sup>2</sup> )	30,084		
Overall Heat Transfer Coefficient (BTU/h*ft <sup>2</sup> *R)	70		
Heat Duty (BTU/h)	360,714,029		
<b>Purchase Cost:</b>		\$271,316	
<b>Bare Module Cost:</b>		\$860,073	
<b>Annual Utilities Cost:</b>		\$0	

R101			
<b>Block Type:</b>		Fixed Bed Catalytic Reactor	
<b>Function:</b>		Convert hot ethanol from S104 into ethylene	
<b>Materials:</b>	<i>Inlet</i>	<i>Outlet</i>	
Stream	S104	S105	
Mass Flow (lb/h)	578,839	578,839	
Volumetric Flow (ft <sup>3</sup> /h)	265,590	435,582	
<b>Breakdown (lb/h):</b>			
Ethanol	549,897	161,532	
Water	28,942	179,995	
Ethylene	0	234,402	
Diethyl-Ether	0	2,212	
Methane	0	38	
Acetaldehyde	0	421	
Ethane	0	36	
Acetic Acid	0	179	
Hydrogen	0	24	
<b>Operating Conditions:</b>	<i>Inlet</i>	<i>Outlet</i>	
Temperature (°F)	752	590	
Pressure (psi)	618.0	616.0	
<b>Design Data:</b>			
Construction Material	Cr-Mo Steel SA-387B	Catalyst	Γ-Alumina
Vessel Weight (lb)	17,759	Residence Time (s)	3.14
Volume (ft <sup>3</sup> )	224	Catalyst Volume (ft <sup>3</sup> )	157.00
Diameter (ft)	5.81	Catalyst Weight (lb)	36,111
Length (ft)	8.46	Catalyst Cost	\$180,555
Wall Thickness (in)	1.84	Catalyst Life (days)	90
<b>Purchase Cost:</b>	\$63,104		
<b>Bare Module Cost:</b>	\$192,467		
<b>Annual Catalyst Cost:</b>	\$15,885		

R102			
<b>Block Type:</b>		Fixed Bed Catalytic Reactor	
<b>Function:</b>		Convert ethanol in S106 to ethylene	
<b>Materials:</b>	<i>Inlet</i>	<i>Outlet</i>	
Stream	S106	S107	
Mass Flow (lb/h)	578,839	578,839	
Volumetric Flow (ft <sup>3</sup> /h)	271,109	435,582	
Breakdown (lb/h):			
Ethanol	161,532	43,816	
Water	179,995	225,728	
Ethylene	234,402	305,225	
Diethyl-Ether	2,212	3,187	
Methane	38	72	
Acetaldehyde	421	529	
Ethane	36	46	
Acetic Acid	179	211	
Hydrogen	24	26	
<b>Operating Conditions:</b>	<i>Inlet</i>	<i>Outlet</i>	
Temperature (°F)	752	590	
Pressure (psi)	608.0	606.0	
<b>Design Data:</b>	Cr-Mo Steel SA-387B		Catalyst $\Gamma$ -Alumina
Construction Material			
Vessel Weight (lb)	24,731	Residence Time (s)	3.73
Volume (ft <sup>3</sup> )	256	Catalyst Volume (ft <sup>3</sup> )	179.46
Diameter (ft)	6.36	Catalyst Weight (lb)	41,277
Length (ft)	8.07	Catalyst Cost	\$206,383
Wall Thickness (in)	2.01	Catalyst Life (days)	90
<b>Purchase Cost:</b>	\$77,115		
<b>Bare Module Cost:</b>	\$235,202		
<b>Annual Operating Cost:</b>	\$573,286		

R103			
<b>Block Type:</b>		Fixed Bed Catalytic Reactor	
<b>Function:</b>		Convert remaining ethanol in S109 to ethylene	
<b>Materials:</b>	<i>Inlet</i>	<i>Outlet</i>	
Stream	S109	S110	
Mass Flow (lb/h)	594,547	594,547	
Volumetric Flow (ft <sup>3</sup> /h)	535,522	521,378	
Breakdown (lb/h):			
Ethanol	53,834	10,266	
Water	228,889	245,822	
Ethylene	306,083	332,309	
Diethyl-Ether	3,627	3,952	
Methane	72	93	
Acetaldehyde	1,701	1,747	
Ethane	104	111	
Acetic Acid	211	221	
Hydrogen	26	26	
<b>Operating Conditions:</b>	<i>Inlet</i>	<i>Outlet</i>	
Temperature (°F)	752	590	
Pressure (psi)	600.0	597.0	
<b>Design Data:</b>	Cr-Mo Steel SA-387B		Catalyst $\Gamma$ -Alumina
Construction Material	27,290		Residence Time (s) 4.05
Vessel Weight (lb)	310	Catalyst Volume (ft <sup>3</sup> ) 216.83	
Volume (ft <sup>3</sup> )	7.12	Catalyst Weight (lb) 49,872	
Diameter (ft)	7.78	Catalyst Cost \$249,359	
Length (ft)	2.24	Catalyst Life (days) 90	
Wall Thickness (in)			
<b>Purchase Cost:</b>	\$82,071		
<b>Bare Module Cost:</b>	\$250,316		
<b>Annual Catalyst Cost:</b>	\$775,784		

F101		
<b>Block Type:</b>	Fired Heater	
<b>Function:</b>	Heat stream S103	
<b>Materials:</b>	<i>Inlet</i>	<i>Outlet</i>
Material Stream	S103	S104
Mass Flow (lb/h)	578,839	578,839
Fuel Stream	FUEL-1	FLUE-1
<b>Operating Conditions:</b>	<i>Inlet</i>	<i>Outlet</i>
Temperature (°F)	572	752
Pressure (psi)	598.9	588.0
<b>Design Data:</b>		
Construction Material	Cr-Mo Steel SA-387B	
Heat Duty (BTU/h)	63,111,000	
Fuel Type	Natural Gas	
Fuel Flow (SCF/h)	60,106	
<b>Purchase Cost:</b>	\$1,836,640	
<b>Bare Module Cost:</b>	\$4,022,242	
<b>Annual Utilities Cost:</b>	\$2,176,170	

F102		
<b>Block Type:</b>	Fired Heater	
<b>Function:</b>	Heat stream S105	
<b>Materials:</b>	<i>Inlet</i>	<i>Outlet</i>
Material Stream	S105	S106
Mass Flow (lb/h)	578,839	578,839
Fuel Stream	FUEL-2	FLUE-2
<b>Operating Conditions:</b>	<i>Inlet</i>	<i>Outlet</i>
Temperature (°F)	590	752
Pressure (psi)	616.0	608.9
<b>Design Data:</b>		
Construction Material	Cr-Mo Steel SA-387B	
Heat Duty (BTU/h)	55,553,211	
Fuel Type	Natural Gas	
Fuel Flow (SCF/h)	52,908	
<b>Purchase Cost:</b>	\$1,665,130	
<b>Bare Module Cost:</b>	\$3,646,634	
<b>Annual Utilities Cost:</b>	\$1,915,565	

F103		
<b>Block Type:</b>	Fired Heater	
<b>Function:</b>	Heat stream S108	
<b>Materials:</b>	<i>Inlet</i>	<i>Outlet</i>
Material Stream	S108	S109
Mass Flow (lb/h)	578,839	578,839
Fuel Stream	FUEL-3	FLUE-3
<b>Operating Conditions:</b>	<i>Inlet</i>	<i>Outlet</i>
Temperature (°F)	591	752
Pressure (psi)	607.0	599.6
<b>Design Data:</b>		
Construction Material	Cr-Mo Steel SA-387B	
Heat Duty (BTU/h)	56,420,329	
Fuel Type	Natural Gas	
Fuel Flow (SCF/h)	53,734	
<b>Purchase Cost:</b>	\$1,685,002	
<b>Bare Module Cost:</b>	\$4,690,155	
<b>Annual Utilities Cost:</b>	\$1,945,465	

## Flash Separation Section

HX201		
<b>Block Type:</b>		Floating Head Shell and Tube Heat Exchanger
<b>Function:</b>		Cool SEP for flash separation using cooling water
<b>Shell:</b>		<i>Inlet</i>
	Stream	CW201
	Temperature (°F)	90
	Pressure (psi)	14.7
		<i>Outlet</i>
	Stream	CW202
	Temperature (°F)	120
	Pressure (psi)	14.7
<b>Tube:</b>	Stream	SEP
	Temperature (°F)	179
	Pressure (psi)	577.0
		S202
	Temperature (°F)	122
	Pressure (psi)	574.6
<b>Operating Conditions:</b>		
Shell Flow Rate (lb/h)		903,320
Tube Flow Rate (lb/h)		594,547
<b>Design Data:</b>		
Construction Material		Carbon Steel
Flow Direction		Countercurrent
Number of Tubes		182
Number of Tube Passes		2
Number of Shell Passes		2
Transfer Area (ft <sup>2</sup> )		7,630
Overall Heat Transfer Coefficient (BTU/h*ft <sup>2</sup> *R)		80
Heat Duty (BTU/h)		-27,014,000
<b>Purchase Cost:</b>		\$79,870
<b>Bare Module Cost:</b>		\$253,186
<b>Annual Utilities Cost:</b>		\$55,068



HX202		
<b>Block Type:</b>	Shell and Tube Heat Exchanger	
<b>Function:</b>	Heat stream S205 for flash separation	
<b>Shell:</b>	<i>Inlet</i>	<i>Outlet</i>
Stream	CRYO-OUT	PRODUCT
Temperature (°F)	-34	52
Pressure (psi)	276	276
<b>Tube:</b>	S205	S206
Stream	S205	S206
Temperature (°F)	122	57
Pressure (psi)	565.0	562.0
<b>Operating Conditions:</b>		
Shell Flow Rate (lb/h)	330,473	
Tube Flow Rate (lb/h)	667,938	
<b>Design Data:</b>		
Construction Material	Carbon Steel	
Flow Direction	Countercurrent	
Number of Tubes	250	
Number of Tube Passes	2	
Number of Shell Passes	1	
Transfer Area (ft <sup>2</sup> )	2,629	
Overall Heat Transfer Coefficient (BTU/h*ft <sup>2</sup> *R)	60	
Heat Duty (BTU/h)	12,630,433	
<b>Purchase Cost:</b>	\$46,879	
<b>Bare Module Cost:</b>	\$148,607	
<b>Annual Operating Cost:</b>	\$0	

FL201			
<b>Block Type:</b>	Flash Drum		
<b>Function:</b>	Remove most of the water and ethanol from S203		
<b>Materials:</b>	<i>Inlet</i>	<i>Overhead</i>	<i>Bottoms</i>
Stream	S203	S205	S204
Phase	MIX	VAP	LIQ
Mass Flow (kg/h)	594,547	337,465	257,082
Volumetric Flow (L/h)	4,391	100,528	24
Breakdown (kg/h):			
Ethanol	10,266	592	9,674
Water	245,822	1,046	244,776
Ethylene	332,309	331,472	837
Ether	3,952	3,542	410
Methane	93	93	0
Acetaldehyde	1,747	640	1,107
Ethane	111	54	57
Acetic Acid	221	1	220
Hydrogen	26	26	0
<b>Operating Conditions:</b>			
Pressure (psi)	565.0		
Temperature (°F)	122		
Equilibrium	Vapor-Liquid Equilibrium		
<b>Design Data:</b>			
Construction Material	Carbon Steel	Diameter (ft)	6.5
Weight (lb)	31,000	Height (ft)	19.5
Volume (gal)	4,841		
<b>Purchase Cost:</b>	\$60,500		
<b>Bare Module Cost:</b>	\$251,680		
<b>Annual Operating Cost</b>	\$0		

FL202			
<b>Block Type:</b>	Flash Drum		
<b>Function:</b>	Remove further amounts of ethanol and		
<b>Materials:</b>	<i>Inlet</i>	<i>Overhead</i>	<i>Bottoms</i>
Stream	S207	S210	S208
Phase	MIX	VAP	LIQ
Mass Flow (kg/h)	337,465	336,043	1,422
Volumetric Flow (L/h)	78,294	100,528	24
Breakdown (kg/h):			
Ethanol	592	246	346
Water	1,046	88	958
Ethylene	331,472	331,451	21
Ether	3,542	3,511	31
Methane	93	93	0
Acetaldehyde	640	575	65
Ethane	54	53	0
Acetic Acid	1	0	1
Hydrogen	26	26	0
<b>Operating Conditions:</b>			
Pressure (psi)	455.6		
Temperature (°F)	39		
Equilibrium	Vapor-Liquid Equilibrium		
<b>Design Data:</b>			
Construction Material	Carbon Steel	Diameter (ft)	6
Weight (lb)	18,300	Height (ft)	12
Volume (gal)	2,538		
<b>Purchase Cost:</b>	\$43,100		
<b>Bare Module Cost:</b>	\$179,296		
<b>Annual Operating Cost:</b>	\$0		

## Distillation Section

D301			
<b>Block Type:</b>	Seive Tray Distillation Tower		
<b>Function:</b>	Remove water and from S302 and enrich stream S305 in ethanol		
<b>Materials:</b>	<i>Inlet</i>	<i>Distillate</i>	<i>Bottoms</i>
Stream	S302	S305	S311
Phase	LIQ	VAP	LIQ
Mass Flow (kg/h)	258,504	15,708	242,796
Volumetric Flow (L/h)	10,794	109,081	4,351
Temperature (°F)	122	206	253
<b>Breakdown (lb/h):</b>			
Ethanol	10,020	10,019	1
Water	245,735	3,161	242,573
Ethylene	858	858	0
Ether	440	440	0
Methane	0	0	0
Acetaldehyde	1,172	1,172	0
Ethane	57	57	0
Acetic Acid	221	0	221
Hydrogen	0	0	0
<b>Operating Conditions:</b>			
Condenser Pressure (psi)	29.4		
Condenser Temperature (°F)	206		
Reboiler Pressure (psi)	31.18		
Reboiler Temperature (°F)	252		
Reflux Ratio	0.85		
<b>Design Data:</b>			
Construction Material	Carbon Steel	Tray Efficiency	0.69
Weight (lb)	57,900	Number Trays	26
Diameter (ft)	6	Feed Stage	7
Height (ft)	64	Tray Spacing (ft)	2
<b>Exterior Components:</b>			
Condenser	HX301		
Reflux Accumulator	AC301		
Pump	P301		
Reboiler	HX302		
<b>Purchase Cost:</b>	\$194,400		
<b>Bare Module Cost:</b>	\$808,704		
<b>Annual Operating Cost:</b>	\$0		

HX301		
<b>Block Type:</b>	Fixed Head Shell and Tube Partial Condenser	
<b>Function:</b>	Condense vapor product from D301 using cooling water	
<b>Shell:</b>	<i>Inlet</i>	<i>Outlet</i>
Stream	S312	TO-REBOIL
Temperature (°F)	90	120
Pressure (psi)	14.7	14.7
<b>Tube:</b>	S303	S304
Stream	S303	S304
Temperature (°F)	206	206
Pressure (psig)	31.2	30.0
<b>Operating Conditions:</b>		
Shell Flow Rate (lb/h)	258,504	
Tube Flow Rate (lb/h)	18,480	
<b>Design Data:</b>		
Construction Material	Carbon Steel	
Flow Direction	Countercurrent	
Number of Tubes	122	
Number of Tube Passes	1	
Number of Shell Passes	1	
Transfer Area (ft <sup>2</sup> )	642	
Overall Heat Transfer Coefficient (BTU/h*ft <sup>2</sup> *R)	180	
Heat Duty (BTU/h)	9,063,300	
<b>Purchase Cost:</b>	\$17,900	
<b>Bare Module Cost:</b>	\$84,000	
<b>Annual Utilities Cost:</b>	\$24,100	

HX302		
<b>Block Type:</b>	U Tube Kettle Reboiler	
<b>Function:</b>	Vaporize liquid product from D301 using 50psi steam	
<b>Tube:</b>	<i>Inlet</i>	<i>Outlet</i>
Stream	STEAM301	STEAM302
Temperature (°F)	298	298
Pressure (psig)	50.0	50.0
<b>Shell:</b>		
Stream	S309	S310
Temperature (°F)	253	253
Pressure (psig)	31.2	29.8
<b>Operating Conditions:</b>		
Tube Flow Rate (lb/h)	54,267	
Shell Flow Rate (lb/h)	258,504	
<b>Design Data:</b>		
Construction Material	Carbon Steel	
Transfer Area (ft <sup>2</sup> )	5,684	
Overall Heat Transfer Coefficient (BTU/h*ft <sup>2</sup> *R)	80	
Heat Duty (BTU/h)	49,469,600	
<b>Purchase Cost:</b>	\$119,800	
<b>Bare Module Cost:</b>	\$379,766	
<b>Annual Utilities Cost:</b>	\$1,091,736	

AC301		
<b>Block Type:</b>	Reflux Accumulator - Horizontal Vessel	
<b>Function:</b>	Accumulate reflux from D301	
<b>Materials:</b>	<i>Inlet</i>	<i>Outlet</i>
Stream	S306	S307
<b>Operating Conditions:</b>		
Pressure (psi)	28.0	
Temperature (°F)	206.383	
<b>Design Data:</b>		
Construction Material	Carbon Steel	
Storage Volume (gal)	264	
Diameter (ft)	3	
Height (ft)	5	
<b>Purchase Cost:</b>	\$10,500	
<b>Bare Module Cost:</b>	\$32,025	
<b>Annual Utilities Cost:</b>	\$0	

P301 A/B		
<b>Block Type:</b>	Centrifugal Pump	
<b>Function:</b>	Return reflux to D301	
<b>Materials:</b>	<i>Inlet</i>	<i>Outlet</i>
Stream	S307	S308
<b>Operating Conditions:</b>		
Discharge Pressure (psi)	29.4	
Pressure Head (ft)	76	
Flow Rate (gpm)	44	
<b>Design Data:</b>		
Construction Material	Cast Iron	
Number of Stages	1	
Pump Efficiency	0.7	
Consumed Power (BTU/h)	1,356	
Power Source	Electricity	
<b>Purchase Cost:</b>	\$4,900	
<b>Bare Module Cost:</b>	\$16,170	
<b>Annual Utilities Cost:</b>	\$160	



P302 A/B		
<b>Block Type:</b>	Centrifugal Pump	
<b>Function:</b>	Pump purge water	
<b>Materials:</b>	<i>Inlet</i>	<i>Outlet</i>
Stream	S311	TREAT
<b>Operating Conditions:</b>		
Pressure Increase (psi)	14.7	
Pressure Head (ft)	38	
Flow Rate (gpm)	597	
<b>Design Data:</b>		
Construction Material	Cast Iron	
Number of Stages	1	
Pump Efficiency	0.711	
Consumed Power (BTU/h)	16,426	
Power Source	Electricity	
<b>Purchase Cost:</b>	\$8,300	
<b>Bare Module Cost:</b>	\$27,390	
<b>Annual Operating Cost:</b>	\$1,941	

C301		
<b>Block Type:</b>	Multistage Compressor	
<b>Function:</b>	Compress S305 so it can be recycled to the reactor section	
<b>Materials:</b>	<i>Inlet</i>	<i>Outlet</i>
Stream	S305	RECYCLE
<b>Operating Conditions:</b>		
Pressure Change (psi)	570.0	
Temperature Rise (°F)	428	
Inlet Flow Rate (ft <sup>3</sup> /h)	109,081	
Outlet Flow Rate (ft <sup>3</sup> /h)	8,027	
<b>Design Data:</b>		
Construction Material	Carbon Steel	
Number of Stages	3	
Interstage Cooling	N/A	
Consumed Power (BTU/h)	2,936,625	
Power Source	Electricity	
<b>Purchase Cost:</b>	\$1,403,400	
<b>Bare Module Cost:</b>	\$4,631,220	
<b>Annual Operating Cost:</b>	\$452,562	

Product Storage Tank	
<b>Block Type:</b>	Spherical Storage Tank
<b>Number of Units:</b>	2
<b>Function:</b>	Stores one hour of ethylene product
<b>Materials:</b>	
Mass Fraction:	
Ethylene	0.99960
Hydrogen	0.00003
Methane	0.00008
<b>Operating Conditions:</b>	
Pressure (psi)	14.7
Temperature (°F)	80
<b>Design Data:</b>	
Construction Material	Carbon Steel
Volume (gal)	1,000,000
Diameter (ft)	63.439
<b>Purchase Cost:</b>	\$1,343,000
<b>Bare Module Cost:</b>	\$4,257,310
<b>Annual Operating Cost:</b>	\$0

## Adsorption Section

C401		
<b>Block Type:</b>	Multistage Compressor	
<b>Function:</b>	Compress the nitrogen to both raise the temperature and	
<b>Materials:</b>	<i>Inlet</i>	<i>Outlet</i>
Stream	NITROGEN	S408
Temperature (°F)	80	350
<b>Operating Conditions:</b>		
Pressure Change (psi)	26.0	
Temperature Rise (°F)	247	
Inlet Flow Rate (ft <sup>3</sup> /h)	67,506	
Outlet Flow Rate (ft <sup>3</sup> /h)	36,171	
<b>Design Data:</b>		
Construction Material	Carbon Steel	
Number of Stages	1	
Interstage Cooling	N/A	
Consumed Power (BTU/h)	295,482	
Power Source	Electricity	
<b>Purchase Cost:</b>	\$87,800	
<b>Bare Module Cost:</b>	\$289,740	
<b>Annual Nitrogen Cost</b>	\$91,800	
<b>Annual Utilities Cost:</b>	\$45,547	

AD401 A/B			
<b>Block Type:</b>		Adsorption Column	
<b>Function:</b>		Remove trace water and ethanol from ADSORB so it cannot damage D501	
<b>Materials:</b>		<i>Inlet</i>	<i>Overhead</i>
Stream		ADSORB	CRYO
Mass Flow (lb/h)		335,339	335,005
Volumetric Flow (GPM)		12,533	12,574
Temperature (°F)		39.00	39.6
Pressure (psi)		455.6	441.0
Breakdown (lb/h):			
Ethylene		331,451	331,451
Ethanol		246	0
Water		67.7	0
Diethylether		3,511.3	3,511.3
Methane		42.0	42.0
Acetaldehyde		260.9	260.9
Hydrogen		11.8	11.8
Acetic Acid		0.035	0.035
<b>Operating Conditions:</b>			
Breakthrough Time (h)		24	Pressure Drop (psi) 15
Maximum Capacity (lb)		7,320	Residence Time (s) 22
Heat of Adsorption (BTU/hr)		113,400	
<b>Regeneration:</b>			
Eluent		NITROGEN	Temperature (°F) 350
Mass Flow (lb/h)		4,800	Regeneration Time (h) 24
<b>Design Data:</b>			
Construction Material		Carbon Steel	Volume (ft <sup>3</sup> ) 839
Vessel Weight (lb)		75,890	Diameter (ft) 7.50
<b>Adsorbant:</b>			
Adsorbant Type		Zeolite 13X	Adsorbant Weight (lb) 13,550
Spherical Diameter (mm)		3	Adsorbant Cost \$15,000
Adsorbant Volume (ft <sup>3</sup> )		772	Adsorbant Life (yrs) 3
<b>Purchase Cost:</b>		\$221,000	
<b>Bare Module Cost:</b>		\$729,300	
<b>Annual Adsorbant Cost:</b>		\$10,000	

## Cryogenic Distillation Section

D501			
<b>Block Type:</b>		Seive Tray Distillation Tower	
<b>Function:</b>		Purify ethylene product	
<b>Materials:</b>	<i>Inlet</i>	<i>Distillate</i>	<i>Bottoms</i>
Stream	S503	S506	S511
Phase	MIX	VAP	LIQ
Mass Flow (kg/h)	335,710	330,473	5,237
Volumetric Flow (L/h)	139,354	102,938	122
Temperature (°F)	-35	-68	-21
Breakdown (kg/h):			
Ethanol	0	0	0
Water	0	0	0
Ethylene	331,451	330,327	1,124
Ether	3,511	0	3,511
Methane	93	93	0
Acetaldehyde	575	0	575
Ethane	53	28	26
Acetic Acid	0	0	0
Hydrogen	26	26	0
<b>Operating Conditions:</b>			
Condenser Pressure (psi)	279.2		
Condenser Temperature (°F)	-67.5		
Reboiler Pressure (psi)	279.8		
Reboiler Temperature (°F)	-21.15		
Reflux Ratio	0.75		
<b>Design Data:</b>			
Construction Material	Stainless Steel	Tray Efficiency	0.75
Weight (lb)	76,800	Number Trays	8
Diameter (ft)	10.5	Feed Stage	3
Height (ft)	24	Tray Spacing (ft)	2
<b>Exterior Components:</b>			
Condenser	HX502		
Reflux Accumulator	AC501		
Pump	P501		
Reboiler	HX503		
<b>Purchase Cost:</b>		\$173,000	
<b>Bare Module Cost:</b>		\$719,680	
<b>Annual Operating Cost:</b>		\$0	

HX501		
<b>Block Type:</b>	Shell and Tube Heat Exchanger	
<b>Function:</b>	Heat CRYO-IN and cool S507	
<b>Shell:</b>	<i>Inlet</i>	<i>Outlet</i>
Stream	S507	CRYO-OUT
Temperature (°F)	-68	-35
Pressure (psi)	279.2	275.6
<b>Tube:</b>	CRYO-IN	S502
Stream	CRYO-IN	S502
Temperature (°F)	40	7
Pressure (psi)	455.6	452.5
<b>Operating Conditions:</b>		
Shell Flow Rate (lb/h)	330,473	
Tube Flow Rate (lb/h)	335,710	
<b>Design Data:</b>		
Construction Material	Stainless Steel	
Flow Direction	Countercurrent	
Number of Tubes	144	
Number of Tube Passes	1	
Number of Shell Passes	1	
Transfer Area (ft <sup>2</sup> )	2,951	
Overall Heat Transfer Coefficient (BTU/h*ft <sup>2</sup> *R)	30	
Heat Duty (BTU/h)	6,591,610	
<b>Purchase Cost:</b>	\$49,673	
<b>Bare Module Cost:</b>	\$157,463	
<b>Annual Operating Cost:</b>	\$0	

HX502		
<b>Block Type:</b>	Floating Head Shell and Tube Partial Condenser	
<b>Function:</b>	Condense vapor product from D501 using propylene refrigerant	
<b>Shell:</b>	<i>Inlet</i>	<i>Outlet</i>
Stream	R501	R502
Temperature (°F)	-90	-70
<b>Tube:</b>	S504	S505
Stream	-68	-68
Temperature (°F)	279.2	240.0
Pressure (psig)		
<b>Operating Conditions:</b>		
Shell Flow Rate (lb/h)	420,000	
Tube Flow Rate (lb/h)	2818	
<b>Design Data:</b>		
Construction Material	Stainless Steel	
Number of Tubes	1,122	
Number of Tube Passes	8	
Number of Shell Passes	2	
Transfer Area (ft <sup>2</sup> )	188,500	
Overall Heat Transfer Coefficient (BTU/h*ft <sup>2</sup> *R)	50	
Heat Duty (BTU/h)	56,357,300	
<b>Purchase Cost:</b>	\$2,985,500	
<b>Bare Module Cost:</b>	\$9,464,035	
<b>Annual Utilities Cost:</b>	\$5,368,643	



HX503		
<b>Block Type:</b>	U Tube Kettle Reboiler	
<b>Function:</b>	Vaporizes the bottoms to return as boilup	
<b>Tube:</b>	<i>Inlet</i>	<i>Outlet</i>
Stream	S512	REBOIL-OUT
Temperature (°F)	120	100
Pressure (psig)	14.7	14.7
<b>Shell:</b>	S510	S511
Stream	S510	S511
Temperature (°F)	-21.2	-21.2
Pressure (psig)	279.8	272.0
<b>Operating Conditions:</b>		
Tube Flow Rate (lb/h)	49,342	
Shell Flow Rate (lb/h)	199,282	
<b>Design Data:</b>		
Construction Material	Stainless Steel	
Transfer Area (ft <sup>2</sup> )	2,105	
Overall Heat Transfer Coefficient (BTU/h*ft <sup>2</sup> *R)	45	
Heat Duty (BTU/h)	49,039,968	
<b>Purchase Cost:</b>	\$59,500	
<b>Bare Module Cost:</b>	\$224,700	
<b>Annual Utilities Cost:</b>	-\$3,930	

AC501		
<b>Block Type:</b>	Reflux Accumulator	
<b>Function:</b>	Accumulate reflux from D501	
<b>Materials:</b>	<i>Inlet</i>	<i>Outlet</i>
Stream	S506	S508
<b>Operating Conditions:</b>		
Pressure (psi)	238.0	
Temperature (°F)	-68	
<b>Design Data:</b>		
Construction Material	Stainless Steel	
Storage Volume (gal)	4,965	
Diameter (ft)	7	
Height (ft)	20	
<b>Purchase Cost:</b>	\$43,900	
<b>Bare Module Cost:</b>	\$267,790	
<b>Annual Operating Cost:</b>	\$0	

P501 A/B		
<b>Block Type:</b>	Centrifugal Pump	
<b>Function:</b>	back into the column	
<b>Materials:</b>	<i>Inlet</i>	<i>Outlet</i>
Stream	S508	S509
<b>Operating Conditions:</b>		
Pressure Rise (psi)	41.0	
Pressure Head (ft)	107	
Flow Rate (gpm)	791	
<b>Design Data:</b>		
Construction Material	Stainless Steel	
Number of Stages	1	
Pump Efficiency	0.70	
Consumed Power (BTU/h)	36,566	
Power Source	Electricity	
<b>Purchase Cost:</b>	\$9,900	
<b>Bare Module Cost:</b>	\$32,670	
<b>Annual Operating Cost:</b>	\$4,321	



# **Section XII**

## **Conclusions and Recommendations**

The profitability of this plant is highly dependent on the prices of ethylene and ethanol, both of which fluctuate often. At currently available market prices, it is not likely to be profitable. The economic analysis conducted in this report shows that ethylene prices must rise significantly and ethanol prices must fall significantly before the plant will return a positive Net Present Value or Internal Rate of Return. While this is not entirely unreasonable, intense market research will be necessary to determine if the risk associated with building a plant at the present time is worthwhile.

There is a strong incentive to find ways to lower the operating cost of this process. Ethanol dehydration is preferable to the currently prevalent ethylene-yielding process of hydrocarbon cracking. For one, ethanol is renewable; it can be derived from sugar cane or corn, two major crops grown in South and North America. Additionally, ethanol dehydration produces far less waste and carbon emissions than cracking does. Governments worldwide are currently incentivizing the preference of “green” industry.

The two factors that make operating this plant expensive are heating the feed to extreme temperatures, and running cryogenic distillation to separate the final product. If more effective systems for heating or refrigeration were developed, this plant could potentially operate closer to profitability. In the future, it is recommended to research these areas to help improve the potential of this plant to succeed.

# **Section XIII**

## **Acknowledgements**

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# **Section XIV**

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# **Section XV**

## **Appendix**



## Appendix Table of Contents

### **Section**

- A. Sample Calculations
- B. ASPEN Printouts
- C. Problem Statement
- D. Relevant Documents
- E. MSDS Reports





# **Appendix A**

## **Sample Calculations**

## CALCULATIONS FOR DISTILLATION COLUMN SIZING (D301)

**Weighted liquid density ( $\rho_L$ )**

$$\rho_L = \sum(p_i)(\text{MassFrac}_i) \quad (0.1)$$

Where  $\rho_i$  = density of each component in the stream

MassFrac<sub>i</sub>= mass fraction of that component within the stream

$$\rho_L = (1000 \text{ kg/m}^3 \text{ H}_2\text{O})(\sim 1.0) = 1000 \text{ kg/m}^3$$

**Weighted gas density ( $\rho_g$ )**

$$MW = \sum(MW_i)(\text{MassFrac}_i) \quad (0.2)$$

Where MW= weighted molecular weight of gas stream

MassFrac<sub>i</sub>= mass fraction of that component within the stream

$$p_g = \frac{MW * P}{R * T} \quad (0.3)$$

Where P= pressure at the top tray

R= ideal gas constant

T= absolute temperature at that tray

$$MW = (0.0461 \text{ kg/mol ethanol})(0.515) + (0.016 \text{ kg/mol H}_2\text{O})(0.318) + (0.0461 \text{ kg/mol ether})(0.049) + (0.026 \text{ kg/mol acetylene})(0.080) = 0.034 \text{ kg/mol}$$

$$p_g = \frac{(0.034 \frac{\text{kg}}{\text{mol}})(20.4 \text{ bar})}{(8.314 \times 10^{-5} \frac{\text{m}^3 \cdot \text{bar}}{\text{K} \cdot \text{mol}})(449 \text{ K})} = 18.5 \frac{\text{kg}}{\text{m}^3}$$

**Flooding Correlation ( $F_{LG}$ )**

$$F_{LG} = \frac{L}{G} \left( \frac{p_G}{p_L} \right)^{0.5} \quad (0.4)$$

Where L= liquid rate

G= gas rate

$$F_{LG} = \left( \frac{88500 \frac{kg}{hr}}{48200 \frac{kg}{hr}} \right) \left( \frac{18.5 \frac{kg}{m^3}}{1000 \frac{kg}{m^3}} \right)^{0.5} = 0.250$$

### Parameter $C_{SB}$

(Use table in Seider et al pg.505)

For 18 inch spacing,  $C_{SB} = 0.2 \text{ft/s}$

### Surface Tension Factor ( $F_{ST}$ )

$$F_{ST} = \left( \frac{\sigma}{20} \right)^{0.20} \quad (0.5)$$

$\sigma =$  surface tension (dyne/cm)  $\sim 20$

$$F_{ST} = \left( \frac{20 \frac{dyne}{cm}}{20} \right)^{0.20} \approx 1$$

### Foaming Factor ( $F_F$ )

For non-foaming systems,  $F_F = 1$

### Hole-Area Factor ( $F_{HA}$ )

1 for

$$\frac{A_h}{A_T} \geq 0.1 \quad (0.6)$$

Where  $A_h$ = total hole area on tray

$A_a$ = is the active area of the tray

### Capacity Parameter (C)

$$C = C_{SB} F_{ST} F_F F_{HA} \quad (0.7)$$

$$C = (0.2 \text{ ft/s})(1)(1)(1) = 0.2 \text{ ft/s}$$

### Flooding Velocity ( $U_f$ )

$$U_f = C \left( \frac{\rho_L - \rho_G}{\rho_G} \right)^{0.5} \quad (1.8)$$

$$U_f = 0.2 \frac{\text{ft}}{\text{s}} \left( \frac{1000 \frac{\text{kg}}{\text{s}} - 18.5 \frac{\text{kg}}{\text{s}}}{18.5 \frac{\text{kg}}{\text{s}}} \right)^{0.5} = 1.46 \frac{\text{ft}}{\text{s}} * \frac{3600 \text{s}}{\text{hr}} = 5248 \frac{\text{ft}}{\text{hr}}$$

### Ratio $A_d/A_T$ (for $0.1 \leq F_{LG} \leq 1.0$ )

$$\frac{A_d}{A_T} = 0.1 + \frac{(F_{LG} - 0.1)}{9} \quad (1.9)$$

$$\frac{A_d}{A_T} = 0.1 + \frac{(0.250 - 0.1)}{9} = 0.117$$

### Fraction of Inside Cross-sectional Area to Vapor Flooding Velocity (f)

$$f = (0.75 \sim 0.85)$$

Assume  $f=0.85$

### Tower Inside Diameter ( $D_T$ )

$$D_T = \sqrt{\frac{4G}{(fU_f)\pi\left(1-\frac{A_d}{A_T}\right)\rho_G}} \quad (1.10)$$

$$D_T = \sqrt{\frac{4 * 48200 \frac{kg}{hr}}{\left(0.85 * 5250 \frac{ft}{hr} * 0.3048 \frac{mft}{hr}\right) \pi (1 - 0.117) * 18.5 \frac{kg}{m^3}}} = 2m = 6 ft$$

### Tower Height (H)

$$H = (N_{trays} - 1) * (spacing) + 4 ft + 10 ft \quad (1.11)$$

$$H = (26-1) * 2.0ft + 4ft + 10ft = 64 \text{ feet}$$

### REACTOR COSTING CALCULATIONS (R101)

$$P_d = \exp \{0.60608 + 0.91615[\ln(P_0)] + 0.0015655[\ln(P_0)]^2\}$$

$$P_d = \exp \{0.60608 + 0.91615[\ln(588psig)] + 0.0015655[\ln(588[psig])]^2\}$$

$$P_d = 673psig$$

$$t_s = \frac{P_d * D_i}{2 * S * E - 1.2 * P_d}$$

$$t_s = \frac{(673psig)(5.81ft)}{2 * 13100 - 1.2(673psig)}$$

$$t_s = 0.154ft$$

$$W = \pi(D_i + t_s)(L + 0.8D_i) * t_s * \rho$$

$$W = \pi(5.81ft + .154ft)(8.46ft + 0.8(5.81ft)) * (.154ft) * (473 \frac{lb}{ft^3})$$

$$W = 17,874lb$$

$$C_V = \exp \{8.9552 - 0.2330[\ln(W)] + 0.04333[\ln(W)]^2\}$$

$$C_V = \exp \{8.9552 - 0.2330[\ln(17874lb)] + 0.04333[\ln(17874lb)]^2\}$$

$$C_V = \$50,400$$

$$C_P = F_M * C_V + C_{PL}$$

$$C_P = (1.2) * (\$50400) + 0$$

$$C_P = \$63,345$$

$$C_{BM} = F_{BM} * C_P$$

$$C_{BM} = (3.05)(\$63345)$$

$$C_{BM} = \$193,201$$

# **APPENDIX B**

## **ASPEN Reports**

The following are ASPEN block results for the blocks representing R101, HX101, FL101, D501, and F101.

BLOCK: R1 MODEL: RSTOIC

-----  
 INLET STREAM: REACTIN  
 OUTLET STREAM: 20  
 PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG  
 HENRY-COMPS ID: HC-1

\*\*\* MASS AND ENERGY BALANCE \*\*\*

DIFF.	IN	OUT	GENERATION	RELATIVE
TOTAL BALANCE				
MOLE (KMOL/HR )	6142.95	9938.61	3795.66	
0.00000				
MASS (KG/HR )	262557.	262557.		
0.00000				
ENTHALPY (GCAL/HR )	-301.338	-272.172		-
0.967891E-01				

\*\*\* CO2 EQUIVALENT SUMMARY \*\*\*

FEED STREAMS CO2E	0.00000	KG/HR
PRODUCT STREAMS CO2E	434.297	KG/HR
NET STREAMS CO2E PRODUCTION	434.297	KG/HR
UTILITIES CO2E PRODUCTION	0.00000	KG/HR
TOTAL CO2E PRODUCTION	434.297	KG/HR

\*\*\* INPUT DATA \*\*\*  
 STOICHIOMETRY MATRIX:

REACTION # 1:						
SUBSTREAM MIXED :						
ETHANOL -1.00	WATER	1.00	ETHYLENE	1.00		
REACTION # 2:						
SUBSTREAM MIXED :						
ETHANOL -2.00	WATER	1.00	ETHER	1.00		
REACTION # 3:						
SUBSTREAM MIXED :						
ETHANOL -1.00	WATER	-1.00	AACID	1.00	HYDROGEN	
2.00						
REACTION # 4:						
SUBSTREAM MIXED :						
ETHANOL -1.00	ACETALD	1.00	HYDROGEN	1.00		
REACTION # 5:						
SUBSTREAM MIXED :						
ETHANOL -1.00	WATER	1.00	METHANE	2.00	HYDROGEN	-
2.00						



REACTION # 6:  
 SUBSTREAM MIXED :  
 ETHANOL -1.00 WATER 1.00 ETHANE 1.00 HYDROGEN -  
 1.00

REACTION CONVERSION SPECS: NUMBER= 6  
 REACTION # 1:  
 SUBSTREAM:MIXED KEY COMP:ETHANOL CONV FRAC: 0.7000  
 REACTION # 2:  
 SUBSTREAM:MIXED KEY COMP:ETHANOL CONV FRAC: 0.5000E-02  
 REACTION # 3:  
 SUBSTREAM:MIXED KEY COMP:ETHANOL CONV FRAC: 0.2500E-03  
 REACTION # 4:  
 SUBSTREAM:MIXED KEY COMP:ETHANOL CONV FRAC: 0.8000E-03  
 REACTION # 5:  
 SUBSTREAM:MIXED KEY COMP:ETHANOL CONV FRAC: 0.1000E-03  
 REACTION # 6:  
 SUBSTREAM:MIXED KEY COMP:ETHANOL CONV FRAC: 0.1000E-03

ONE PHASE TP FLASH SPECIFIED PHASE IS VAPOR  
 SPECIFIED TEMPERATURE C 310.000  
 SPECIFIED PRESSURE BAR 40.2767  
 MAXIMUM NO. ITERATIONS 30  
 CONVERGENCE TOLERANCE 0.000100000  
 SIMULTANEOUS REACTIONS  
 GENERATE COMBUSTION REACTIONS FOR FEED SPECIES NO

## \*\*\* RESULTS \*\*\*

OUTLET TEMPERATURE C 310.00  
 OUTLET PRESSURE BAR 40.277  
 HEAT DUTY GCAL/HR 29.166

## REACTION EXTENTS:

REACTION NUMBER	REACTION EXTENT KMOL/HR
1	3790.0
2	13.536
3	1.3536
4	4.3314
5	0.54142
6	0.54142

BLOCK: FURN1 MODEL: HEATER

-----  
 INLET STREAM: FROMRHX

OUTLET STREAM: REACTIN  
 PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG  
 HENRY-COMPS ID: HC-1

\*\*\* MASS AND ENERGY BALANCE \*\*\*

	IN	OUT	RELATIVE
DIFF.			
TOTAL BALANCE			
MOLE (KMOL/HR )	6142.95	6142.95	0.00000
MASS (KG/HR )	262557.	262557.	0.00000
ENTHALPY (GCAL/HR )	-317.242	-301.338	-0.501316E-

01

\*\*\* CO2 EQUIVALENT SUMMARY \*\*\*

FEED STREAMS CO2E	0.00000	KG/HR
PRODUCT STREAMS CO2E	0.00000	KG/HR
NET STREAMS CO2E PRODUCTION	0.00000	KG/HR
UTILITIES CO2E PRODUCTION	0.00000	KG/HR
TOTAL CO2E PRODUCTION	0.00000	KG/HR

\*\*\* INPUT DATA \*\*\*

TWO PHASE TP FLASH

SPECIFIED TEMPERATURE	C	400.000
SPECIFIED PRESSURE	BAR	42.6072
MAXIMUM NO. ITERATIONS		30
CONVERGENCE TOLERANCE		0.000100000

\*\*\* RESULTS \*\*\*

OUTLET TEMPERATURE	C	400.00
OUTLET PRESSURE	BAR	42.607
HEAT DUTY	GCAL/HR	15.904
OUTLET VAPOR FRACTION		1.0000
PRESSURE-DROP CORRELATION PARAMETER		-1165.8

V-L PHASE EQUILIBRIUM :

COMP	F (I)	X (I)	Y (I)	K (I)
ETHANOL	0.88138	0.96486	0.88138	
1.8458				
WATER	0.11862	0.35136E-01	0.11862	
6.8219				

BLOCK: FLASH1 MODEL: FLASH3

-----

INLET STREAM: SEPFEEDC  
 OUTLET VAPOR STREAM: FTOP  
 FIRST LIQUID OUTLET: FMIDDLE  
 SECOND LIQUID OUTLET: FBOTTOM  
 PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG

HENRY-COMPS ID: HC-1

```

*** MASS AND ENERGY BALANCE ***
                                IN                OUT                RELATIVE
DIFF.
TOTAL BALANCE
  MOLE (KMOL/HR )                11717.4                11717.4                -0.155238E-
15
  MASS (KG/HR )                   269682.                269682.                -0.431676E-
15
  ENTHALPY (GCAL/HR )             -361.947                -361.947                0.743684E-
09

```

```

*** CO2 EQUIVALENT SUMMARY ***
FEED STREAMS CO2E                1051.87                KG/HR
PRODUCT STREAMS CO2E             1051.87                KG/HR
NET STREAMS CO2E PRODUCTION      0.00000                KG/HR
UTILITIES CO2E PRODUCTION        0.00000                KG/HR
TOTAL CO2E PRODUCTION            0.00000                KG/HR

```

```

*** INPUT DATA ***
THREE PHASE PQ FLASH
SPECIFIED PRESSURE BAR                39.5167
SPECIFIED HEAT DUTY GCAL/HR           0.0
MAXIMUM NO. ITERATIONS                30
CONVERGENCE TOLERANCE                 0.000100000
NO KEY COMPONENT IS SPECIFIED
KEY LIQUID STREAM: FBOTTOM

```

```

*** RESULTS ***
OUTLET TEMPERATURE C                 49.971
OUTLET PRESSURE BAR                   39.517
VAPOR FRACTION                        0.46334
1ST LIQUID/TOTAL LIQUID              1.0000

```

V-L1-L2 PHASE EQUILIBRIUM :

COMP	F(I)	X1(I)	X2(I)	Y(I)	K1(I)
K2(I) ETHANOL	0.863E-02	0.151E-01	0.151E-01	0.107E-02	0.709E-01
0.709E-01 WATER	0.528	0.980	0.980	0.485E-02	0.495E-02
0.495E-02 ETHYLENE	0.459	0.215E-02	0.215E-02	0.987	458.
458. ETHER	0.206E-02	0.399E-03	0.399E-03	0.399E-02	10.0
10.0 METHANE	0.224E-03	0.389E-06	0.389E-06	0.483E-03	0.124E+04
0.124E+04 ACETALD	0.154E-02	0.181E-02	0.181E-02	0.121E-02	0.670
0.670 ETHANE	0.143E-03	0.136E-03	0.136E-03	0.150E-03	1.10
1.10					

AACID 0.143E-03 0.265E-03 0.265E-03 0.129E-05 0.485E-02  
 0.485E-02  
 HYDROGEN 0.499E-03 0.819E-06 0.819E-06 0.108E-02 0.131E+04  
 0.131E+04

BLOCK: CRYO MODEL: RADFRAC

-----  
 INLETS - INCRYO STAGE 3  
 OUTLETS - CRYOVER STAGE 1  
 CPURGE STAGE 6

PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG  
 HENRY-COMPS ID: HC-1

\*\*\* MASS AND ENERGY BALANCE \*\*\*

	IN	OUT	RELATIVE
DIFF. TOTAL BALANCE			
MOLE (KMOL/HR )	5395.80	5395.80	-0.384217E-
09 MASS (KG/HR )	152275.	152275.	-0.322460E-
09 ENTHALPY (GCAL/HR )	60.3259	58.4819	0.305663E-
01			

\*\*\* CO2 EQUIVALENT SUMMARY \*\*\*

FEED STREAMS CO2E	1050.87	KG/HR
PRODUCT STREAMS CO2E	1050.87	KG/HR
NET STREAMS CO2E PRODUCTION	0.879258E-04	KG/HR
UTILITIES CO2E PRODUCTION	0.00000	KG/HR
TOTAL CO2E PRODUCTION	0.879258E-04	KG/HR

\*\*\*\*\*  
 \*\*\*\* INPUT DATA \*\*\*\*  
 \*\*\*\*\*

\*\*\*\* INPUT PARAMETERS \*\*\*\*

NUMBER OF STAGES	6
ALGORITHM OPTION	STANDARD
ABSORBER OPTION	NO
INITIALIZATION OPTION	STANDARD
HYDRAULIC PARAMETER CALCULATIONS	NO
INSIDE LOOP CONVERGENCE METHOD	BROYDEN
DESIGN SPECIFICATION METHOD	NESTED
MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS	150
MAXIMUM NO. OF INSIDE LOOP ITERATIONS	10
MAXIMUM NUMBER OF FLASH ITERATIONS	30
FLASH TOLERANCE	0.000100000
OUTSIDE LOOP CONVERGENCE TOLERANCE	0.000100000

\*\*\*\* COL-SPECS \*\*\*\*

MOLAR VAPOR DIST / TOTAL DIST 1.00000  
 MASS REFLUX RATIO 0.75000  
 MASS DISTILLATE RATE KG/HR 149,900.

\*\*\*\* PROFILES \*\*\*\*

P-SPEC STAGE 1 PRES, BAR 19.2518

\*\*\*\*\*  
 \*\*\*\* RESULTS \*\*\*\*  
 \*\*\*\*\*

\*\*\* COMPONENT SPLIT FRACTIONS \*\*\*

COMPONENT:	OUTLET STREAMS	
	CRYOVER	CPURGE
ETHANOL	1.0000	0.0000
WATER	.33271E-07	1.0000
ETHYLENE	.99661	.33920E-02
ETHER	.11471E-04	.99999
METHANE	1.0000	.46106E-06
ACETALD	.28257E-04	.99997
ETHANE	.51445	.48555
AACID	.31932E-10	1.0000
HYDROGEN	1.0000	.80519E-12

\*\*\* SUMMARY OF KEY RESULTS \*\*\*

TOP STAGE TEMPERATURE	C	-55.2971
BOTTOM STAGE TEMPERATURE	C	-29.5271
TOP STAGE LIQUID FLOW	KMOL/HR	4,007.41
BOTTOM STAGE LIQUID FLOW	KMOL/HR	45.9789
TOP STAGE VAPOR FLOW	KMOL/HR	5,349.82
BOILUP VAPOR FLOW	KMOL/HR	3,115.93
MOLAR REFLUX RATIO		0.74907
MOLAR BOILUP RATIO		67.7686
CONDENSER DUTY (W/O SUBCOOL)	GCAL/HR	-14.2018
REBOILER DUTY	GCAL/HR	12.3579

\*\*\*\* MAXIMUM FINAL RELATIVE ERRORS \*\*\*\*

DEW POINT	0.24631E-05	STAGE=	6
BUBBLE POINT	0.18015E-07	STAGE=	6
COMPONENT MASS BALANCE	0.75536E-06	STAGE=	5 COMP=ETHER
ENERGY BALANCE	0.25259E-06	STAGE=	6

\*\*\*\* PROFILES \*\*\*\*

\*\*NOTE\*\* REPORTED VALUES FOR STAGE LIQUID AND VAPOR RATES ARE THE FLOWS

FROM THE STAGE INCLUDING ANY SIDE PRODUCT.

STAGE	TEMPERATURE C	PRESSURE BAR	ENTHALPY KCAL/MOL		HEAT DUTY GCAL/HR
			LIQUID	VAPOR	
1	-55.297	19.252	7.7196	11.238	-14.2018
2	-55.083	19.260	7.2006	11.249	
3	-55.029	19.268	7.1344	11.258	
4	-55.000	19.277	7.0945	11.245	
5	-54.772	19.285	6.5640	11.210	
6	-29.527	19.293	-35.601	11.152	12.3578

STAGE	FLOW RATE KMOL/HR		FEED RATE KMOL/HR			PRODUCT RATE KMOL/HR
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID
VAPOR						
1	4007.	5350.				
5349.8226						
2	3528.	9357.		5392.8552		
3	3530.	3485.	2.9462			
4	3526.	3484.				
5	3162.	3480.				
6	45.98	3116.				45.9789

\*\*\*\* MASS FLOW PROFILES \*\*\*\*

STAGE	FLOW RATE KG/HR		FEED RATE KG/HR			PRODUCT RATE KG/HR
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID
VAPOR						
1	0.1124E+06	0.1499E+06				
.14990+06						
2	0.9997E+05	0.2623E+06		.15209+06		
3	0.1001E+06	0.9778E+05	190.2472			
4	0.1000E+06	0.9775E+05				
5	0.9039E+05	0.9765E+05				
6	2375.	0.8802E+05				2375.3259

STAGE	ETHANOL	**** MOLE-X-PROFILE ****		
		WATER	ETHYLENE	ETHER
METHANE				
1	0.13347E-30	0.45921E-14	0.99965	0.24372E-04
0.78486E-04				
2	0.76656E-31	0.12748E-10	0.99247	0.54650E-02
0.50126E-04				
3	0.17813E-30	0.62459E-10	0.99140	0.60986E-02
0.81251E-05				
4	0.53303E-51	0.62530E-10	0.99019	0.61132E-02
0.13170E-05				
5	0.16056E-71	0.71148E-10	0.98083	0.10081E-01
0.21267E-06				
6	0.10881E-69	0.47946E-08	0.39536	0.46733
0.26274E-07				

**** MOLE-X-PROFILE ****				
STAGE	ACETALD	ETHANE	AACID	HYDROGEN
1	0.10906E-04	0.22100E-03	0.28876E-12	0.11853E-04
2	0.16098E-02	0.39387E-03	0.10782E-07	0.68311E-05
3	0.16824E-02	0.81084E-03	0.16649E-06	0.75451E-07
4	0.16902E-02	0.20048E-02	0.16668E-06	0.83378E-09
5	0.36909E-02	0.53937E-02	0.18670E-06	0.91971E-11
6	0.12879	0.85168E-02	0.12782E-04	0.10224E-12

**** MOLE-Y-PROFILE ****				
STAGE	ETHANOL	WATER	ETHYLENE	ETHER
METHANE				
1	0.45270E-10	0.13710E-17	0.99834	0.46074E-07
2	0.25883E-10	0.19674E-14	0.99890	0.10464E-04
3	0.60285E-10	0.95588E-14	0.99964	0.11760E-04
4	0.18048E-30	0.95147E-14	0.99927	0.11818E-04
5	0.54007E-51	0.97801E-14	0.99805	0.19714E-04
6	0.23695E-73	0.14484E-11	0.98947	0.33336E-02

**** MOLE-Y-PROFILE ****				
STAGE	ACETALD	ETHANE	AACID	HYDROGEN
1	0.31277E-07	0.77554E-04	0.35079E-17	0.10913E-02
2	0.46888E-05	0.13899E-03	0.12367E-12	0.62902E-03
3	0.49305E-05	0.28662E-03	0.19245E-11	0.69253E-05
4	0.49646E-05	0.70915E-03	0.19332E-11	0.76447E-07
5	0.10992E-04	0.19188E-02	0.21971E-11	0.84479E-09
6	0.18450E-02	0.53477E-02	0.84414E-09	0.93313E-11

**** K-VALUES ****					
STAGE	ETHANOL	WATER	ETHYLENE	ETHER	
METHANE					
1	0.10000E+21	0.29856E-03	0.99869	0.18905E-02	6.2402
2	0.10000E+21	0.15433E-03	1.0065	0.19147E-02	6.2568
3	0.10000E+21	0.15304E-03	1.0083	0.19283E-02	6.2520
4	0.10000E+21	0.15216E-03	1.0092	0.19332E-02	6.2508
5	0.10000E+21	0.13746E-03	1.0176	0.19557E-02	6.2728
6	0.21777E-03	0.30210E-03	2.5027	0.71333E-02	8.1988

**** K-VALUES ****				
STAGE	ACETALD	ETHANE	AACID	HYDROGEN
1	0.28678E-02	0.35092	0.12148E-04	92.069
2	0.29127E-02	0.35288	0.11470E-04	92.082
3	0.29307E-02	0.35348	0.11559E-04	91.785
4	0.29373E-02	0.35372	0.11598E-04	91.687
5	0.29782E-02	0.35574	0.11768E-04	91.854
6	0.14326E-01	0.62789	0.66041E-04	91.266

		**** MASS-X-PROFILE ****		
STAGE	ETHANOL	WATER	ETHYLENE	ETHER
METHANE				
1	0.21918E-30	0.29489E-14	0.99964	0.64393E-04
0.44882E-04				
2	0.12465E-30	0.81065E-11	0.98275	0.14298E-01
0.28384E-04				
3	0.28933E-30	0.39672E-10	0.98058	0.15938E-01
0.45957E-05				
4	0.86568E-51	0.39712E-10	0.97927	0.15974E-01
0.74481E-06				
5	0.25874E-71	0.44835E-10	0.96250	0.26137E-01
0.11934E-06				
6	0.97032E-70	0.16720E-08	0.21469	0.67051
0.81590E-08				

		**** MASS-X-PROFILE ****		
STAGE	ACETALD	ETHANE	AACID	HYDROGEN
1	0.17126E-04	0.23688E-03	0.61812E-12	0.85173E-06
2	0.25031E-02	0.41803E-03	0.22855E-07	0.48606E-06
3	0.26130E-02	0.85963E-03	0.35250E-06	0.53626E-08
4	0.26249E-02	0.21252E-02	0.35286E-06	0.59253E-10
5	0.56876E-02	0.56733E-02	0.39219E-06	0.64853E-12
6	0.10982	0.49573E-02	0.14858E-04	0.39896E-14

		**** MASS-Y-PROFILE ****		
STAGE	ETHANOL	WATER	ETHYLENE	ETHER
METHANE				
1	0.74432E-10	0.88150E-18	0.99956	0.12188E-06
0.28042E-03				
2	0.42533E-10	0.12643E-14	0.99959	0.27667E-04
0.17947E-03				
3	0.98997E-10	0.61383E-14	0.99962	0.31071E-04
0.29049E-04				
4	0.29636E-30	0.61096E-14	0.99920	0.31224E-04
0.47072E-05				
5	0.88674E-51	0.62794E-14	0.99787	0.52080E-04
0.76273E-06				
6	0.38644E-73	0.92372E-12	0.98268	0.87474E-02
0.12234E-06				

		**** MASS-Y-PROFILE ****		
STAGE	ACETALD	ETHANE	AACID	HYDROGEN
1	0.49175E-07	0.83228E-04	0.75183E-17	0.78515E-04
2	0.73679E-05	0.14908E-03	0.26491E-12	0.45231E-04
3	0.77423E-05	0.30721E-03	0.41196E-11	0.49763E-06
4	0.77954E-05	0.76005E-03	0.41379E-11	0.54929E-08
5	0.17258E-04	0.20563E-02	0.47024E-11	0.60694E-10
6	0.28773E-02	0.56926E-02	0.17946E-08	0.66593E-12

\*\*\* ASSOCIATED UTILITIES \*\*\*

UTILITY USAGE: HW (WATER)

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REBOILER	2.2428+04		0.4486
	-----		-----
TOTAL:	2.2428+04	KG/HR	0.4486 \$/HR
	=====		

BLOCK: REACTHX MODEL: HEATX

HOT SIDE:

INLET STREAM: REACTOUT  
 OUTLET STREAM: SEPFEEED  
 PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG  
 HENRY-COMPS ID: HC-1

COLD SIDE:

INLET STREAM: TORHX  
 OUTLET STREAM: FROMRHX  
 PROPERTY OPTION SET: NRTL-RK RENON (NRTL) / REDLICH-KWONG  
 HENRY-COMPS ID: HC-1

\*\*\* MASS AND ENERGY BALANCE \*\*\*

	IN	OUT	RELATIVE
DIFF.			
TOTAL BALANCE			
MOLE (KMOL/HR )	17860.4	17860.4	0.00000
MASS (KG/HR )	532239.	532239.	0.00000
ENTHALPY (GCAL/HR )	-672.382	-672.382	-0.169081E-

15

\*\*\* CO2 EQUIVALENT SUMMARY \*\*\*

FEED STREAMS CO2E	1051.87	KG/HR
PRODUCT STREAMS CO2E	1051.87	KG/HR
NET STREAMS CO2E PRODUCTION	0.00000	KG/HR
UTILITIES CO2E PRODUCTION	0.00000	KG/HR
TOTAL CO2E PRODUCTION	0.00000	KG/HR

\*\*\* INPUT DATA \*\*\*

FLASH SPECS FOR HOT SIDE:

TWO PHASE FLASH  
 MAXIMUM NO. ITERATIONS 30  
 CONVERGENCE TOLERANCE 0.000100000

FLASH SPECS FOR COLD SIDE:

TWO PHASE FLASH  
 MAXIMUM NO. ITERATIONS 30  
 CONVERGENCE TOLERANCE 0.000100000

FLOW DIRECTION AND SPECIFICATION:

COUNTERCURRENT HEAT EXCHANGER  
 SPECIFIED COLD OUTLET TEMP  
 SPECIFIED VALUE C 300.0000  
 LMTD CORRECTION FACTOR 1.00000

## PRESSURE SPECIFICATION:

HOT SIDE OUTLET PRESSURE	BAR	39.8000
COLD SIDE OUTLET PRESSURE	BAR	41.0500

## HEAT TRANSFER COEFFICIENT SPECIFICATION:

OVERALL COEFFICIENT	KCAL/HR-SQM-K	1220.6069
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\*\*\* OVERALL RESULTS \*\*\*

## STREAMS:

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-----
REACTOUT  -----> |                | |-----> SEPFEED
T= 3.1000D+02 |                | |                T=
8.1840D+01 |                | |                P=
P= 4.0074D+01 |                | |                V=
3.9800D+01 |                | |                V=
V= 1.0000D+00 |                | |                V=
4.7123D-01 |                | |                V=

FROMRHX  <----- |                | |<----- TORHX
T= 3.0000D+02 |                | |                T=
2.6026D+01 |                | |                P=
P= 4.1050D+01 |                | |                P=
4.1543D+01 |                | |                V=
V= 1.0000D+00 |                | |                V=
0.0000D+00 |                | |                V=
-----

```

## DUTY AND AREA:

CALCULATED HEAT DUTY	GCAL/HR	90.8984
CALCULATED (REQUIRED) AREA	SQM	2794.9152
ACTUAL EXCHANGER AREA	SQM	2794.9152
PER CENT OVER-DESIGN		0.0000

## HEAT TRANSFER COEFFICIENT:

AVERAGE COEFFICIENT (DIRTY)	KCAL/HR-SQM-K	1220.6069
UA (DIRTY)	CAL/SEC-K	947636.8860

## LOG-MEAN TEMPERATURE DIFFERENCE:

LMTD CORRECTION FACTOR		1.0000
LMTD (CORRECTED)	C	26.6448
NUMBER OF SHELLS IN SERIES		1

## PRESSURE DROP:

HOTSIDE, TOTAL	BAR	0.2740
COLD SIDE, TOTAL	BAR	0.4932

## PRESSURE DROP PARAMETER:

HOT SIDE:	154.74
COLD SIDE:	779.31

# **APPENDIX C**

## **Problem Statement**

## **Ethylene from Ethanol**

**(Recommended by Bruce M. Vrana, DuPont)**

Ethylene is conventionally produced from fossil-fuel feedstocks such as ethane or naphtha in huge, expensive ethylene crackers. Typical crackers produce 1 million tonnes of ethylene per year and cost over a billion dollars to build. The ethylene market is large and growing worldwide. The industry needs about 5 million tonnes per year of new capacity by 2030 in the U.S. alone. Ethylene is one of the basic building blocks of the chemical industry, going into a wide variety of products, including polyethylene, polystyrene, ethylene glycol, and PVC. To reduce your company's dependence on fossil fuels, your team has been assembled to design a plant to make 1MM tonnes of ethylene per year from ethanol, made by fermentation of renewable resources. The goal is to be cost competitive with fossil ethylene while reducing greenhouse gas emissions.

Ethanol dehydration to ethylene was practiced commercially in the first half of the 20<sup>th</sup> century in the U.S. and Europe, and in the second half of the century in Brazil and elsewhere, but was abandoned largely with the global expansion of the petrochemical industry. However, with the increase in the cost of, and limited supply of, fossil fuels, and the growing production of ethanol, companies are beginning to consider this technology again.

Ethanol dehydration to ethylene is an endothermic reaction, usually carried out at 300 to 400°C at moderate pressure over an activated alumina or silica catalyst. Ethanol conversion is 98%, and selectivity to ethylene is about 98%. Ethylene must be 99.96% pure to meet polymer grade specs.

There are two different reactor technologies. An isothermal fixed bed reactor can be run at 350°C with a liquid hourly space velocity of 0.2/hr. Catalyst is typically packed in tubes of a heat exchanger, with heating on the outside to maintain isothermal operation. The catalyst must be regenerated to remove coke approximately every 1 to 2 months, so your design should consider this fact. Regeneration takes about 3 days. Most plants built in the 20th century used isothermal technology. (If you cannot find selectivity data, you may assume the same product distribution as in the Petrobras patent for adiabatic reactors without steam co-feed at whatever pressure you wish to operate).

Alternatively, an adiabatic fixed bed reactor can be used, with an inlet temperature of 450°C. Petrobras technology used steam in the feed to solve the coking problem, and catalyst life was about 1 year. The Petrobras patent gives more details. You may use either isothermal or adiabatic reactor technology, and if adiabatic, you may add steam to the feed or not. You should justify your choice based on economic estimates as well as technical feasibility. The United States and Brazil produce most of the world's ethanol by fermentation of local agricultural feedstocks. The U.S. industry is almost entirely based on corn, while Brazil uses sugar cane. Process efficiencies in both countries have improved dramatically in recent years, with increasing ethanol production for use in transportation fuels; thus, do not use process or cost data that is more than 2-3 years old. You may locate your plant in either the U.S. or Brazil, using appropriate construction costs for your location, and local ethanol costs and specs.

If you decide to locate in Brazil, one important factor to consider in your economics is that ethanol price increases dramatically during the inter-harvest period, typically 3-4 months of the year when sugar cane cannot be harvested and local ethanol plants shut down. In recent years, Brazil has imported ethanol from the U.S. during this part of the year. Corn ethanol in the U.S. has no such restriction, as corn can be stored year-round. Be sure to include freight to your plant site in the cost of the ethanol.

You will need to make many assumptions to complete your design, since the data you have is far from complete. State them explicitly in your report, so that management may understand the uncertainty in your design and economic projections before considering the next step toward commercialization – designing and running a pilot plant. Test your economics to reasonable ranges of your assumptions. If there are any possible “showstoppers” (i.e., possible fatal flaws, if one assumption is incorrect that would make the design either technically infeasible or uneconomical), these need to be clearly communicated and understood before proceeding.

The plant design should be as environmentally friendly as possible, at a minimum meeting Federal and state emissions regulations. Recover and recycle process materials to the maximum economic extent. Also, energy consumption should be minimized, to the extent economically justified. The plant design must also be controllable and safe to operate. Remember that you will

be there for the plant start-up and will have to live with whatever design decisions you have made.

#### References

U.S. Patent 4,232,179, November 4, 1980, assigned to Petrobras.

The Renewable Fuels Association web site has a good description of the fuel ethanol process and industry. <http://www.ethanolrfa.org>

# **APPENDIX D**

## **MSDS Reports**

# **APPENDIX E**

## **Relevant Documents**



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*
* Calculations were completed normally
*
* All Unit Operation blocks were completed normally
*
* All streams were flashed normally
*
* All Utility blocks were completed normally
*
* All Convergence blocks were completed normally
*
*****
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