

Production of Ethylene from Ethanol

Senior Design and Professionalism

CHEG 4247-P01

Presented by group 3:

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Outline

- Introduction
- Gantt Chart
- Design Basis / Chemical Conditions
- Catalyst Selection
- Uses and Client List
- Location
- Block Flow and Process Flow Diagram
- Material and Energy Balance
- Aspen HYSYS
- Summary of Economics
- Cash Flow Diagram
- P&ID/ Specification sheet
- HAZOP
- Process Safety

Problem Statement / Introduction

- The project aims to produce high purity ethylene from ethanol through catalytic dehydrogenation of ethanol.
- Must meet state regulations, follow codes, and stay within legal limits to work.
- How much can our plant produce a year?
- Is this plant built to last 20-30 years?

Gantt Chart

Production of Ethylene from Ethanol

Project Start:

Mon, 1/24/2022

Display Week:

1

Jan 24, 2022

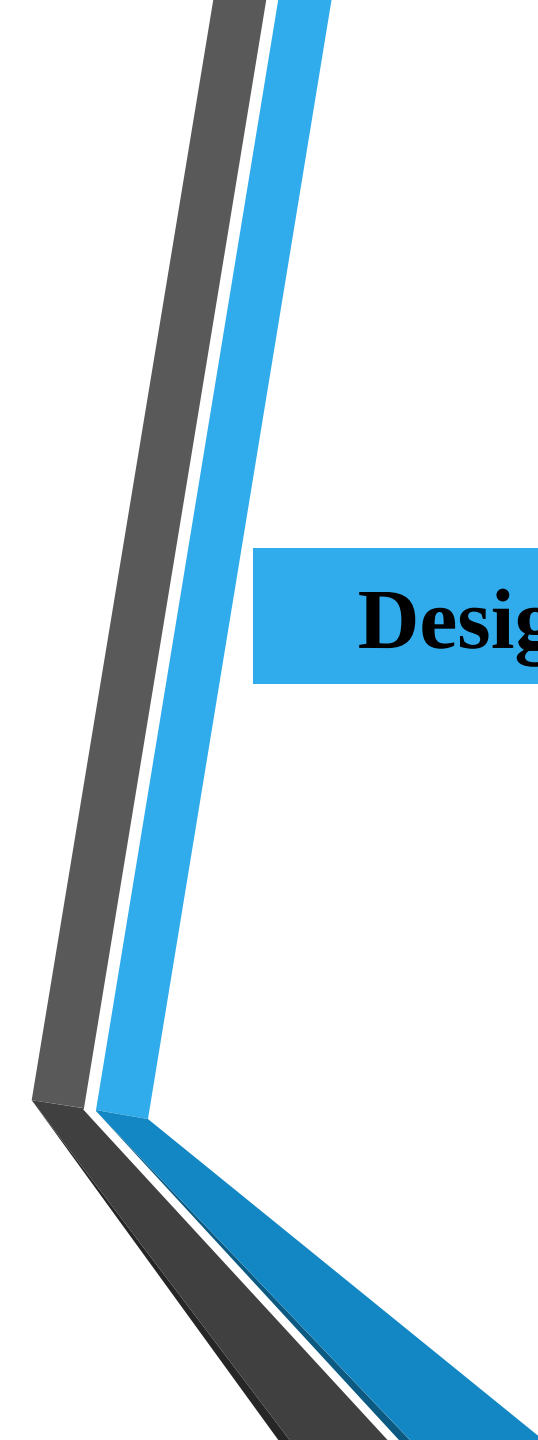
Jan 31, 2022

Feb 7, 2022

24 25 26 27 28 29 30 31 1 2 3 4 5 6 7 8 9 10

M T W T F S S M T W T F S S M T W

TASK	PROGRESS	START	END	ASSIGNED TO	DURATION	DAYS	M	T	W	T	F	S	S	M	T	W	T	F	S	S	M	T	W
Process Design	PROGRESS				5 WEEKS																		
ASPEN/PLUS Simulation of Process	100%	1/24/22	2/9/22	Ryan L.	2.5 WEEKS																		
Major Equipments Calculations	100%	2/9/22	3/2/22	All members	5 WEEKS																		
Design of Major Equipment	100%	3/3/22	3/24/22	All members	3 WEEKS																		
Equipments Specification	100%	3/25/22	4/1/22	All members	2 WEEKS																		
Financial Analysis	100%	4/1/22	4/8/22	Alexus L.	1 WEEK																		
Safety and HAZOP Analysis					2 WEEKS																		
HAZID	100%	4/1/22	4/5/22	Rafid & Reema M.	5 DAYS																		
Hazard and Operability Study (HAZOP)	100%	4/1/22	4/15/22	Rafid & Reema M.	2 WEEKS																		
Reporting					4 MONTHS																		
Final Report	100%	1/24/22	4/30/22	ALL	4 MONTHS																		
Final Presentation	100%	4/16/22	4/21/22	ALL	6 DAYS																		
ASPEN/PLUS Report	100%	4/18/22	4/18/22	Ryan L.	1 DAY																		



Design Basis

**Plant
Capacity:** 400,000
lbs/yr

Raw materials:
Ethanol

Process:
Assume Steady
State

Process Selection:
Catalytic
Dehydrogenation

**Initial Mass Flow
Rate:** 77,525 lbs/hr

Chemical Conditions

	Ethanol	Ethylene
Boiling Point Temperature	173 °F	-155 °F
Flash Point Temperature	55 °F	-213 °F
Melting point Temperature	-173 °F	-274 °F
Autoignition Temperature	689 °F	842 °F
Freezing point	-173 °F	-328 °F
Storage Temperature	Below 73 °F	Near 32°F

Table 1

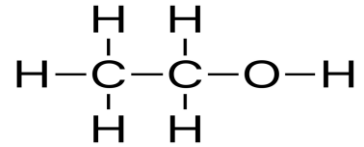
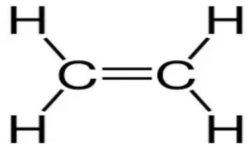
	Ethanol	Ethylene
Molecular Formula	C ₂ H ₅ OH	C ₂ H ₄
Structure Formula		

Table 2

By-Products
(C ₂ H ₅) ₂ O+H ₂ O
C ₂ H ₄ O+H ₂
H ₂

Table 3

Catalytic Dehydrogenation

γ -Al₂O₃ (Alumina)



The removal/
production of
hydrogen which is an
efficient renewable
energy source.

Requires a high
reaction temperature
of about 805 degrees
Fahrenheit.

Life Expectancy is
about 400 hours.

Ethanol Conversion
at 95.6% with 98%
Ethylene purity

Ethylene

Uses:

- Production of fabricated plastics
- Antifreeze



Client List

Companies Names	Product
Shell Polymers	They use ethylene to manufacture polyethylene which in turn is used for piping irrigation of water and gas.
Petro Extrusion Technologies, In	They are specialized in extrusion of polyethylene to mold in specific shape.
Chevron Corporation	Ethylene is polymerized in polyethylene to produce a wide range of plastics.
Twin Specialties	They use ethylene to produce ethylene glycol in both liquid and powder form.

Location

North Dakota

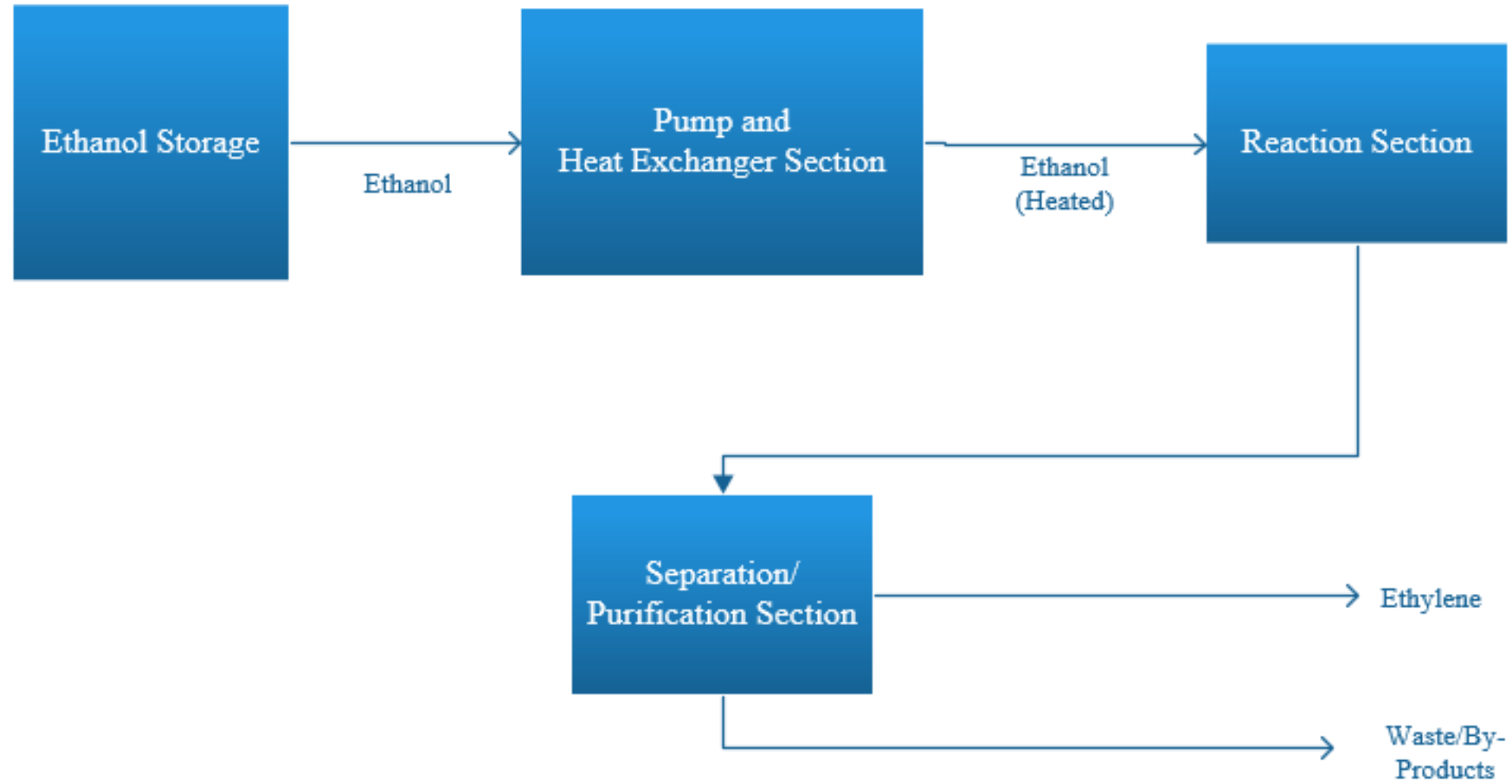


Why ?

- Major ethanol production from corn, closer to raw material.
- Access to waste-water treatments.
- 440 million gallons of ethylene produced a year.
- 10% sold within the state / 90% is shipped.
- Seven order concentration units, which cannot be 100 feet from schools, churches, etc. (Construction Permit)
- An air pollution permit, and a hazardous air pollutant permit (Clean air act).

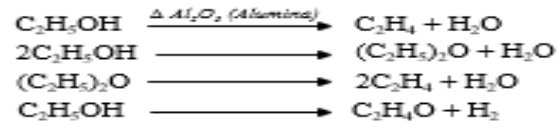


Block Flow Diagram

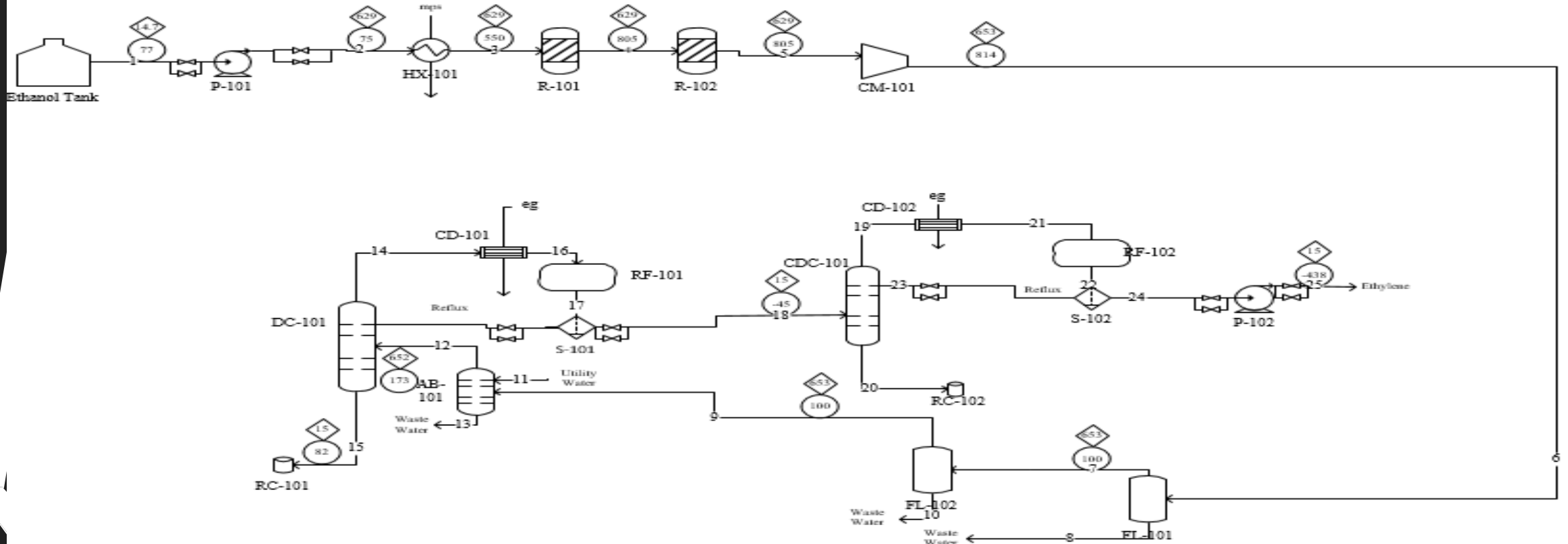


Process Flow Diagram

Catalytic Dehydration of Ethanol to Ethylene



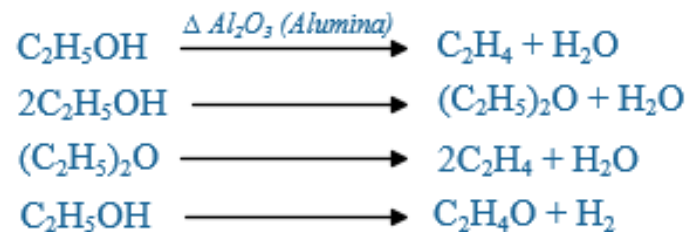
 Pressure (psia)
 Temperature (°F)



P-101/102 Pump	HX-101/102 Heat Exchanger	R-101/102 Reactor	CM-101 Compressor	C-101/102 Cooler	FL-101/102 Flash Drum
AB-101 Absorber	DC-101 Distillation Column	CD-101/102 Condenser	CDC-101 Cryogenic Distillation Column	RC-101/102 Receiver	RF-101/102 Reflux Drum

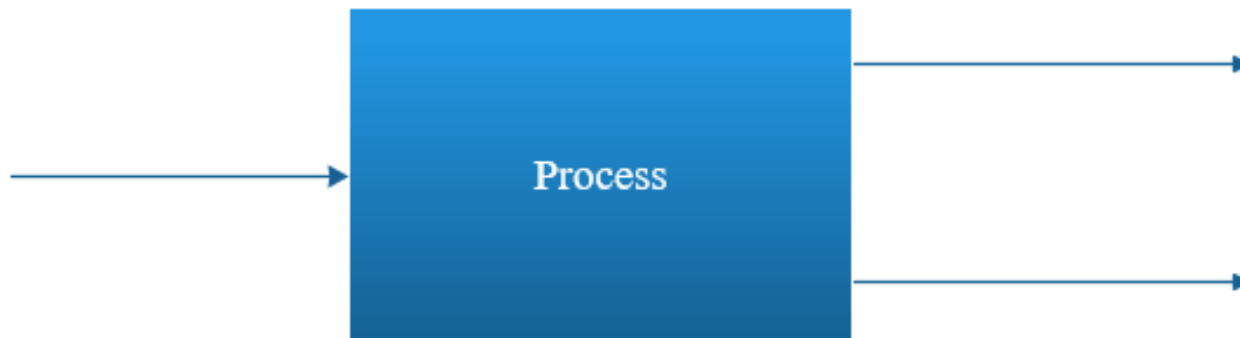
Overall Material Balance

Overall Material Balance (Highly Endothermic Reaction)



Feed

$F_A = 77,525 \text{ lbs/hr}$
 $X_A = 1.00$
 $T_i = 77^\circ\text{F}$
 $P = 14.7 \text{ psia}$



Desired Product

$F_B = 45,662 \text{ lbs/hr}$
 $X_B = .98$
 $T_{FB} = -200^\circ\text{F}$
 $P_B = 15 \text{ psia}$

By-Products

$F_C = 12,745 \text{ lbs/hr}$
 $F_D = 19,117 \text{ lbs/hr}$
 $X_C = .40$
 $X_D = .60$
 $T_{FC} = -149.62^\circ\text{F}$
 $T_{FD} = -149.62^\circ\text{F}$
 $P_C = 14.7 \text{ psia}$
 $P_D = 14.7 \text{ psia}$

Overall Material Balance Basis

Overall Material Balance Basis

The following material balance was based off of literature received on the largest Ethylene plants in production.

We expect to produce .2MT (400,000 lbs./yr.) per annum according to the following calculations.

After establishing our plant capacity, we performed the following dimensional analysis to get our product stream:

$$F_{BF} = 400,000 \frac{\text{lbs.}}{\text{yr.}} * \left(\frac{1 \text{ yr.}}{365 \text{ days}} \right) * \left(\frac{1 \text{ day}}{24 \text{ hours}} \right) = 45,662.10 \frac{\text{lbs.}}{\text{hr.}} \cong 46,000 \frac{\text{lbs.}}{\text{hr.}}$$

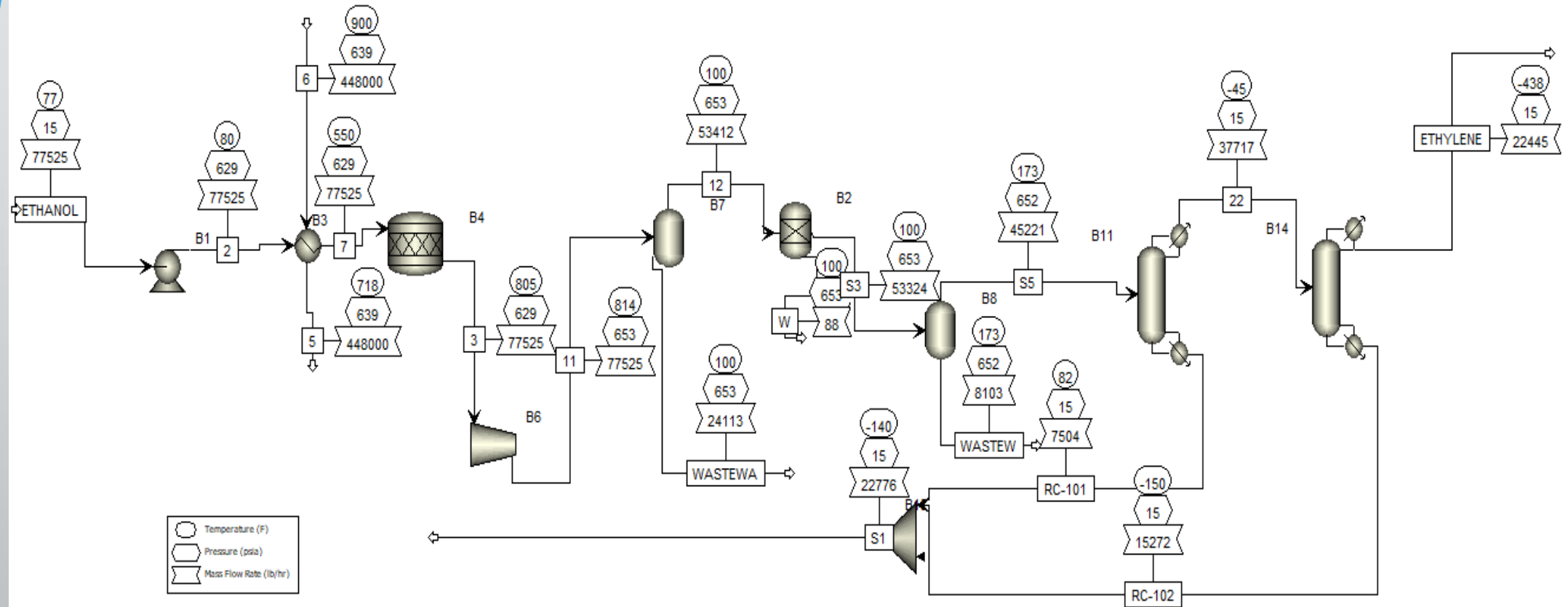
Now we can use the following algorithm to calculate the amount of Ethanol being consumed during the process:

$$\left(\frac{1 \text{ mol } C_2H_5OH}{1 \text{ mol } C_2H_4} \right) * \left(\frac{1 \text{ mol } C_2H_4}{.062 \frac{\text{lb.}}{\text{mol}} C_2H_4} \right) * \left(45,662.1 \frac{\text{lbs.}}{\text{hr.}} \right) * \left(\frac{.1 \frac{\text{lb.}}{\text{mol}} C_2H_5OH}{1 \text{ mol } C_2H_4} \right) = 73,648.55 \frac{\text{lb.}}{\text{hr.}} C_2H_5OH$$

With the conversion rate we received through literature review, we can now calculate the initial flow rate of Ethanol into our system.

$$F_{Ai} = \frac{\text{EtOH consumption}}{\text{EtOH conversion}} = \frac{73,648.55 \frac{\text{lbs.}}{\text{hr.}}}{.95} \cong 77,525 \frac{\text{lbs.}}{\text{hr.}}$$

ASPEN Plus Simulation

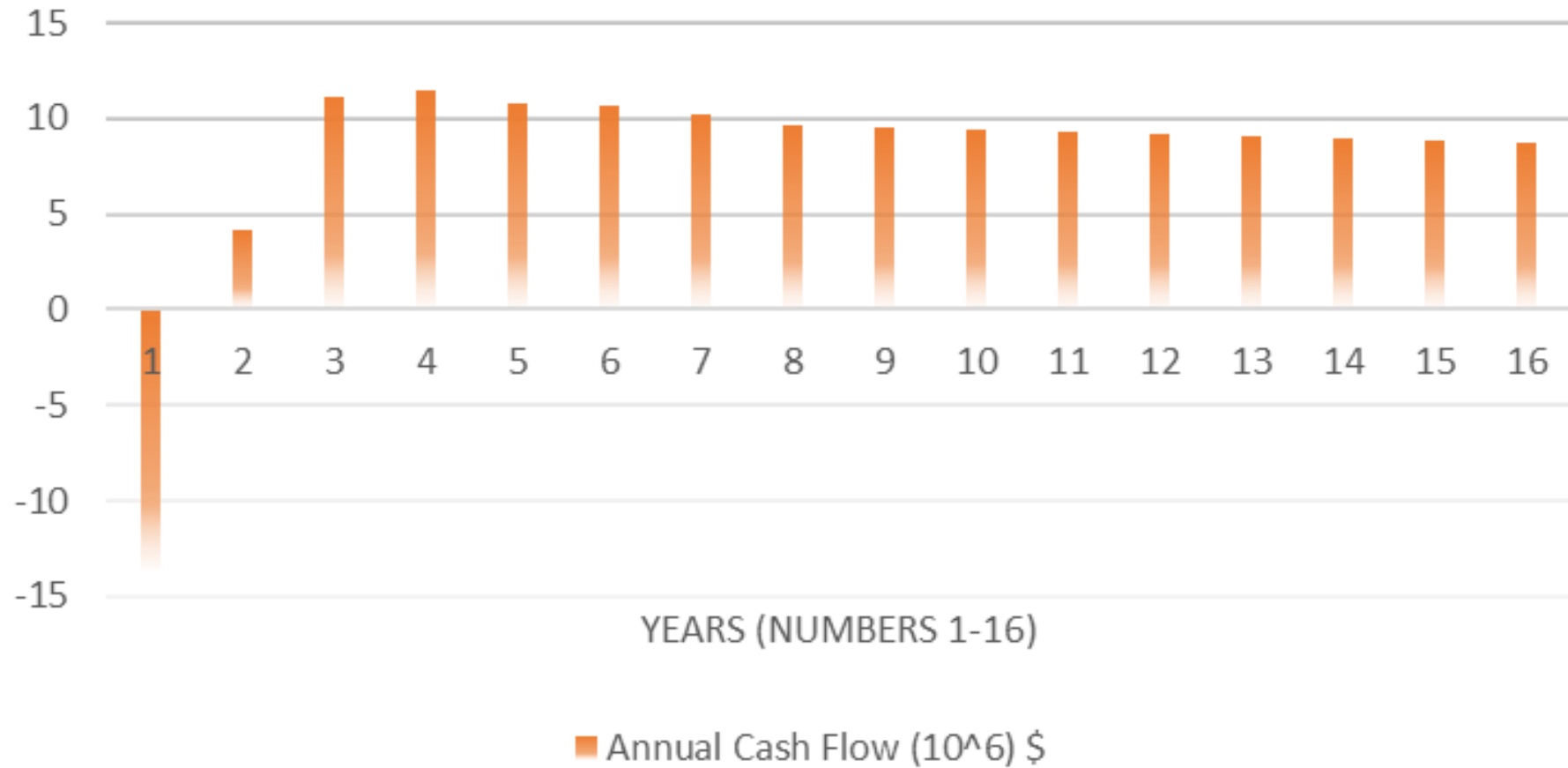


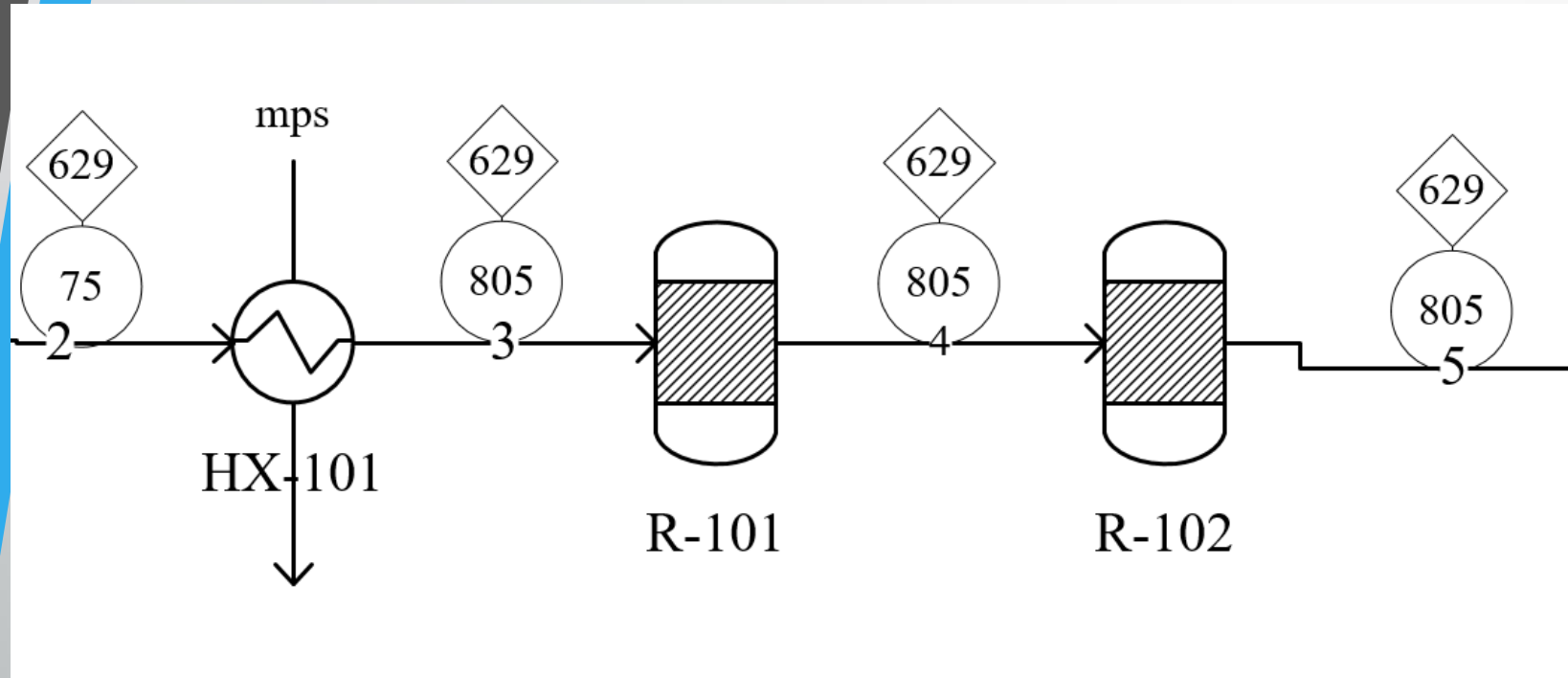
Summary of Economics

Summary of Economics			
Total Capital Investment (TCI)	Invested Capital	Total Operating Assets- Total Operating Liabilities + Total Non-Current Assets	31.89 million
Net Present Value (NPV)	Difference between the current or expected future cash flows at different time.	$NPV = \frac{R_t}{(1+i)^t}$	22.23million
Return on Investment	View of profitability of the plant after tax earnings the third year of operation if they remain unchanged during the project.	$ROI = \frac{(S - C)(1 - t)}{C_{TCI}}$	32.6% per year
Discounted Rate of Return on Investment (DR	Time required for annual earnings to equal the original Investment.	$PBP = \frac{C_{TDC}}{(1 - t)(S - C) + D}$	14.1% per year
Net Return (IRR)	Internal rate of return after fees and carried interest are factored in.	$NPV = \sum_{n=0}^N \frac{C_n}{(1 - r)^n}$	4.2 million
Pay Back Period	Amount of time for the investment to recover our initial pay out in terms of profits and savings.	Initial investment/ Cash Flow per year	2.1 years

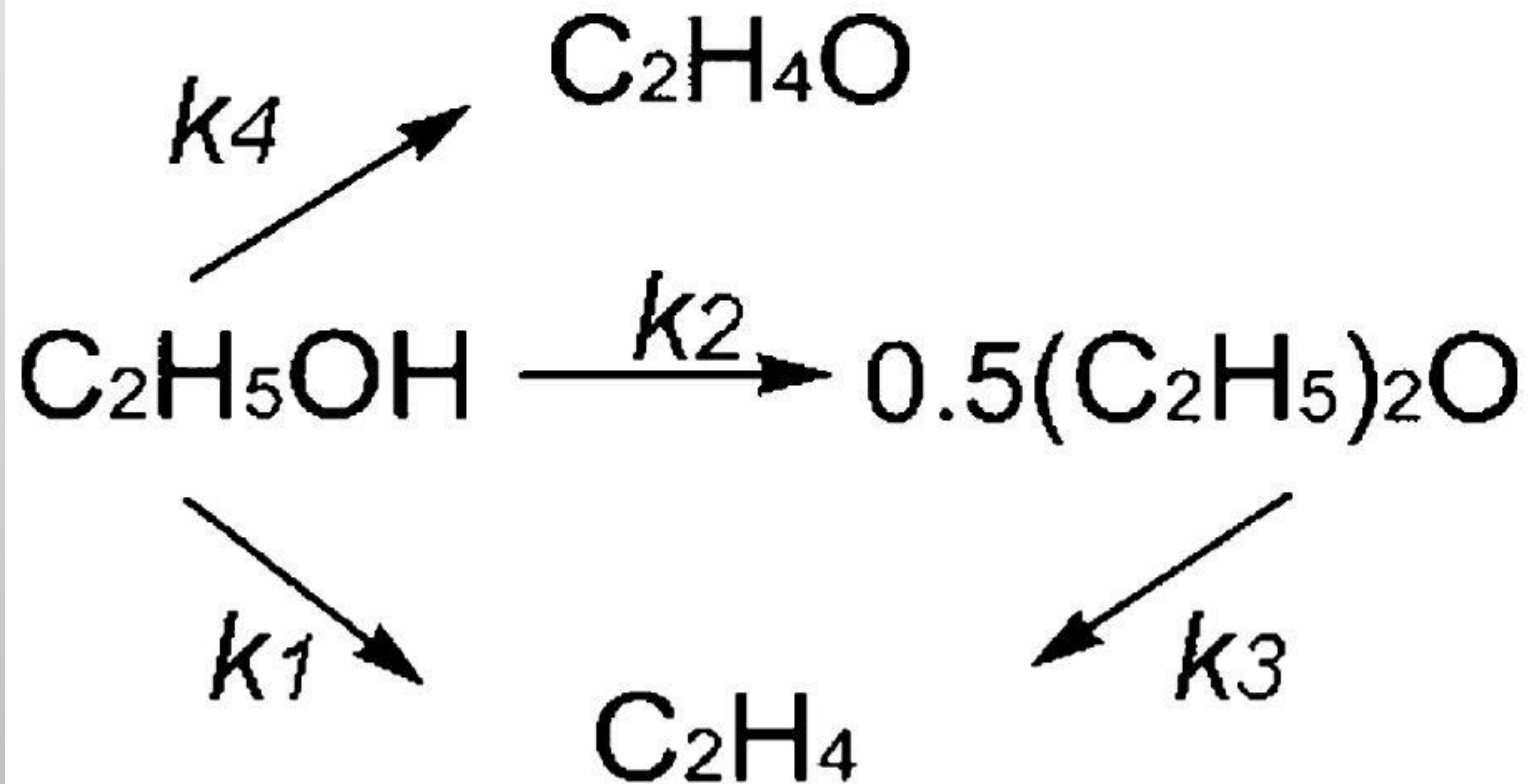
Figure 1: Considered within a 15-year span.

CASH FLOW DIAGRAM





Reactor Section



Reaction Network

Packed Bed Reactor Material and Energy Balance

1) Mole Balance

$$\frac{dF_A}{dW} = r'_A \quad \frac{dF_B}{dW} = r'_B \quad \frac{dF_C}{dW} = r'_C$$

$$\frac{dF_D}{dW} = r'_D \quad \frac{dF_E}{dW} = r'_E \quad \frac{dF_F}{dW} = r'_F$$

2) Rate Law

Rates of Formation

$$\sum r_A = r_{1A} + r_{2A} + r_{4A}$$

$$\sum r_B = r_{1B} + r_{3B}$$

$$\sum r_C = r_{1C} + r_{2C} + r_{3C}$$

$$\sum r_D = r_{2D} + r_{3D}$$

$$\sum r_E = r_{4E}$$

$$\sum r_F = r_{4F}$$

Relative Rates

$$1) \frac{r_A}{-1} = \frac{r_B}{1} = \frac{r_C}{1}; -r_A = r_B = r_C$$

$$2) \frac{r_A}{-2} = \frac{r_D}{1} = \frac{r_C}{1}; -2r_A = r_{2D} = r_{2C}$$

$$3) \frac{r_{3D}}{-1} = \frac{r_{3B}}{2} = \frac{r_{3C}}{1}; -r_{3D} = r_{3B} = r_{3C}$$

$$4) \frac{r_{4A}}{-1} = \frac{r_{4E}}{1} = \frac{r_{4F}}{1}; -r_{4A} = r_{4E} = r_{4F}$$

Net Rate Laws (Rates of Formation)

$$r_A = r_{1A} + r_{2A} + r_{4A} = [k_1 C_A + k_2 C_A^2 + k_4 C_A]$$

$$r_B = r_{1B} + r_{3B} = [k_1 C_A + k_3 C_D]$$

$$r_C = r_{1C} + r_{2C} + r_{3C} = [k_1 C_A + k_2 C_A^2 + k_3 C_D]$$

$$r_D = r_{2D} + r_{3D} = [k_2 C_A^2 + k_3 C_D]$$

$$r_E = r_{4E} = [k_4 C_A]$$

$$r_F = r_{4F} = [k_4 C_A]$$

recall from kinetics textbook

$$k_j = A_j \exp\left(\frac{-E_{a,j}}{RT}\right); k = \text{rate constants}$$

$$k_1 = A_1 \exp\left(\frac{-E_{a1}}{RT}\right) = (5.41 \times 10^6) \exp\left(\frac{-(147.7 \times 10^3 \text{ J/mol})}{(8.314 \text{ J/mol}\cdot\text{K})(702.92 \text{ K})}\right) = 5.716 \times 10^{-5}$$

$$k_2 = A_2 \exp\left(\frac{-E_{a2}}{RT}\right) = (9.55 \times 10^7) \exp\left(\frac{-(101.0 \times 10^3 \text{ J/mol})}{(8.314 \text{ J/mol}\cdot\text{K})(702.92 \text{ K})}\right) = 2.980$$

$$k_3 = A_3 \exp\left(\frac{-E_{a3}}{RT}\right) = (2.79 \times 10^{10}) \exp\left(\frac{-(135 \times 10^3 \text{ J/mol})}{(8.314 \text{ J/mol}\cdot\text{K})(702.92 \text{ K})}\right) = 2.589$$

$$k_4 = A_4 \exp\left(\frac{-E_{a4}}{RT}\right) = (2.78 \times 10^8) \exp\left(\frac{-(138.4 \times 10^3 \text{ J/mol})}{(8.314 \text{ J/mol}\cdot\text{K})(702.92 \text{ K})}\right) = 1.442 \times 10^{-2}$$

3) Stoichiometry

Recall from kinetics

$$C_j = C_{T0} \frac{F_i}{F_T} \frac{T_0}{T} \frac{P}{P_0}$$

$$C_A = C_{T0} \frac{F_A}{F_T} \frac{T_0}{T} \frac{P}{P_0}$$

$$C_D = C_{T0} \frac{F_D}{F_T} \frac{T_0}{T} \frac{P}{P_0}$$

4) Combine

$$\frac{dF_A}{dW} = r'_A = -\left[k_1 k_4 \left(C_{T0} \frac{F_A}{F_T} \frac{T_0}{T} \frac{P}{P_0}\right) + k_2 \left(C_{T0} \frac{F_A}{F_T} \frac{T_0}{T} \frac{P}{P_0}\right)^2\right]$$

$$\frac{dF_B}{dW} = r'_B = -\left[k_2 \left(C_{T0} \frac{F_A}{F_T} \frac{T_0}{T} \frac{P}{P_0}\right)^2 + k_3 \left(C_{T0} \frac{F_D}{F_T} \frac{T_0}{T} \frac{P}{P_0}\right)\right]$$

5) Energy Balance

$$\frac{dT}{dW} = \frac{r'_A H_{rx}(T) - \frac{U_a}{P_0} (T - T_a)}{\sum F_i C_{p,i}}$$

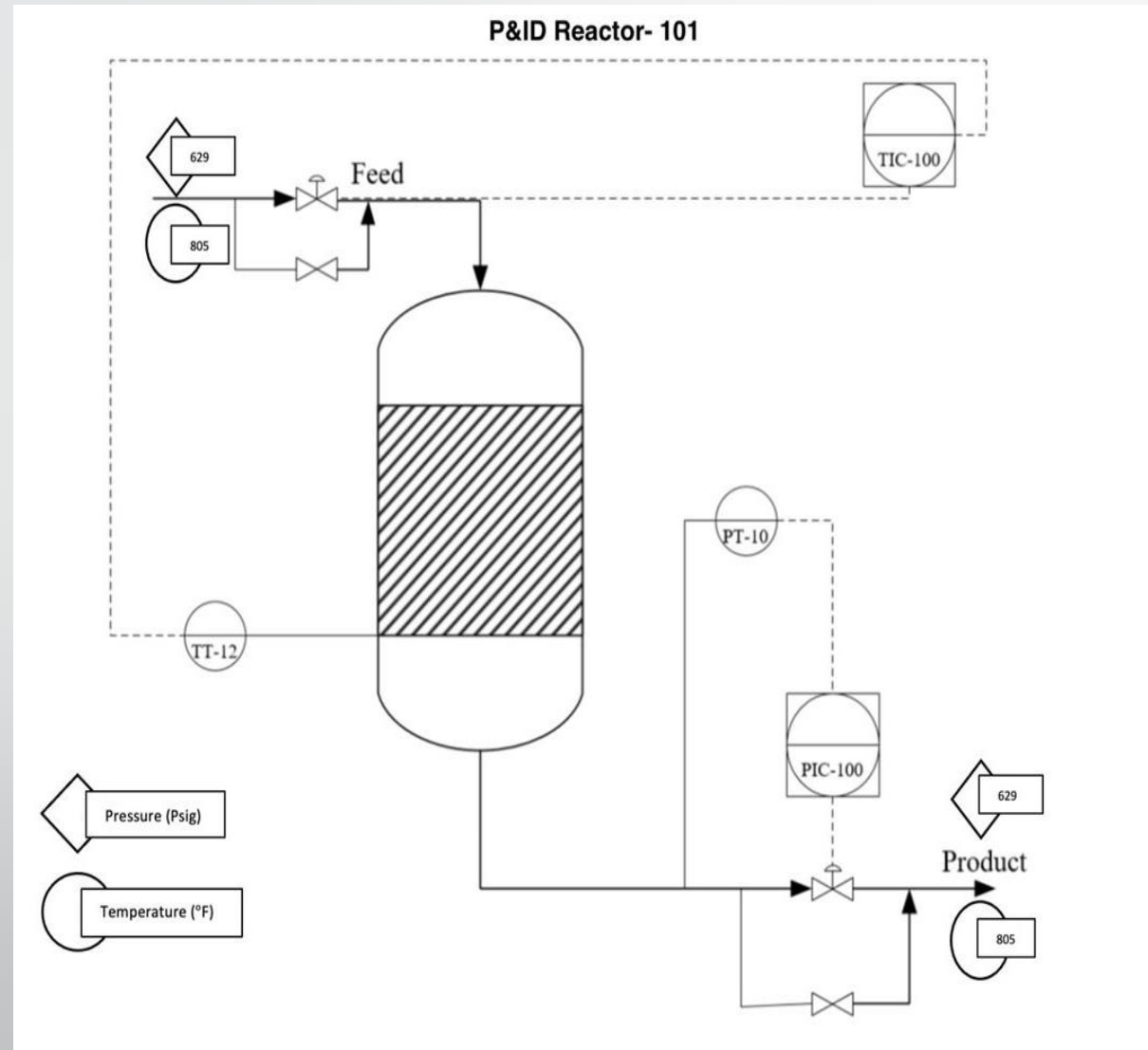
$$r'_A = -\left[k_1 k_4 \left(C_{T0} \frac{F_A}{F_T} \frac{T_0}{T} \frac{P}{P_0}\right) + k_2 \left(C_{T0} \frac{F_A}{F_T} \frac{T_0}{T} \frac{P}{P_0}\right)^2\right]$$

$$H_{rx}(T) = -119.346 \text{ Btu/lb}\cdot\text{mol}$$

$$U_a = (3.3288 \times 10^4 \text{ Btu/lb}\cdot\text{K})(22237.8 \text{ ft}^2)$$

$$P_0 = 34 \text{ lbs/ft}^2$$

P&ID



Specification sheet

Ethanol and Water Reactor				
Identification:	Item:	Packed Bed Reactor (PBR) Alumina Catalyst		
	Item No:	R-101	Date	04/12/2022
	No. Required	1	By:	Group # 3
	C _{TPI} (\$)			\$89,500
Function:	To convert the reaction into the product			
Operation:	Continuous Batch Reactor (Agitated)			
	In	Out		
Materials Handled				
Mass Flow (lb/hr)	77525	77525		
Component Flow (Lb/Hr):				
Water	0	23646.6		
Ethylene	0	33990.4		
Ethanol	77525	3876.25		
Dimethyl-ether	0	7484.03		
Acetaldehyde	0	8154.29		
Hydrogen	0	373.156		
Temperature (F)	550	805		
Pressure (psig):	629	629		
Design Data:				
Material	Stainless Steel			
Volume	2072.14 ft ³			
Partial Size	(.01-.02) inches			
Catalyst Weight	9252.8 lbs			
Catalyst Bed Volume (gallons)	2035.75			

Hazard and Operability Analysis (HAZOP)

No.	Parameter	Guideword	Deviation	What if?	Possible Causes	Consequences	Safeguards	Action
1	Flow	None	No flow to R-101	There is no flow of ethanol into the reactor	- Feed line valve is closed. - Blockage in the feed line.	-No reactant enters the reactor	- Alarm/monitoring system at the feed line valve.	- Opening the feed line valve. - The installation of a bypass system in case of blockages.
2	Temperature	More	Increase in feed Temperature	There is a sudden increase in temperature at the feed of R-101	-Incorrectly calibrated temperature gauge.	-Thermal runaway and risk of explosion. -Ineffectiveness of the catalyst	-Temperature alarm at feed entry point. -Recalibration of temperature gauge.	-Installation of a temp gauge. - Checking maintenance schedule and procedures.
3	Pressure	More	Pressure build-up in the feed line	There is pressure build up in the feed line leading into the reactor	-Clogging/Blockage in the line. - Failed reaction in the reactor.	-Failure of feed line tube -Risk of expansion and bursting of the reactor.	-Installation of quick-pressure relief valves at strategic locations before and after the reactor	- Installation of a secondary pressure relief device. - Checking maintenance schedule and procedures
1	Pressure	Less	Pressure decreases in the reactor	There are sudden pressure losses in the reactor	- Leakages within the in the feed line. -Influx of flow rate in the product lines.	- Less reactant is converted to product. - inefficiencies within the reactor.	Pressure monitoring devices before and after the reactor	- Installation of pressure gauge. -Checking and following maintenance schedule and procedures
2	Temperature	More	Temperature increases	-There is a sudden increase in temperature within the reactor	-Failure of reactor cooling devices.	-Deactivation of the Alumina catalyst. - Incomplete conversion of reactant to product	-Installation of a cooling jacket or other cooling techniques	Installation of a temp gauge -Checking and following maintenance schedule and procedures
1	Flow	Reverse	Back flow to R-101	There is a backflow of the product stream back to the reactor	- Pressure loss in the product line.- Clogging and blockage down the product line	-Mixing of reactant and product in the reactor. -Inefficiencies within the reactor	- Check valve to prevent back flow	-Monitoring pressure in the product line. -Following the stipulated maintenance schedule and procedures
2	Temperature	More	Increase in product line temperature	There is sudden increase in temperature within product line transporting ethylene	- Incorrectly calibrated temperature gauge within the line. - Product buildup downstream	-Risk of thermal runaway. -Failure of product line including expansion and bursting.	-Recalibration of temperature gauge within the line. -Flow regulation throughout the product line	-Installation of a temp gauge - checking and following maintenance schedule and procedures
3	Pressure	More	Pressure increases in the product line	There is pressure build up in the product line transporting ethylene from the reactor	-Blockage further up the product line. -Incomplete reaction in the reactor.	- Failure of the product line tube. -Risk of expansion, bursting and/or damage to the product stream	-Installation of quick pressure relief valves at strategic locations within the product line	-Installation of a secondary pressure relief device. -Checking and following maintenance schedule and procedures

Process Safety

Ethanol

- Keep away from heat, sparks, open flames, hot surfaces
- Store in a well-ventilated place, Keep cool
- Keep container tightly closed, Protect from sunlight.
- Storage Temperature 59 – 77 °F
- Conventional carbon steel storage tanks

Ethylene

- Keep away from heat, hot surfaces, sparks, open flames and other ignition sources
- Keep container tightly closed. Protect from sunlight.
- Storage temperatures near 32°F
- Cryogenic tanks are commonly employed

Conclusion

- Using proper tools, and our knowledge of **engineering** we were able to identify a base design for our Production plant. With the consideration of our location, cost of raw materials, etc. Our Annual cost of our Chemical Plant were determined to be profitable

Acknowledgements

- Dr. Emmanuel Dada
- Dr. Lealon Martin
- Special Thanks to our Panel of Attendees



QUESTIONS ?



Backup slides

Material Streams

Stream Name	Units	2	3	5	6	7	11	12	22	ETHANOL	ETHYLENE	RC-101	RC-102	S1	S3	S5	W	WASTEW	WASTEW
Description																			
From		B1	B4	B3		B3	B6	B7	B11		B14	B11	B14	B15	B2	B8	B2	B8	B7
To		B3	B6		B3	B4	B7	B2	B14	B1		B15	B15		B8	B11			
Stream Class		CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN
Phase		Liquid Phase	Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase	Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase			Vapor Phase	Liquid Phase	Liquid Phase	Liquid Phase
Temperature	F	79.7481	805	718	900	549.843	813.868	100	-45.3753	77	-438.339	81.7953	-149.62	-140.117	100	172.833	100	172.833	100
Pressure	psia	628.696	628.696	639	639	628.696	653	653	14.7	14.7	14.7	14.7	14.7	14.7	653	652	653	652	653
Volume Flow	cuft/hr	1558.63	64780.2	454626	542414	23128.6	62807.2	9615.29	434608	1555.19	550.953	159.769	368.37	31366.9	9540.32	13320.3	1.44277	214.94	395.279
Vapor Phase																			
Enthalpy Flow	Btu/hr		-1.05E+08	-2.47E+09	-2.42E+09	-1.57E+08	-1.05E+08	2.04E+06	2.21E+07					2.80E+06	1.84E+07	1.35E+07			
Mass Flows	lb/hr		77525	448000	448000	77525	77525	53412.4	37717					3826.14	31553.7	45221.1			
C2H5OH	lb/hr		3876.25	0	0	77525	3876.25	3474.89	8.47E-06					0.000377443	171.498	1393.3			
C2H4	lb/hr		33990.4	0	0	0	33990.4	33988	32666.9					3823.37	27721.2	32666.9			
H2O	lb/hr		23646.6	0	0	0	23646.6	88.4068	0					0	0	0			
C2H4O	lb/hr		8154.59	0	0	0	8154.59	8003.94	4522.36					2.46992	2068.16	5920.66			
DIETH-01	lb/hr		7484.03	0	0	0	7484.03	7484.03	155.832					0.301071	1224.17	4868.37			
STEAM	lb/hr		0	448000	448000	0	0	0	0					0	0	0			
H2	lb/hr		373.156	0	0	0	373.156	373.149	371.903					0	368.613	371.903			
Mass Fractions																			
C2H5OH			0.05	0	0	1	0.05	0.0650577	2.25E-10					9.86E-08	0.00543513	0.0308108			
C2H4			0.438444	0	0	0	0.438444	0.636331	0.866106					0.999276	0.878542	0.722381			
H2O			0.305019	0	0	0	0.305019	0.00165517	0					0	0	0			
C2H4O			0.105187	0	0	0	0.105187	0.149852	0.119902					0.000645538	0.0655443	0.130927			
DIETH-01			0.096537	0	0	0	0.096537	0.140118	0.00413162					7.87E-05	0.0387965	0.107657			
STEAM			0	1	1	0	0	0	0					0	0	0			
H2			0.00481336	0	0	0	0.00481336	0.00698619	0.00986035					0	0.0116821	0.0082241			

Material Streams																			
Stream Name	Units	2	3	5	6	7	11	12	22	ETHANOL	ETHYLENE	RC-101	RC-102	S1	S3	S5	W	WASTEW	WASTEW
Description																			
From		B1	B4	B3		B3	B6	B7	B11		B14	B11	B14	B15	B2	B8	B2	B8	B7
To		B3	B6		B3	B4	B7	B2	B14	B1		B15	B15		B8	B11			
Stream Class		CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN
Phase		Liquid Phase	Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase	Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase			Vapor Phase	Liquid Phase	Liquid Phase	Liquid Phase
Temperature	F	79.7481	805	718	900	549.843	813.868	100	-45.3753	77	-438.339	81.7953	-149.62	-140.117	100	172.833	100	172.833	100
Pressure	psia	628.696	628.696	639	639	628.696	653	653	14.7	14.7	14.7	14.7	14.7	14.7	653	652	653	652	653
Volume Flow	cuft/hr	1558.63	64780.2	454626	542414	23128.6	62807.2	9615.29	434608	1555.19	550.953	159.769	368.37	31366.9	9540.32	13320.3	1.44277	214.94	395.279
Liquid Phase																			
Enthalpy Flow	Btu/hr	-2.01E+08								-2.01E+08	7.49E+06	-1.22E+07	1.51E+06	-1.35E+07	-1.86E+07		-604715	-9.78E+06	-1.62E+08
Mass Flows	lb/hr	77525								77525	22445	7504.11	15272	18949.9	21770.3		88.4068	8102.87	24112.6
C2H5OH	lb/hr	77525								77525	3.65E-24	1393.3	8.47E-06	1393.3	3303.39		0	2081.59	401.363
C2H4	lb/hr	0								0	22073.1	4.19E-10	10593.8	6770.39	6266.72		0	1321.08	2.42031
H2O	lb/hr	0								0	0	0	0	0	0		88.4068	0	23558.2
C2H4O	lb/hr	0								0	2.93E-06	1398.29	4522.37	5918.19	5935.78		0	2083.29	150.651
DIETH-01	lb/hr	0								0	1.16E-11	4712.52	155.832	4868.05	6259.86		0	2615.67	0.0011675
STEAM	lb/hr	0								0	0	0	0	0	0		0	0	0
H2	lb/hr	0								0	371.903	4.54E-25	2.01E-22	0	4.53614		0	1.24621	0.0066246
Mass Fractions																			
C2H5OH		1								1	1.63E-28	0.185671	5.55E-10	0.0735251	0.151738		0	0.256895	0.0166454
C2H4		0								0	0.983431	5.59E-14	0.693674	0.357278	0.287857		0	0.163039	0.0001003
H2O		0								0	0	0	0	0	0		1	0	0.977006
C2H4O		0								0	1.31E-10	0.186337	0.296122	0.312307	0.272655		0	0.257105	0.0062478
DIETH-01		0								0	5.19E-16	0.627992	0.0102038	0.25689	0.287541		0	0.322807	4.84E-08
STEAM		0								0	0	0	0	0	0		0	0	0
H2		0								0	0.0165695	6.05E-29	1.32E-26	0	0.000208364		0	0.000153799	2.75E-07

Economics Considerations

Raw Materials				
Name of Material	Price, \$/kg	Annual Amount, million kg/y	Annual raw materials cost, million \$/y	
Ethanol	0.27	3.240	0.87	
			0.00	
			0.00	
			0.00	
			0.00	
Total annual cost of raw materials =			0.87	\$

Direct Costs					
Purchased equipment, E'					3.500
Delivery, fraction of E'	0.00	0.00	0.10	0.10	0.350
Subtotal: delivered equipment					3.850
Purchased equipment installation	0.45	0.39	0.47	0.47	1.810
Instrumentation&Controls(installed)	0.18	0.26	0.36	0.36	1.386
Piping (installed)	0.16	0.31	0.68	0.68	2.618
Electrical systems (installed)	0.10	0.10	0.11	0.11	0.424
Buildings (including services)	0.25	0.29	0.18	0.18	0.693
Yard improvements	0.15	0.12	0.10	0.10	0.385
Service facilities (installed)	0.40	0.55	0.70	0.70	2.695
Total direct costs	1.69	2.02	2.60	2.60	13.860
Indirect Costs					
Engineering and supervision	0.33	0.32	0.33	0.33	1.271
Construction expenses	0.39	0.34	0.41	0.41	1.579
Legal expenses	0.04	0.04	0.04	0.04	0.154
Contractor's fee	0.17	0.19	0.22	0.22	0.847
Contingency	0.35	0.37	0.44	0.44	1.694
Total indirect costs	1.28	1.26	1.44	1.44	5.544

2	Process Identifier: Illustration 101				
3	Required user input		Notes & comments		
4	Default, may be changed				
5	RESULT				
6	Products, Coproducts and Byproducts				
7	Name of	Price,	Annual	Annual	
8	Material	\$/kg	Amount,	value of	
9			million	product,	
10			kg/y	million \$/y	
11	Ethylene	1.12	11.200	12.54	
12	Ethylene Oxide	0.85	10.200	8.67	
13	Diethyl Ether	0.43	5.160	2.22	
14				0.00	
15				0.00	
16				0.00	
17	Total annual value of products =			23.43	Sent to 'Evaluation
18					and 'Year-0 \$'
19					

Process Identifier: Illustration 101			
Required user input		Notes & comments	
Default, may be changed			
RESULT			
Operating Labor			
Number of operators per shift*	Shifts per day**	Operator rate, \$/h #	Annual operating labor cost, million \$/y
3	3	40	1.051
Sent to 'Annual TP			

*See Tables 6-13 and Fig. 6-9.

**Default = 3 for continuous process.

Enter appropriate value for batch operation.

#To obtain current, local value, enter (latest local ENR skilled labor index)/6067 = 1

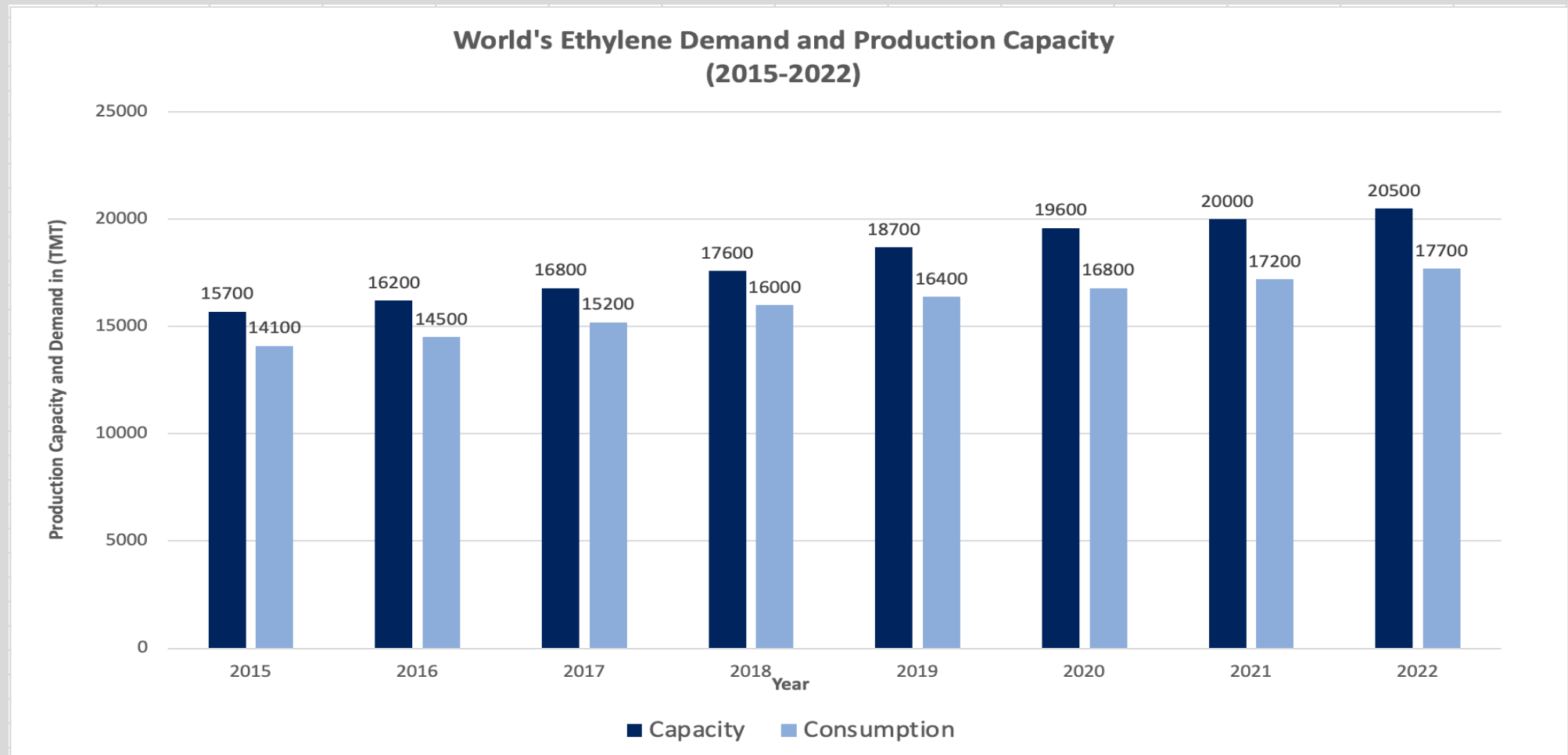
Theoretical Market Analysis

Gross Profit= 24.36 cents/ pound

$$19.3(1) + .642(0.0015) - 26.62(1.64) = 24.35$$

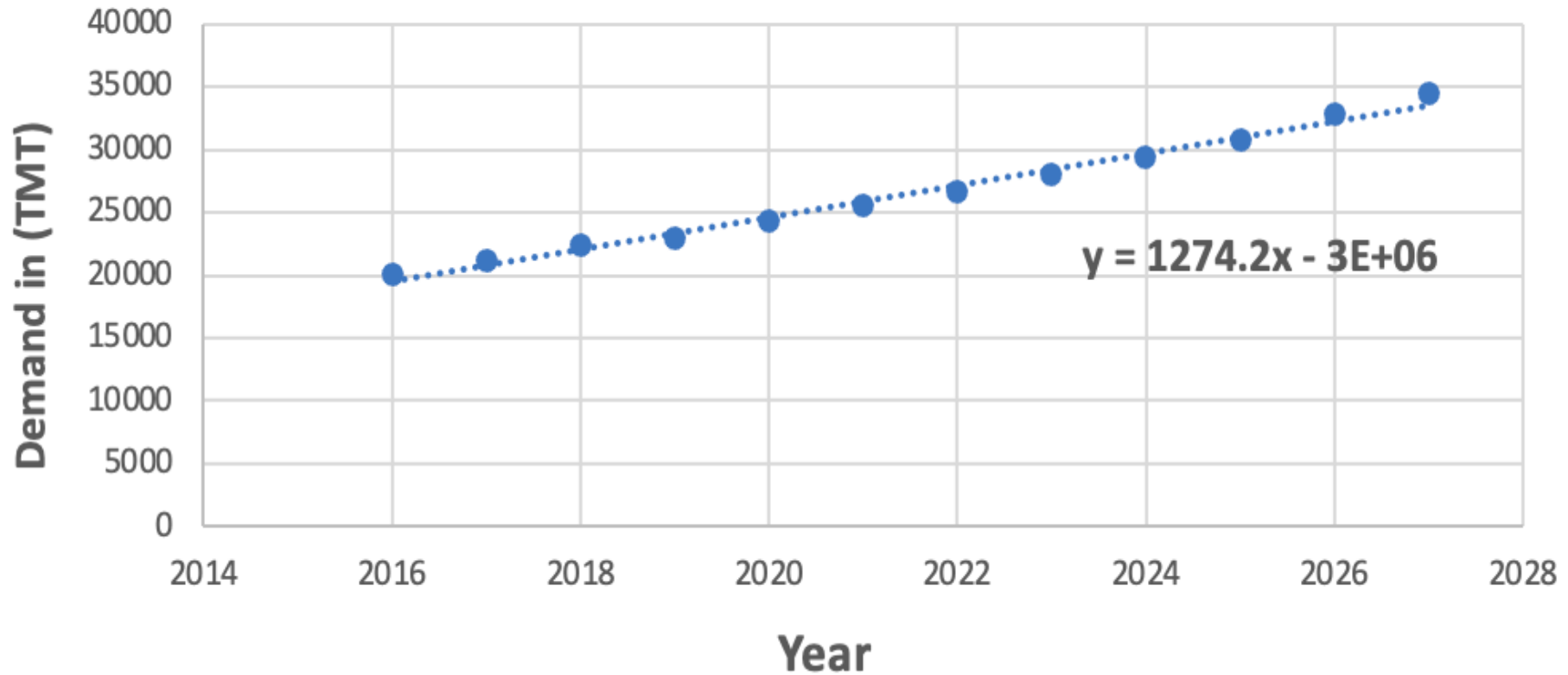
$\text{C}_2\text{H}_5\text{OH} \longrightarrow \text{C}_2\text{H}_4 + \text{H}_2\text{O}$			
Pound-mole	1	1	1
Molecular Weight	0.1016 lb-mol	0.0612 lb-mol	0.0397 lb-mol
Pound / Pound of ethylene	1.64	1	.642
Cents per Pound	26.62	19.3	0.0015

Supply and Demand



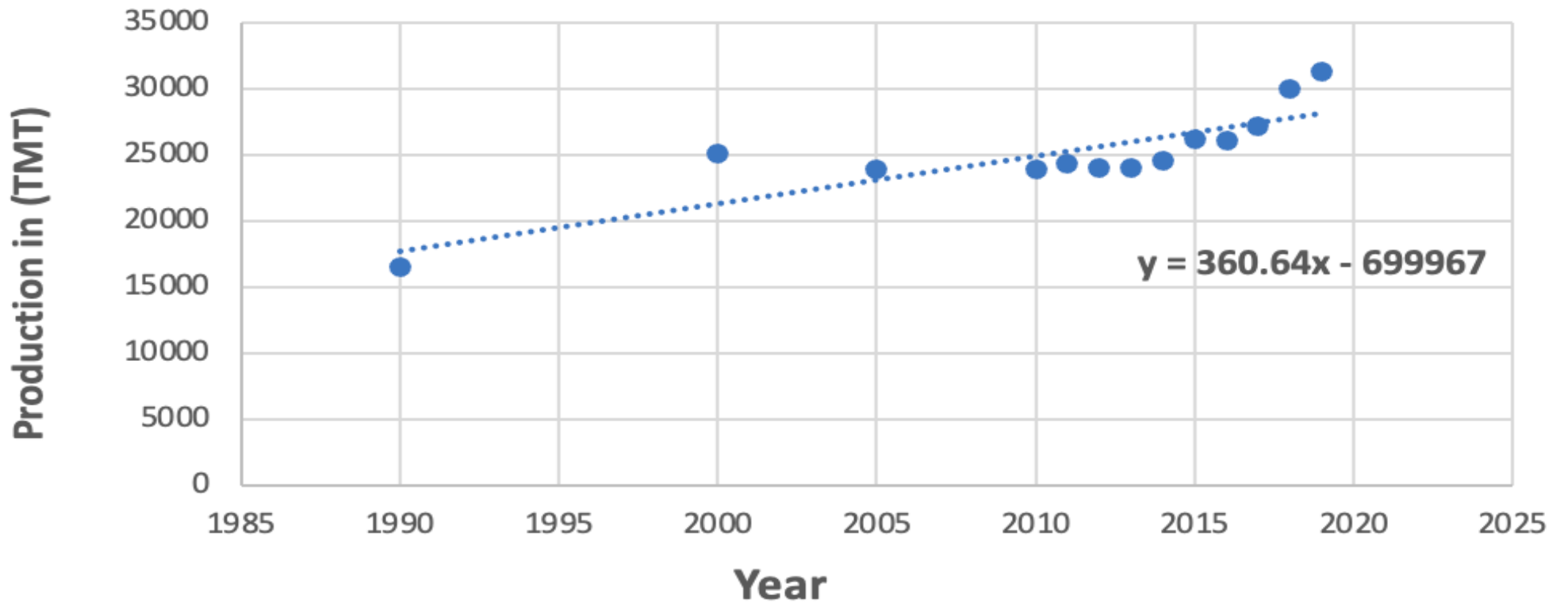
Market Demand

U.S. Ethylene Market Demand (2016-2027)



Ethylene Production

U.S. Ethylene Production (1990-2019)



Driving this Process Reactor Calculations

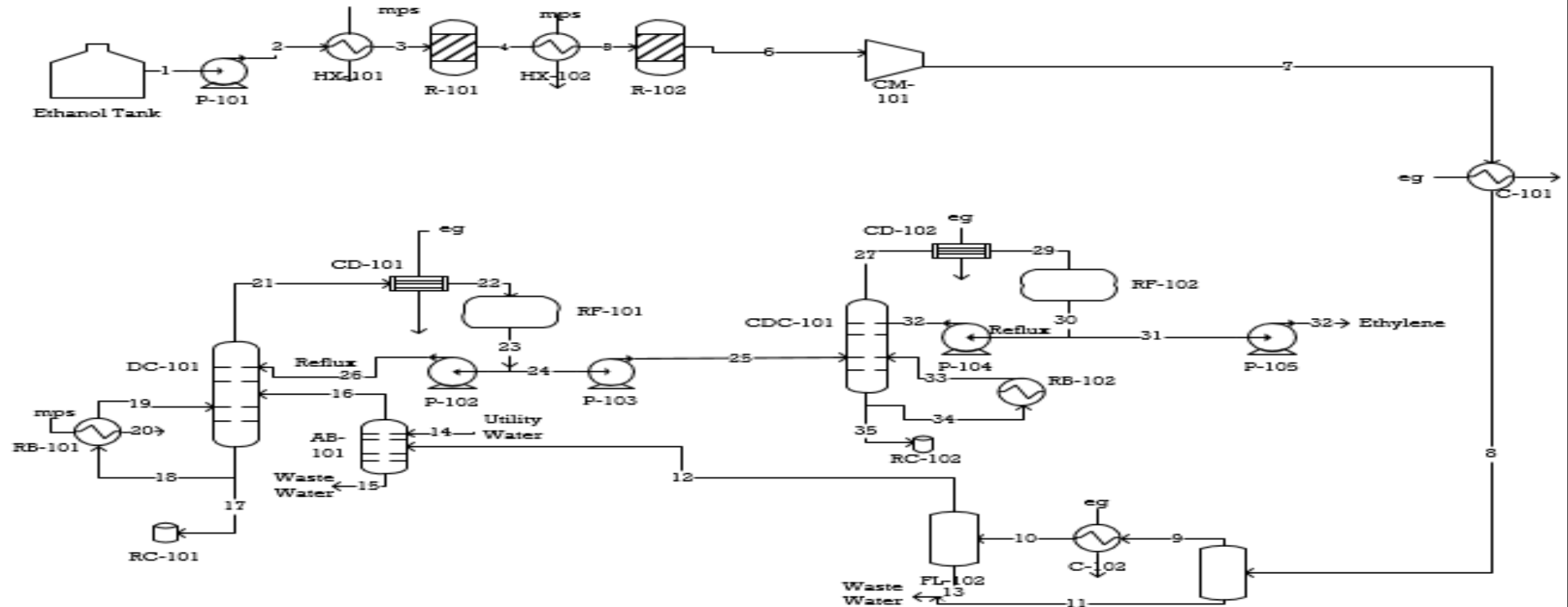
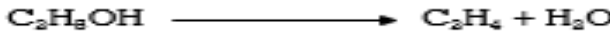
Pump		
	Equation	Value
k	$k = \frac{C_p}{C_v}$	1.101
a	$a = \frac{k-1}{k}$	0.092
p	$P = \frac{mzRT_1 \left[\left(\frac{P_2}{P_q} \right)^a - 1 \right]}{a}$	64 kw
v	The volumetric flow rate is determined from Aspen.	77 %
Exit T	$T_2 = T_1 \left(\frac{P_2}{P_q} \right)^a$	298 °F

Process Hazards

Process Equipment	Hazard	Mitigation
Storage tank of ethanol	Leakage of ethanol , is highly flammable.	- Storage tank should be tightly enclosed. - There should be display of MSDS of ethanol near the storage tank
Reactors R-101, R-102	- Hot spots may occur - Ethylene is flammable if heated for prolonged time.	- Rigorous temperature control can avoid hot spots. - Quenching can also be employed. - Product should be drawn continuously from the reactor and should be cooled down.
Flash drum, FL-101, FL-102	- They are dealing with flammable component (ethylene) - Equipment would burst out if vacuum created.	Vapor flow rate can be manipulated to avoid vacuum.
Absorber, AB-101	There would be ethanol and water present in process stream after coming out of absorber which may impact downstream equipment.	- Absorbent with high affinity towards ethanol and water should be used. - High pressure and low temperature should be kept to make absorption effective.

Process Flow Diagram (Fall Design)

Catalytic Dehydration of Ethanol to Ethylene



P-101/102/103/104/105 Pump	HX-101/102 Heat Exchanger	R-101/102 Reactor	CM-101 Compressor	C-101/102 Cooler	FL-101/102 Flash Drum	AB-101 Absorber
DC-101 Distillation Column	RB-101/102 Reboiler	CD-101 Condenser	CDC-101 Cryogenic Distillation Column	RC-101/102 Receiver	RF-101/102 Reflux Drum	

Pump

Pump Type

The type of the pump used is centrifugal pump.

Power Estimation

The constant volume and constant pressure specific heat values are obtained from ASPEN. The value of k is;

$$k = \frac{C_p}{C_v} = 1.101$$

Thus, value of “a” is as follows;

$$a = \frac{k - 1}{k} = \frac{1.101 - 1}{1.101} = 0.092$$

Thus, reversible adiabatic power is;

$$P = \frac{mzRT_1 \left[\left(\frac{P_2}{P_q} \right)^a - 1 \right]}{a} = \frac{\left[\frac{4754}{3600} \right] 0.004331 (8.314) 298 \left[\left(\frac{629}{14.7} \right)^{0.092} - 1 \right]}{0.092}$$
$$P = 64 \text{ kW}$$

Pump Efficiency

The volumetric flow rate determined from HYSYS is as follows;

$$V = 252.7 \frac{\text{m}^3}{\text{h}} = \frac{252.7 \text{ m}^3}{3600 \text{ s}} = 0.07 \frac{\text{m}^3}{\text{s}}$$

For this volumetric flow rate, pump efficiency is 77%.

Exit Temperature

The exit temperature of the pump is determined from adiabatic compression, therefore,

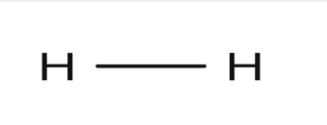
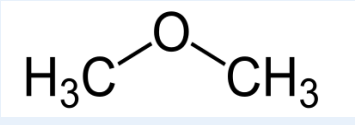
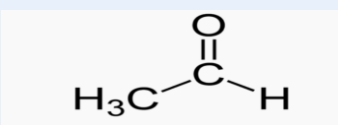
$$T_2 = T_1 \left(\frac{P_2}{P_q} \right)^a = 298 \left(\frac{629}{14.7} \right)^{0.092} = 421 \text{ K}$$

Covert to K

$$(421 \text{ K} - 273.15) * \frac{9}{5} + 32 = 298.13^\circ\text{F}$$

Side Reactions Chemical Conditions

Temperatures	Hydrogen	Dimethyl-ether	Acetaldehyde
Boiling Point	-423.2 °F	-11 °F	69.36 °F
Flash Point	None	105.98 °F	-36 °F
Melting point	-434.5 °F	221.8°F	-190 °F
Autoignition Point	995 °F	662°F	348.8 °F (30–60% of acetaldehyde) 302°F(mixtures with oxygen contained 60–80°
Freezing Point	-435 F		-190 °F
Storage	(5,000–10,000 psi)	None (Store in cool, dry area)	35.6- 46.4 °F

	Hydrogen	Dimethyl-ether	Acetaldehyde
Molecular Formula	H ₂	CH ₃ OCH ₃	C ₂ H ₄ O
Structure Formula			

Reactor Volume Calculations

$$1) V_{PBR} = \frac{W_c}{\rho_b}$$

$W_c = 4197 \text{ kg / literature)} \rightarrow 9252.80 \text{ lbs For } 69000 \text{ tons}$

Now to upscale the catalyst weight

$$\text{UPSC}_{\text{factor}} = \frac{400,000,000 \text{ lb/yr}}{120,000,000 \text{ lb/yr}} = 3.3\bar{3}$$

$$W_c (\text{catalyst weight}) = 9252.8 \text{ lbs} \cdot 3.3\bar{3} = 30,811.82 \text{ lbs}$$

Now to use W_c to get V_{PBR}

$$V_{PBR} = \frac{W_c}{\rho_b} = \frac{30,811.82}{34 \text{ lbs/ft}^3} = 906.23 \text{ ft}^3 = 6709 \text{ gal}$$

