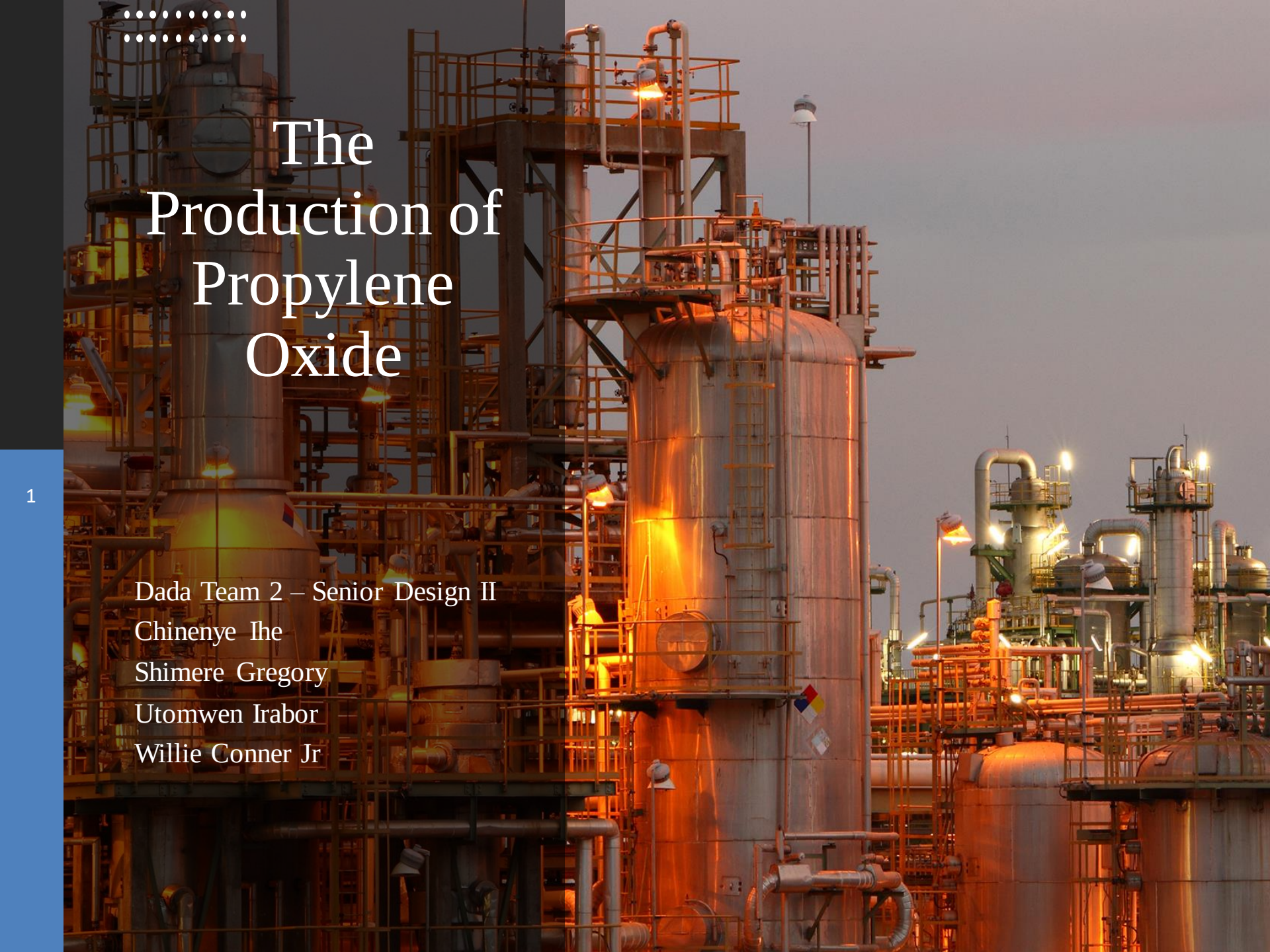


A photograph of a large industrial chemical plant at night. The scene is dominated by tall, cylindrical storage tanks and a complex network of pipes, walkways, and scaffolding. Several bright lights are visible, illuminating parts of the structure and creating a warm, orange glow. The sky is dark, suggesting dusk or dawn. The overall impression is one of a busy, large-scale industrial facility.

The Production of Propylene Oxide

Dada Team 2 – Senior Design II
Chinenye Ihe
Shimere Gregory
Utomwen Irabor
Willie Conner Jr

OUTLINE

- Introduction
- Gantt chart
- Design Basis
- Location
- Process Flow Diagram (PFD)
- Material and Energy Balance
- Aspen Simulation
- Shell & Tube Heat Exchanger
- Distillation Column Design
- Flash Drum
- Cash Flow Diagram
- Summary of Economics
- Piping and Instrumental Diagram
- Hazard Analysis of unit Equipment
- Recommendation & Future Work

GANTT CHART

TASK	Assigned Team Member	PROGRESS	START	END	DAYS
HYSYS/ASPEN Simulation of Process					
Reiterate Previous Semester's Project Presentation Comments as a Team with Dr. Dada	Everyone	99%	1/18/22	1/28/22	11
Work on Converging ASPEN HYSYS Simulation from Last Semester	David Irabor	70%	1/28/22	2/14/22	18
Make Corrections to the Material Balance	David Irabor	50%	2/14/22	2/18/22	5
Chemical Engineering Design					
<i>Design of Major Equipment</i>					
The Shell and Tube Reactor	Shimere Gregory	10%	2/19/22	2/25/22	7
Distillation Columns and Flash Drums	Willie Connor	2%	2/25/22	3/2/22	6
Pumps and Heat Exchangers	David Irabor	4%	3/2/22	3/6/22	5
Economic Evaluation					
External constraints and Internal constraints	Willie Connor	1%	3/10/22	3/12/22	3
Research Details of raw materials that are available to be transported to our company's location	Shimere Gregory	2%	3/13/22	3/15/22	3
Generate a Cash flow Diagram	Chinenye Ihe	4%	3/16/22	3/18/22	3
Rate of Return Calculations and Payback Time	David Irabor	5%	3/19/22	3/23/22	5
Investment Incentives and Corporate Taxes	Willie Connor	6%	3/16/22	3/20/22	5
TASK	Assigned Team Member	PROGRESS	START	END	DAYS
Safety and HAZOP Analysis					
Potential Hazards in Business Operation	David Irabor	3%	3/21/22	3/23/22	3
Past incidents that had likelihood for catastrophic consequences	Chinenye Ihe	5%	3/24/22	3/26/22	3
Human-controlled factors	Shimere Gregory	4%	3/27/22	3/29/22	3
Consequences of failure of applied control measures	Willie Connor	1%	3/30/22	4/1/22	3
Risk Communication	David Irabor	30%	4/2/22	4/4/22	3

DESIGN BASIS

Plant Capacity	220 Million lb/yr
Operating Days	330 days/yr
Operating Time	7920 hr/yr
Production Rate of Product	30,000 lb/hr
Raw Materials	Propene (gas) Hydrogen Peroxide (Liquid)
Catalyst	Titanium Silicalite (TS-1)
Plant Location	Channelview, TX
Ambient Conditions at Channelview, TX	Max Temp: 82°F Min Temp: 72°F Relative Humidity: 75%



LOCATION & CLIENTS

- Channel view, Texas

Why ?

- Access to Feed stock
- Raw Material
- Water Source

Clients

- Textile Rubber & chemical
- Sigma-Aldrich
- Dow Chemical company

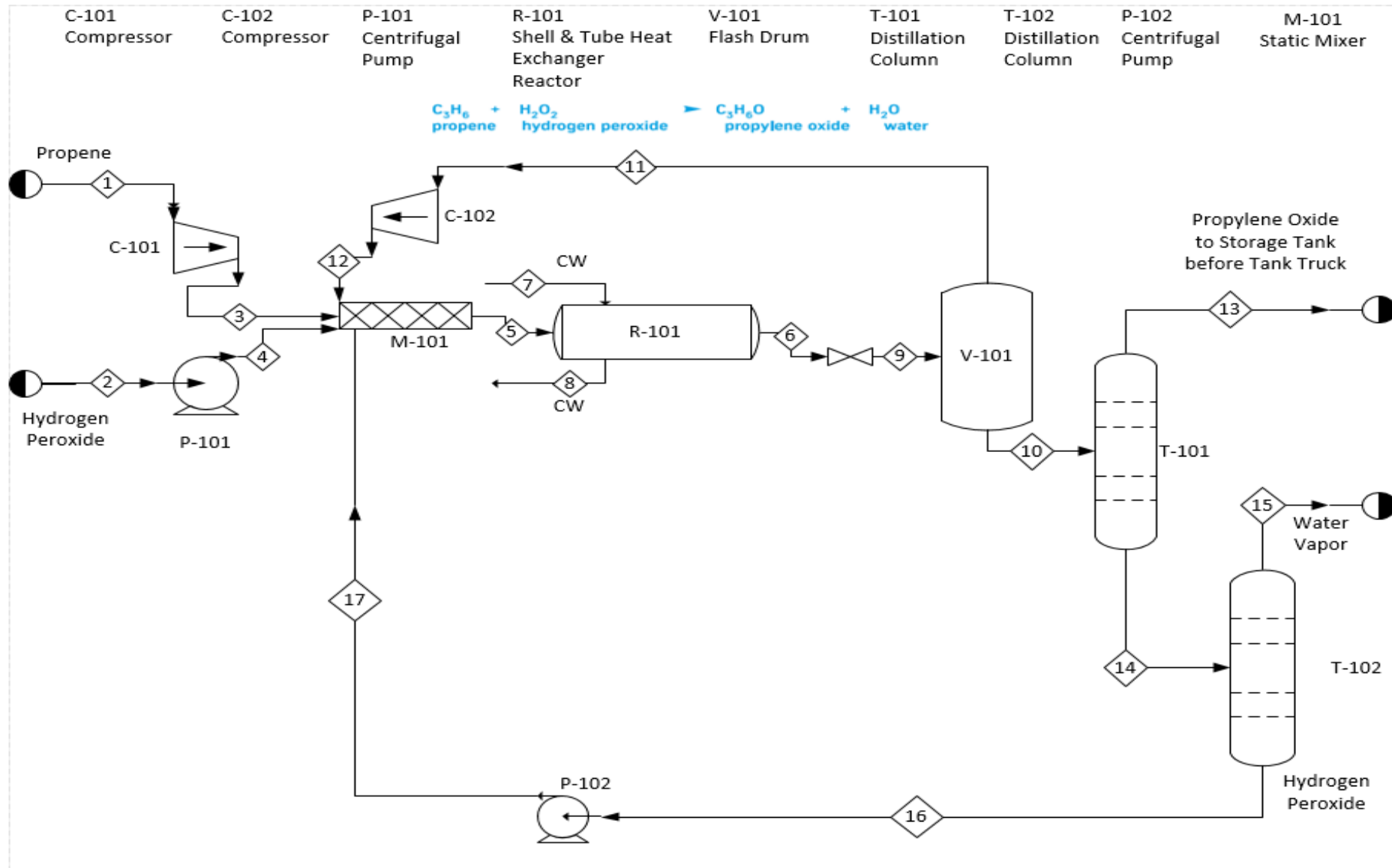


SIGMA-ALDRICH

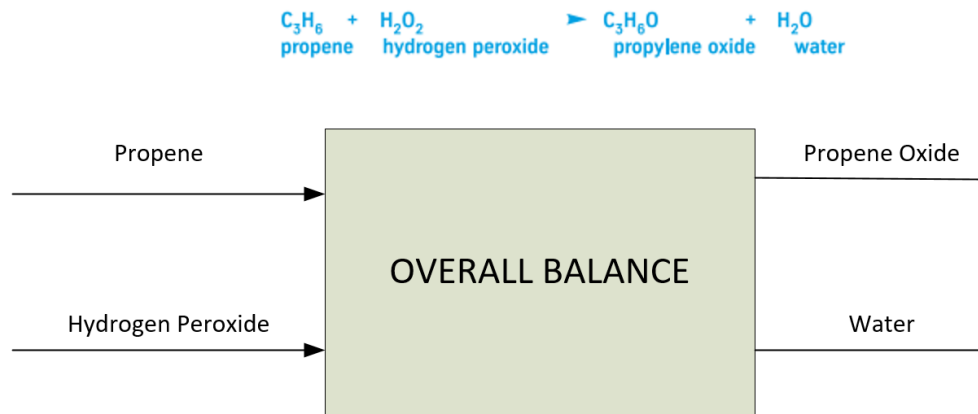


**PRAIRIE VIEW
A&M UNIVERSITY**

PROCESS FLOW DIAGRAM



MATERIAL BALANCE



The Capacity of Our Propylene Oxide Plant
 220,462,262 lbs/yr

If the plant operates at 330 days/year

$$220,462,262 \frac{\text{lbs}}{\text{yr}} \times \frac{1 \text{ yr}}{330 \text{ days}} \times \frac{1 \text{ day}}{24 \text{ hrs}}$$

thus, $m_3 = 27,836.14 \text{ lb/hr}$

The plant can produce 27,836.14 lb/hr of $\text{C}_3\text{H}_6\text{O}$



PRAIRIE VIEW
A&M UNIVERSITY

ENERGY BALANCE

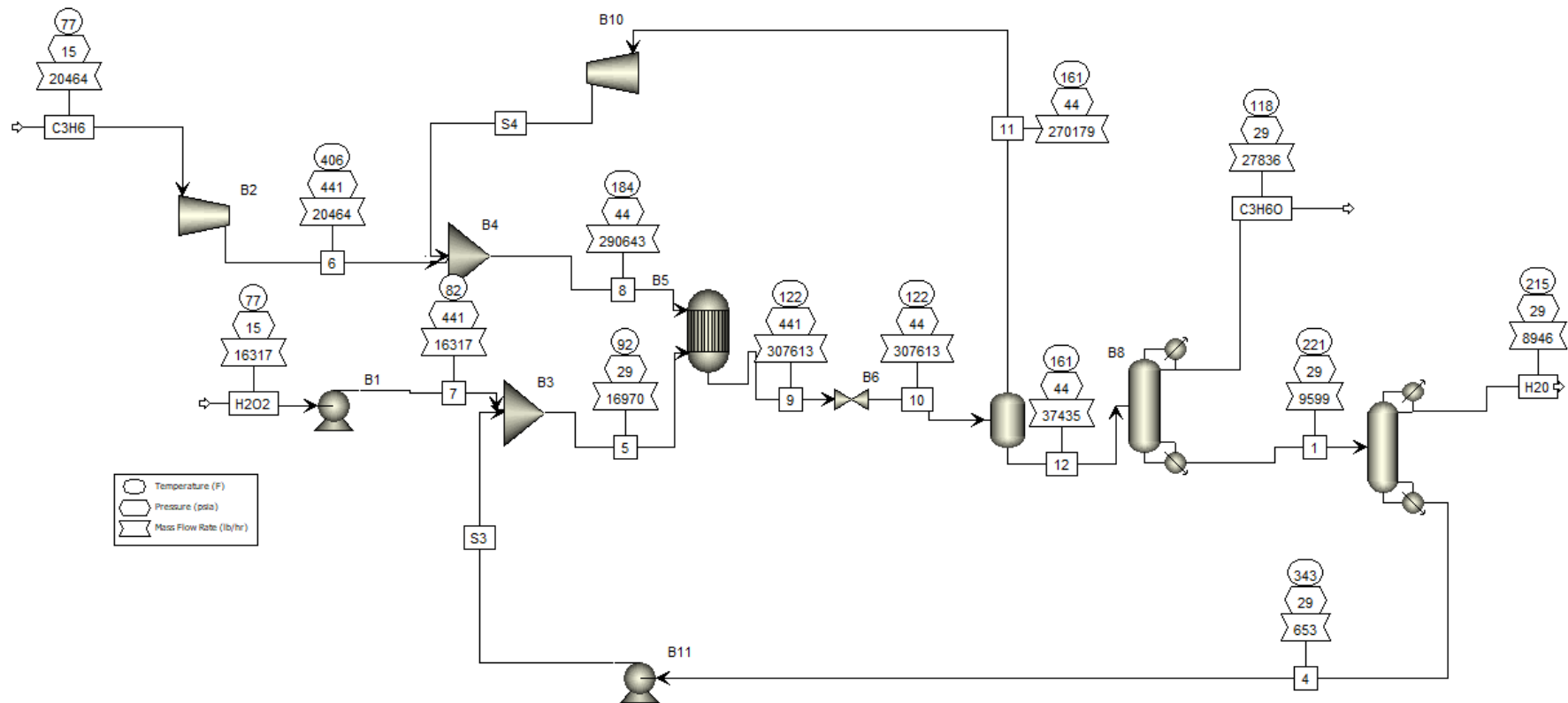


Figure 1: ASPEN Simulation of the Production of Propylene Oxide



UNIT DESIGN



REACTOR DESIGN

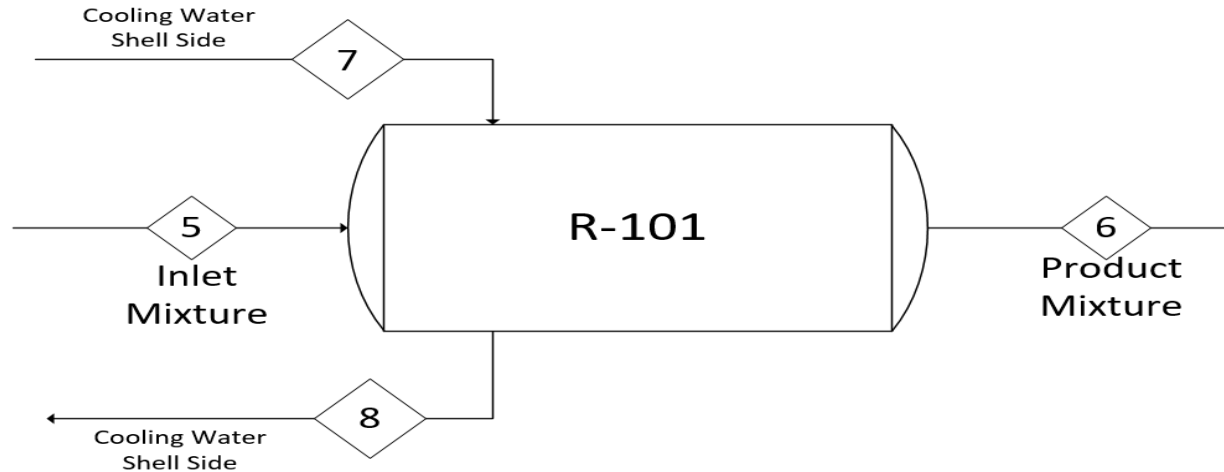


Figure 2: Showing PFD of the Shell and Tube Reactor showing Counterflow

Parameter	Design Equation	Terms
Heat Transfer	$Q = m C_p \Delta T$	m = mass ΔT = temperature change C_p = specific heat
Weight of Catalyst	$w = \frac{V_o}{k C_{Ao}} \int_0^{0.96} \frac{(1+x)^2}{(1-x)^2}$	V_o = Vol. flowrate k = rate constants C_{Ao} = inlet conc.
Number of Tubes	$N_T = \frac{A_{overall}}{\pi \times OD \times L}$	$A_{overall}$ = Overall Heat Transfer OD = Tube Outer Diameter L = Tube Length
Log Mean Temperature	$Q = u A \Delta T_{LM}$	u = Heat Transfer Coefficient ΔT_{LM} = Log Mean Temp. A = Area
Heat Transfer Coefficient	$190 \frac{BTU}{hr ft^2 F}$	Shell and Tube Side Constants for Light Hydrocarbons

R-101 SPECIFICATION SHEET

The Shell and Tube Heat Exchanger Reactor			
Identification: R-101	Product:	Propylene Oxide	
	Item No:	101	
	Reactor Type:	Packed Bed Conversion Reactor	
Function: To Convert 96% Hydrogen Peroxide to produce Propylene oxide, Propylene, Water			
Operation: Continuous			
Design Data			
Tube Diameter (inches)	2		
Tube Length (ft)	12		
Material of Construction	Stainless Steel	Medium	Cooling Water
		Mass of Water (Shell)	202,146 lbs.
Number of Tubes based on Heat Transfer	109 tubes	Shell Side Temperature inlet and Outlet	Inlet: 77°F Outlet: 122°F
		Q (Heat Transfer) (BTU/hr)	4.9×10^6
Heat Transfer Surface Area (ft²)	820		
Max. Operating Temp. (°F)	122		
Flowrate Rate (lb/hr)	307,613		

DRUM DESIGN

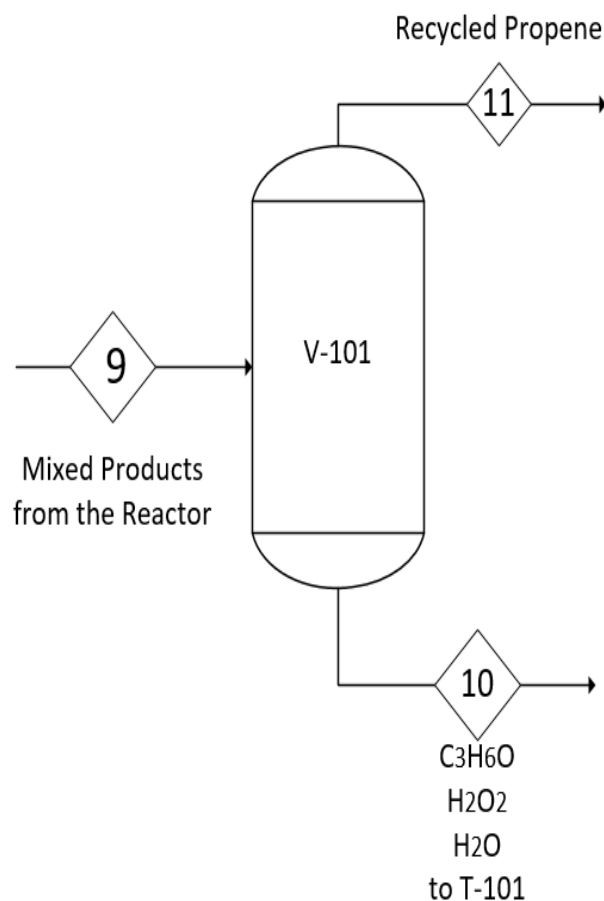


Figure 4: Flash Drum Design

Molecular weight of Liquid	$MW_L = X_{H2O2} MW_{H2O2} + X_{C3H6O} MW_{C3H6O} + X_{H2O} MW_{H2O}$
Molecular weight of Vapor	$MW_V = X_{C3H6}$
Density of Liquid	$\rho_L = \frac{MW_L}{V_L}$
Density of Vapor	$\rho_V = \frac{P_{atm} MW_V}{R T}$
Flow Parameter	$FL_V = \frac{W_L}{W_V} \sqrt{\frac{\rho_V}{\rho_L}}$
Permissible Vapor Velocity	$U_{perm} = K_{drum} \sqrt{\frac{\rho_L - \rho_V}{\rho_V}}$
Area of the Vessel	$A_C = \frac{V MW_V}{(U_{perm})(3600) \rho_V}$
Diameter	$D = \sqrt{\frac{4 A_C}{\pi}}$
Total Height	$H_{Total} = 3D$
Maximum Volume	$V = \frac{\pi \times D^2 \times H}{4}$

MW_L	MW_V	ρ_L	ρ_V	FL_V	U_{perm}	A_C	D	H_{Total}	V
48.628 lb/mol	42.08 lb/mol	52.30 lb/ft ³	0.1086 lb/ft ³	0.006	5.6 ft/s	109.8 ft ²	11.8 ft	35.5 ft	3882 ft ³



V-101 SPECIFICATION SHEET

Flash Drum				
Identification	Item:	<i>Vertical Vessel</i>		
	Item No: V-101		Date:	4/21/2022
	No. Required	1	By:	Team 2
Function: Separates vapor- liquid mixture of Propene, Hydrogen Peroxide, Propylene Oxide and Water				
Operation: Isobaric				
	Feed Stream(lb/hr)	Vapor Stream(lb/hr)	Liquid Stream (lb/hr)	
Material Handled:				
Propene	241685	241658	0	
Hydrogen Peroxide	557	0	662	
Propylene Oxide	27844	0	27844	
Water	8353	0	8276	
Total	278439	241658	36782	
Temperature (F)	122	161	161	
Pressure (psia)	44	44	44	
Design Data:				
Area (ft²)	10			
Height (ft)	35.5			
Diameter (ft)	11.8			
Volume within the vessel (ft³)	121.7			
Maximum Volume (ft³)	3822.24			
Material of Construction	Stainless Steel			
Vapor Velocity (ft/s)	5.63			



ECONOMICS

SUMMARY OF MATERIALS

Continuous Operation:

- 330 days/year
- Operating Factor: 0.9
- Production Capacity: 90% of Design Capacity
- Start Production at 50% of Production Capacity
- Cost of Capital: 15%

Materials	Cost (\$/lb)
Propylene	0.27
Hydrogen Peroxide	0.74
Propylene Oxide	0.85

Equipment Description	Type	Purchase Cost	Bare Module Factor	Bare Module Cost
Name	(must be filled-in!)		(Default 3.21 if blank)	
Shell and Tube Reactors	Process Machinery	\$87,900		\$282,159
Flash drum	Process Machinery	\$122,000		\$391,620
DistillationC1	Process Machinery	\$38,900		\$124,869
Storage Tank	Storage	\$175,000		\$561,750
10% Utilities Factor	-	-		\$1,682,874
Total				3,043,272



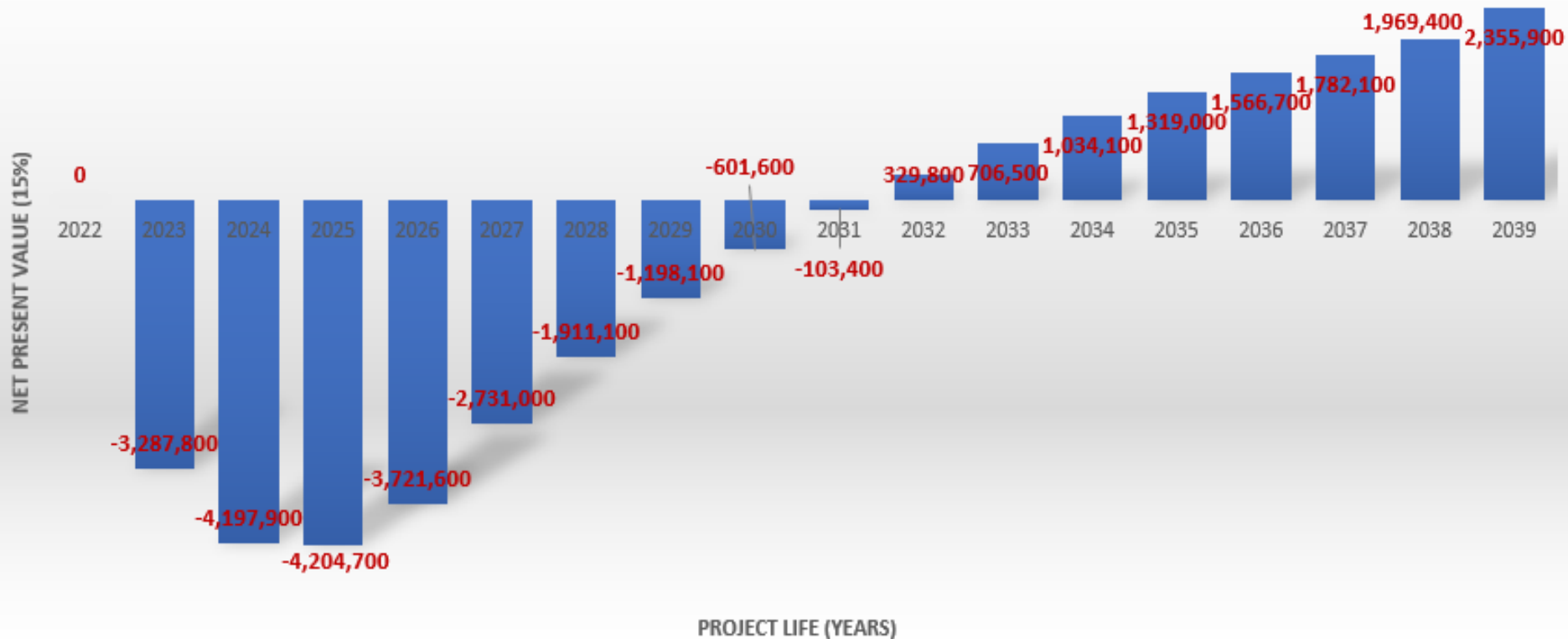
SUMMARY OF ECONOMICS

Parameters	Values	Units	Parameters	Equations	Terms
Total Capital Investment (TCL)	5,430,837	\$	Total Capital Investment (TCL)	$C_{TCL} = C_{TDC} + C_{start} + C_{WC}$	C_{TCL} = Total Capital Investment C_{TDC} = Total depreciable capital investment C_{start} = Start-up capital C_{WC} = Working Capital
Total Annual Value of Products	76,605,754	\$	Return on Investment	$\frac{(S - C)x(1 - t)}{C_{TCL}}$	S = Total annual sales revenue C = Total annual production cost D = Depreciation
Total Annual Cost of Raw Materials	70,309,061	\$	Payback Period	$\frac{C_{TDC}}{(1 - t)x(S - C) + D}$	
Capital Cost (Capex)	-3,780,939	\$	Net Present Value	$NPV = \frac{R_t}{(1+i)^t}$	R_t = net cash flow at time i = discount rate t = time of the cash flow
Operating Cost (Opex)	1,128,360	\$			
Return on Investment	25.24	%			
Payback Period	3	years			
Internal rate of return (IRR) Or Discounted Cash Flow Rate of Return (DCFRR)	22.26	%			
Net Present Value	2,355,900	\$			



CASH FLOW DIAGRAM

Production of Propylene Oxide



P&ID

HAZOP
Analysis



V-101 HAZOP

Flow				
Process Parameter	Deviations	Possible causes	Possible Consequences	Action required
Flow	Low	Valve fully open	Unreacted Propene won't fully be flashed back to recycle meaning that it won't fully separate.	Always check the condition of valve and test the openings
Flow	High	Valve opening too small	Flow of the product too slow causing impurities	Install pump to move the product flow for purification
Pressure				
Process Parameter	Deviations	Possible causes	Possible Consequences	Action required
Pressure	Low	1. Lower feed drum temperature 2. A possible temperature lower than the operating temperature of the flash drum (T=161F)	1. Higher liquid level 2. Gas products will be less generated	1. Install pressure & temperature controller for the drum.
		2. Leakage in the flash drum	2. Lower Propene vapor recovered at the top of flash drum.	2. Install pressure indicator in flash drum
Pressure	High	1. Higher feed temperature 2. May heat up the liquid component into gas phase	1. Lower liquid level. 2. Less propylene oxide being generated	1. Install pressure & temperature controller for the drum.
		2. Blockage in vapor stream.	2. Risk of drum explosion.	2. Install pressure alarm.
Level				
Process Parameter	Deviations	Possible causes	Possible Consequences	Action required
Level	Low	1. Blockage in inlet stream	1. No separation occurs.	1. Low Level alarm
		2. The inlet stream too hot.	2. No separation occurs. The pump might get damaged due to high temperature	2. Install temperature controller at the feed stream to check the level
		3. Fewer separation occurs		
Level	High	1. Inlet stream too cold.	1. No separation occurs.	1. Install temperature controller at the feed to check the level
		2. Blockage in vapor stream.	2. Risk of drum explosion. Risk of pipeline bursting	2. Install pressure alarm to alert the operator



V-101 P&ID

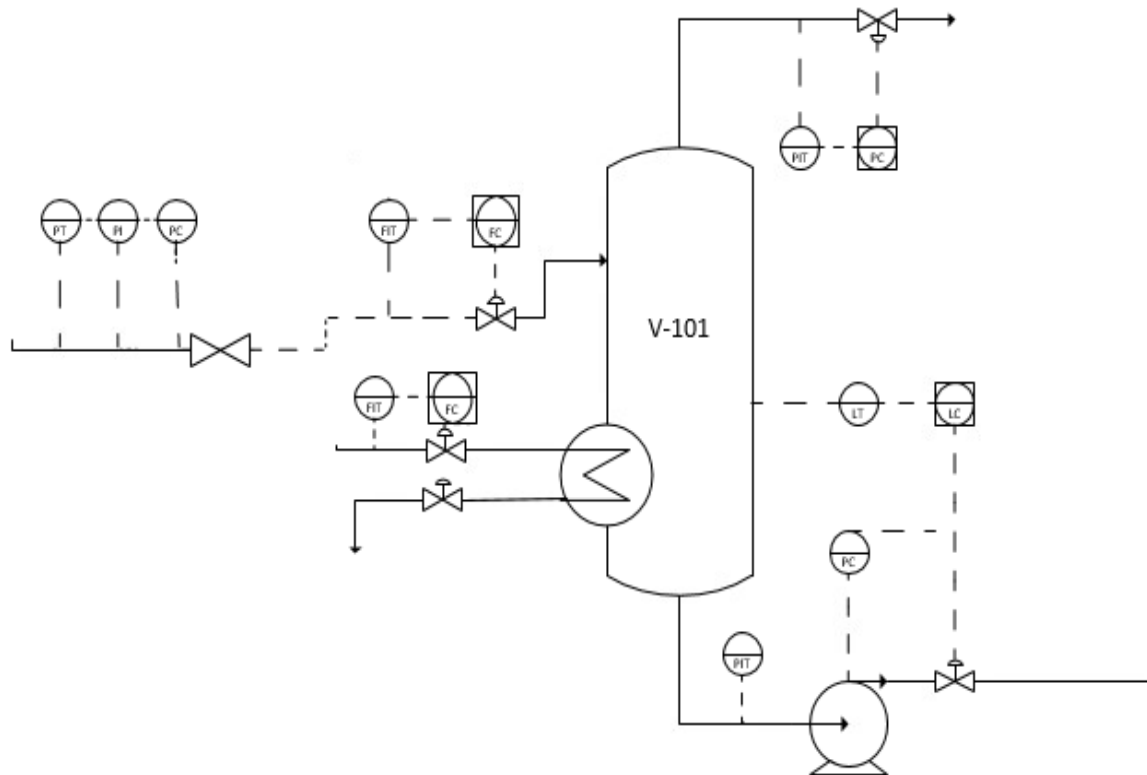


Figure 5: A P&ID Illustration on the Flash Drum (V-101)



CONCLUSION





RECOMMENDATIONS AND FUTURE WORK

REFERENCES

- <https://www.globenewswire.com/en/news-release/2022/03/03/2396000/28124/en/Global-Propylene-Oxide-Market-Report-2022-Increasing-Demand-from-Building-and-Construction-Automotive-Industries-Forecast-to-2026.html>
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