

**SENIOR DESIGN AND PROFESSIONALISM II
SPRING 2020
ORAL PRESENTATION**

TOPICS COVERED IN PROJECT

- 1. Apply a systematic design process, incorporate engineering codes, standards, and realistic constraints that include economic; environmental; sustainability; manufacturability; ethical; health and safety; social; and political considerations in solving the design problem.**
- 2. Work in groups**

The grading rubrics for evaluation of the Senior Design II projects CHEG 4482 (a continuation of the the fall 2019 Senior Design I CHEG 4472) are presented below. The students are to be evaluated as outlined in the rubrics with emphasis on the following:

- Justification of plant location, major raw material sources and capacity
- Provide a process description and Process Flow Diagram (PFD) for the plant showing the major items of equipment, and indicating the materials of construction and the operating temperatures and pressures
- Design temperatures/pressures (or MAWP/MAWT) of major equipment
- Material and energy balances with summary table for the process with streams information showing a mass balance for each major equipment
- Understanding of uses, sources and impacts of utilities (i.e. steam, cooling water, chill water, cooling tower, electricity etc) for the plant
- A complete HYSYS/ASPEN simulation report of the process
- Chemical engineering design of major equipment such as (i) reactor(s), (ii) absorption column(s) and (iii) distillation columns
- Estimates of the Major Equipment Capital Cost (Capex)
- Estimates of Operating Cost (Opex)
- Preparation of a net present value and investor's rate of return analysis for the investment over a 15-year life, assuming the company's current capital hurdle rate is 15%.
- Preparation of a project milestone schedule
- Preparation of a P&ID for a section of the process showing the control scheme to ensure safe operation of the unit, and carrying out a HAZOP analysis of the section of the process selected with correct equipment symbology
- Preparation of a safety report indicating the engineered safety measures required for the plant bearing in mind any toxic and flammable materials handled
- Knowledge or mention of external discharges from the plant (i.e. wastewater, flare or thermal oxidizer discharges)

In addition, the names of the presenters for each design project have been included in the rubrics to enable each presenter to be evaluated as well.

References:

- 1. Gael D. Ulrich and Palligarnai T. Vasudevan, " Chemical Engineering : Process Design and Economics, A practical Guide", second edition, 2004, Process Publishing, New Hampshire, USA, ISBN 0-9708768-2-3**
- 2. Gavin Towler and Ray innott, "Chemical Engineering Design : Principles, Practice and Economics of Plant and Process Design" Butterworth-Heinemam, ISBN 978-0-08-096659-5, second edition, 2013**
- 3. Perry's Chemical Engineering Handbook, sith edition or latest**
- 4. Turton, R., Bailie, R., Whiting, W., and Shaeiwits, J. A. "Analysis, Synthesis, and Design of Chemical Processes," 4th Edition Prentice-Hall PTR, Upper Saddle River, New Jersey 07458, 2008.**

5. “Plant Design and Economics for Chemical Engineers” by Peters, M.S., K.D. Timmerhaus and R.E. West, 5th edition, 2003, McGraw-Hill, ISBN 0—07-239266-5.

**SENIOR DESIGN & PROFESSIONALISM II CHEG 4482
Oral Design Presentation Evaluation Form**

Title of Presentation:
Date of Presentation: April 25, 2020
Name of Examiner/Appraiser:

Performance Criteria	Not Acceptable (0-59.9%)	Below Expectations (60-69.9%)	Average meets minimal expectations 70-79.9	Very Good Meets Expectations (80-89.9%)	Excellent Exceeds Expectations (90-100%)
1. Ability to Organize, Plan, Design/Prepare and Use Appropriate Visual Aids for communication/Presentation**	20 40 59	60 65 69	70 75 79	80 85 89	90 95 99
Presentation is organized in well structured logical sequence making it easy for audience to follow the content with clear understanding.	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
Slides are well prepared and are effective in helping audience to understand (<i>adequate and relevant technical content and view graphs that are legible, completely labeled, annotated, dimensioned to illustrate important features of the work being presented</i>)	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
Modern presentation techniques are used (<i>may include visually enhanced transitions, animations, video, and sound clips</i>).	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
Average for this Performance Criteria					
2. Ability to Articulate Subject Knowledge (Technical Content)*					
Client identification and recognition of need	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
Project goals and objectives, and planning	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
Process screening and selection, PFD and process description	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
Process chemistry, and material and energy balances	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
Quality of chemical engineering design/and analysis, and design constraints	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
Design within economic, societal and environmental constraints (including contemporary issues and broader impact on society)	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
Hazard and Safety considerations****	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
Questions are responded to in a clear professional manner after restating questions to audience	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
Average for this Performance Criteria					
3. Appearance and Ability to Provide Good Oral Delivery**					
Correct grammatical English and technical terms appropriate to technical area and audience are used; and presenters speak with clarity and confidence	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
Good posture and eye contact with the audience are maintained (<i>should not read from prepared notes</i>) and elicits the attention of the audience	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
Presenters dress appropriately for the occasion.	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
Efforts of all group members/Group dynamics***	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
Average for this Performance Criteria					
OVERALL AVERAGE GROUP PERFORMANCE					
NAME OF PRESENTER	OVERALL PERFORMANCE OF PRESENTER				

	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐
	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐	☐ ☐ ☐

ABET Student Outcome 2 ; ** ABET Student Outcome 3; *** ABET Student Outcome 5; *Program Criterion 9b**

**ABOVE AVERAGE
PROJECT PRESENTATION**

Ethylene Oxide Production
by
Direct Oxidation
of
Ethylene
in
Catalytic Multi-tubular Reactors

Chloe Sanders

Natalie Russell

Leah McClellan

Ariel Taylor

Francis Saneii



Project Scope

❖ Problem Statement

- Design a grass-roots ethylene oxide plant to produce 550 M tons per year (1,100 MM lbs per year)

❖ Goals

- Produce ethylene oxide with a purity of 99.7%
 - ❖ Direct catalytic oxidation of ethylene
 - ❖ Silver-supported catalyst
 - AgAl_2O_3
 - ❖ High selectivity of ethylene to ethylene oxide
 - ❖ Plant location: Texas Gulf Coast



Project Deliverables

- ❖ Process Description and PFD
- ❖ Detailed Chemical Engineering Design of Major Equipment
- ❖ HAZOP Analysis and P&ID of Most Critical Piece of Equipment
- ❖ Converged ASPEN Simulation Report of Process
- ❖ Estimate of Equipment Capital Cost (CAPEX)
- ❖ Estimate of Operating Cost (OPEX)
- ❖ Cash Flow Diagram of 15 Year Plant Life with ROROI hurdle of 15%



Design Basis

❖ Plant Capacity:

- 1,100 MM lbs/year (550,000 tons/year)
- 15% Supply Gap

❖ Plant Production Time

- 92% of the year
- 336 Days
- 8,064 Hours

❖ Hourly Production Rate:

- 136 M lb/hr

❖ Production of ethylene oxide with 99.7% purity

❖ Texas Gulf Coast; Ethylene feedstock

- Max T: 105 °F
- Min T: 30 °F



Preliminary Design Assumptions

- ❖ Feed impurities negligible
 - Polymer grade ethylene (99.999% Purity)
 - Oxygen (99.9% pure)
- ❖ Water to EO ratio 22:1
 - High T & P application
- ❖ Methane used as an inert gas to keep reactor feed and reactor affluent below flammability limits
- ❖ Negligible formation of aldehydes
- ❖ Negligible losses of ethylene oxide in EO stripping column



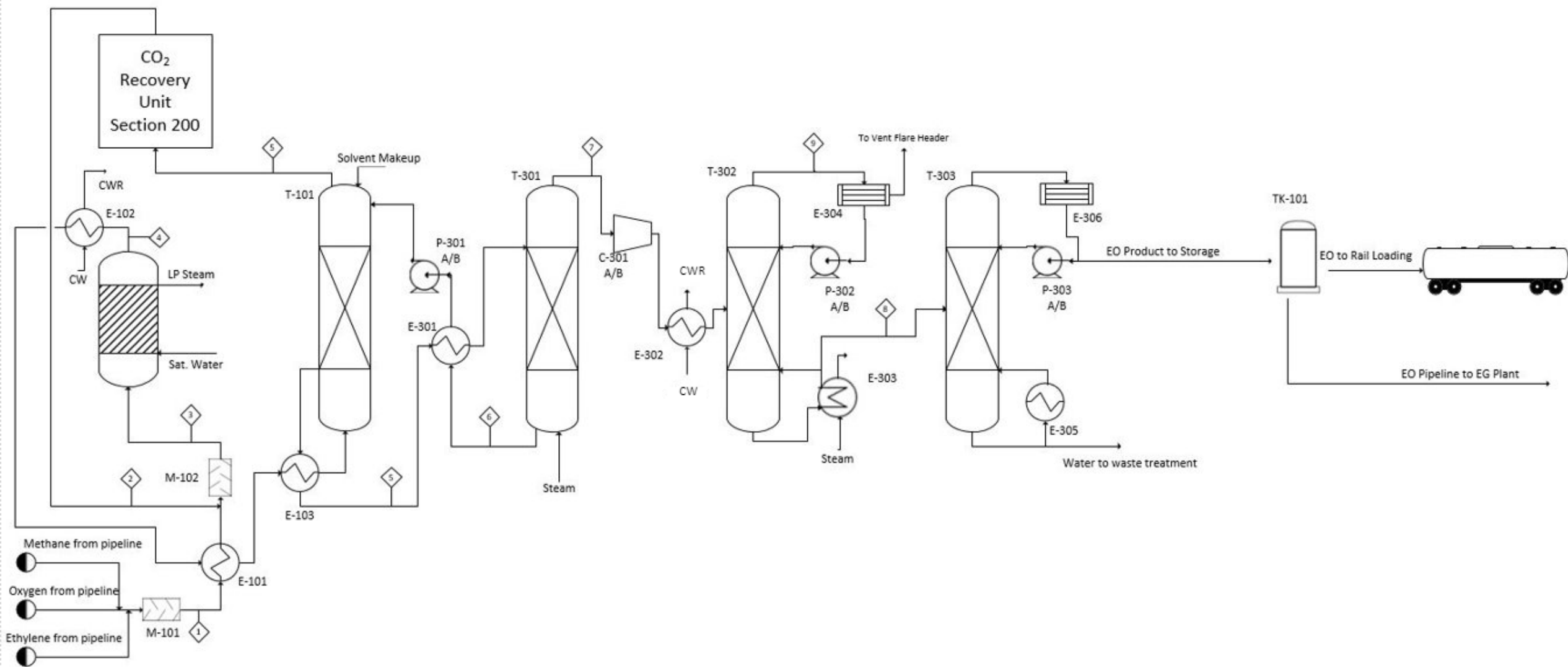
R-101
Reactor
OT 480 °F
OP 230 psi

T-101
EO Absorber
OT 75 °F
OP 215 psig

T-301
EO Stripper
OT 150 °F
OP 15 psig

T-302
Light-ends removal
OT 75 °F
OP 80 psig

T-303
EO Distillation
OT 75°F
OP 14.7 psia



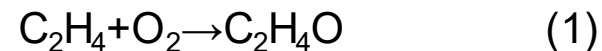
Detailed Design of Major Equipment



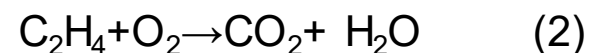
R-101 Detailed Design

	Item No:	R-101	Date:	4/24/2020
	No Required:	8		
	TIC (\$)	\$ 1,536,000.00	CBM(\$)	\$ 7,728,000.00
Function: Convert ethylene and oxygen to produce to ethylene oxide				
Operation: Continuous				
	Feed	Outlet		
Materials Handled:				
Total flow (MMSCF/hr):	19.1	18.5		
Component Flows (MMSCF/hr)				
Ethylene	7.7	6.3		
Oxygen	3.8	2.3		
Methane	7.6	7.6		
Ethylene Oxide		1.2		
Water		0.6		
Carbon Dioxide		0.6		
	Operating	Design		
Temperature (F):	480	720		
Pressure (psia):	230	480		
Design Data: PER REACTOR				
Height	70 ft	Material		
Total Diameter	30 ft	Shell	316L SS clad carbon steel	
# Tubes	6943	Tubes	316 L SS	
Tube I.D	0.083 ft	Tubesheet	316L SS clad carbon steel	
Tube Length	70 ft			
Tube Formation	Triangular	Q(MMBTU/hr)	14.65	
Amount of Catalyst (lbs)	108,000			

Process Chemistry



$$\Delta H_{\text{rxn}} = -101.1 \text{ BTU/lbmol}$$



$$\Delta H_{\text{rxn}} = -1254 \text{ BTU/lbmol}$$

$$\diamond \text{ Total Bed Volume} = \frac{V(\text{SCF})}{GHSV}$$

$$\diamond \text{ Total Amount of Catalyst Required} = \text{Catalyst Density} \times \text{Total Bed Volume}$$

$$\diamond \text{ Bed Volume Per Tube} = \pi \times \left(\frac{D^2}{4}\right) \times h$$

$$\diamond \text{ Catalyst Volume Required} = \frac{\text{Total Amount of Catalyst}}{\text{Density of Catalyst}}$$

$$\diamond \text{ Total Number of Tubes} = \frac{\text{Catalyst Volume Required}}{\text{Bed Volume Per Tube}}$$

$$\diamond \text{ Total Number of Reactors} = \frac{\text{Total Number of Tubes}}{8}$$

$$\diamond \text{ Catalyst Weight Per Tube} = \frac{\text{Total Catalyst needed}}{\text{Total Number of Tubes}}$$



T-101 Detailed Design

Identification:	Item: Ethylene Oxide Absorber			
	Item No:	T-101	Date:	4/24/2020
	No Required:	1		
	TIC (\$)	\$ 730,658.00	CBM(\$)	\$ 5,020,658.00
Function:	Recover 99% of Ethylene Oxide by scrubbing with water			
Operation:	Continuous			
	Inlet		Outlet	
	Feed	Solvent	Overhead	Bottoms
Materials Handled:				
Total flow (MMSCF/hr):	18.4	0.02	17.16	1.248
Component Flows (MMSCF/hr)				
Ethylene	6.1		6.09	0.006
Oxygen	2.3		2.30	0.002
Methane	7.6		7.59	0.008
Ethylene Oxide	1.2		0	1.2
Water	0.6	0.02	0.579	0.021
Carbon Dioxide	0.6		5.99E-01	7.59E-04
	Operating	Design		
Temperature (F):	75	112.5		
Pressure (psig):	215	480		
Design Data:				
Tower Height (ft)	127			
Tower Diameter (ft)	12.5			
Total Packing Height (ft)	117			
Packing Diameter (ft)	12.5			
	Internal	External		
Material	316L SS clad to carbon steel	Carbon steel		
Packing	Mellpak 125X			



Design Equations for EO Abs (T-101)

Number of transfer units, N_{OG} :

$$N_{OG} = \frac{A}{A-1} \ln \left\{ \frac{(A-1)(y_{in} - K * x_{in})}{A(y_{out} - K * x_{in})} + \frac{1}{A} \right\}$$

Where:

y_{in} = mole fraction of EO entering in the gas stream; 0.07

y_{out} = mole fraction of EO exiting in the gas stream; 0.0007

x_{in} = mole fraction of EO entering in the liquid stream; 0

K = dimensionless equilibrium distribution coefficient; 0.85

A = Absorption factor; $A = \frac{L}{KV}$

Where:

L = solvent flowrate entering (lbmol/hr)

V = vapor flowrate entering (lbmol/hr)

i. Height of transfer units, H_{OG} :

$$H_{OG} = \frac{V}{K_y a * S}$$

Where:

S = cross-sectional area of the column in ft²; 38.5

$K_y a$ = overall mass transfer coefficient; $K_y a = \left(\frac{1}{k_y a} + \frac{K}{k_x a} \right)^{-1}$

Where:

$k_y a$ = volumetric mass transfer coefficient in the gas phase in lbmol/(hr*ft³); 200

$k_x a$ = volumetric mass transfer coefficient in the liquid phase in lbmol/(hr*ft³); 165

i. Total height of packing

$$\text{Packing height} = N_{OG} * H_{OG}$$



T-301 Detailed Design

Identification:	Ethylene Oxide Stripper			
Item:	Item No:	T-301	Date:	4/24/2020
	No Required:	1		
	TIC (\$)	\$ 475,927.41	CBM(\$)	\$ 1,186,927.41
Function:	Recover 99% Ethylene Oxide and regenerate T-101 Solvent by steam stripping			
Operation:	Continuous			
	Inlet		Outlet	
	Feed	Steam	Overhead	Bottoms
Materials Handled:				
Total flow (MMSCF/hr):	1.248	5.3	6.53	0.021
Component Flows (MMSCF/hr)				
Ethylene	0.006		0.006	
Oxygen	0.002		0.002	
Methane	0.008		0.008	
Ethylene Oxide	1.21		1.2	0.012
Water	0.021	5.3	5.3	0.02
Carbon Dioxide	7.59E-04		7.59E-04	
	Operating	Design		
Temperature (F):	150	225		
Pressure (psig):	15	400		
Design Data:				
Tower Height (ft)	70.5			
Tower Diameter (ft)	13.4			
Total Packing Height (ft)	60.5			
Packing Diameter (ft)	13.4			
	Internal	External		
Material	316L SS clad to carbon steel	Carbon steel		
Packing	Mellapak 125X			

$$N_{OL} = \frac{x_1 - x_2}{(x^* - x)_{LM}}$$

$$H_{OL} = \frac{L}{K_x a (1 - x)^*_{LM}}$$

$$(1 - x)^*_{LM} = \frac{(x_1^* - x_1) - (x_2^* - x_2)}{\ln\left(\frac{(x_1^* - x_1)}{(x_2^* - x_2)}\right)}$$

T-302 Detailed Design

Identification:	Item:	Light-ends Column		
	Item No:	T-302	Date:	4/24/2020
	No Required:	1		
	TIC (\$)	\$ 4,414.84	CBM(\$)	\$ 130,014.84
Function:	Remove VOC from Ethylene Oxide and Water Stream			
Operation:	Continuous			
	Inlet	Outlet		
	Feed	Overhead	Bottoms	
Materials Handled:				
Total flow (MMSCF/hr):	6.5	0.017	6.5	
Component Flows (MMSCF/hr)				
Ethylene	0.006	0.006		
Oxygen	0.002	0.002		
Methane	0.008	0.008		
Ethylene Oxide	1.2	-	1.2	
Water	5.3	-	5.3	
Carbon Dioxide	7.49E-04	0.00075		
	Operating	Design		
Temperature (F):	75	112.5		
Pressure (psig):	80	400		
Design Data:				
Tower Height (ft)	22.5			
Tower Diameter (ft)	5.68			
Total Packing Height (ft)	12.5			
Packing Diameter (ft)	5.68			
	Internal	External		
Material	316L SS clad to carbon steel	Carbon steel		
Packing	Mellapak 125Y			

◆ Feed Operating Line

$$y = \frac{q}{q-1} x - \frac{z_F}{q-1}$$

◆ Rectifying Section Operating Line

$$y = \frac{R}{1+R} + \frac{1}{1+R} x_D$$

◆ Stripping Section Operating Line

$$y = \frac{\bar{L}}{\bar{V}} x - + \frac{B}{\bar{V}} x_B$$

◆ Height Equivalent to Theoretical Plate (HETP)

$$H_{packed} = N_{ideal} * HETP$$

T-303 Detailed Design

Identification:	Ethylene Oxide Distillation			
	Item:			
	Item No:	T-303	Date:	4/24/2020
	No Required:	1		
	TIC (\$)	\$ 134,391.11	CBM(\$)	318,49.11
Function:	Recover Ethylene Oxide Product with 99.7% purity by distillation			
Operation:	Continuous			
	Inlet	Outlet		
	Feed	Overhead	Bottoms	
Materials Handled:				
Total flow (MMSCF/hr):	6.5	1.18	5.32	
Component Flows (MMSCF/hr)				
Ethylene				
Oxygen				
Methane				
Ethylene Oxide	1.2	1.18	0.02	
Water	5.3	2.70E-05	5.3	
Carbon Dioxide				
	Operating	Design		
Temperature (F):	75	112.5		
Pressure (psig):	0	400		
Design Data:				
Tower Height (ft)	31			
Tower Diameter (ft)	12.5			
Total Packing Height (ft)	21			
Packing Diameter (ft)	12.5			
	Internal	External		
Material	316L SS clad to carbon steel	Carbon steel		
Packing	Mellapak 452Y			

♦ Feed Operating Line

$$y = \frac{q}{q-1} x - \frac{z_F}{q-1}$$

♦ Rectifying Section Operating Line

$$y = \frac{R}{1+R} + \frac{1}{1+R} x_D$$

♦ Stripping Section Operating Line

$$y = \frac{\bar{L}}{\bar{V}} x - + \frac{B}{\bar{V}} x_B$$

♦ Height Equivalent to Theoretical Plate (HETP)

$$H_{packed} = N_{ideal} * HETP$$

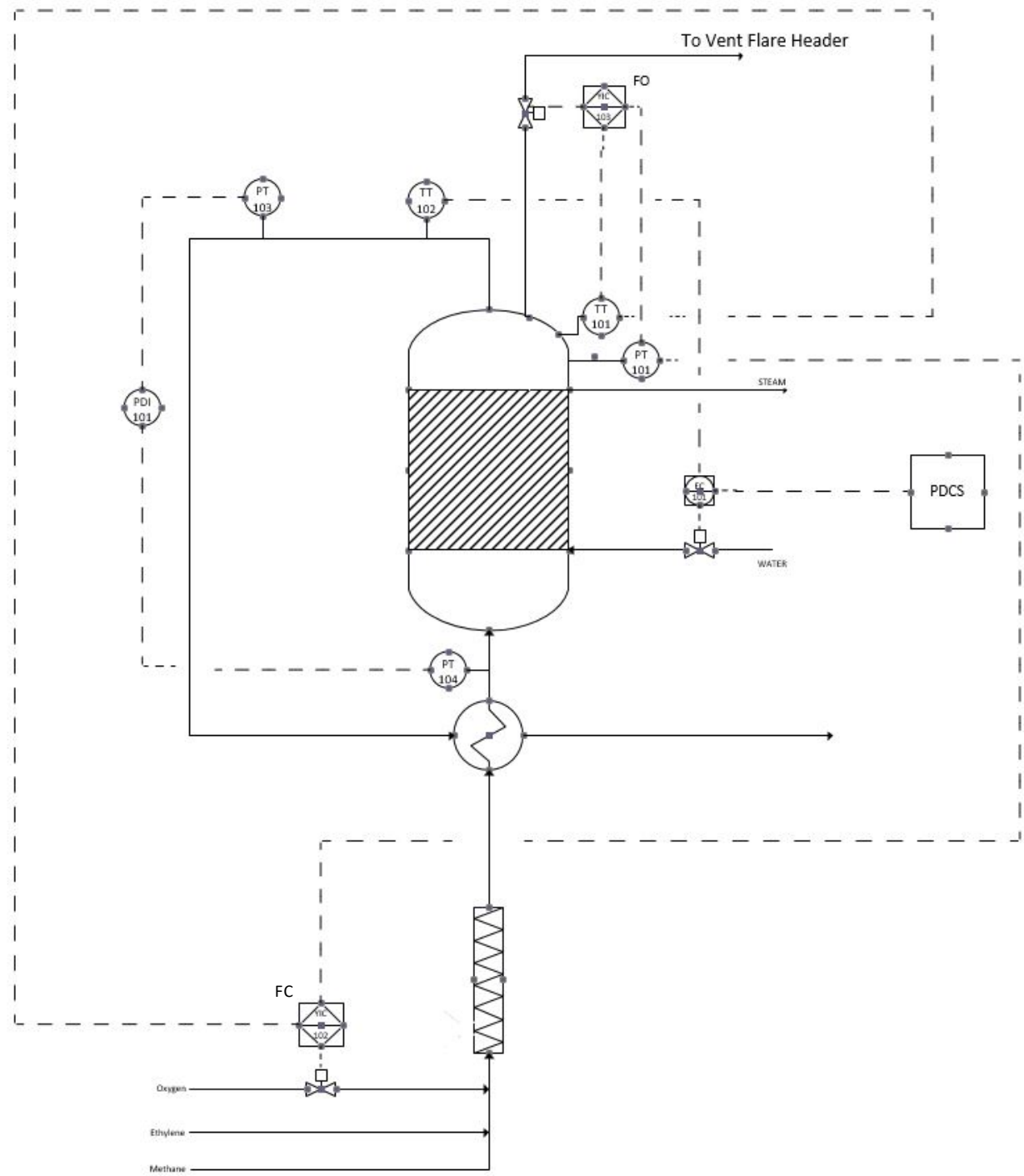


Process Safety



Deviation		Possible Causes	Consequences	Recommendation
Parameter	Guideword			
Flow to the reactor	No	Feed inlet control valve failed closed	No reaction takes place	Install low flow alarm to monitor and regularly measure the flow entering the reactor
	More	Valve failed open	Too much flow into the reactor causes a runaway heat reaction and possible explosion	Install high flow alarm and backup control valve
	Less	Leaking of pipe	Desired amount not produced possible accumulation in pipeline can lead to potential	Install Pressure indicator and bypass valve
Pressure in the reactor	Less	High pressure downstream due to pump/compressor failure	EO line could back flow into reactor and uncontrolled amounts of oxygen and ethylene oxide could cause Runaway reaction	Monitor reactor temperature and pressure on DCS system and have an emergency shutdown procedure in place. Add thermal jacket to reactor
	More	Reactor material/valve failure	Temperature will increase runaway reaction takes place leading to potential explosion	Monitor reactor temperature and pressure on DCS and have emergency shutdown procedures. Add thermal jacket to reactor. Include pressure release valve to reactor.
Temperature in the reactor	Low	Cooling water valve failed open	Reaction kinetics would be affected, and pressure could decrease	Install temperature alarm for jacketed cooling. Add thermal control jacket to reactor. Monitor reactor temperature and pressure on DCS and have an emergency shutdown procedure in place
	High	Cooling water valve failed closed	Increase Temperature in reactor could cause Explosion	Add thermal control jacket to reactor and monitor reactor temperature and pressure on DCS system and have automatic shutdown procedures





Process Safety Handling

Effects of Exposure:

- Short term effects of the chemicals such as (OSHA):
 - Respiratory irritation
 - Lung injury
 - Headaches
- Chronic long-term damage includes:
 - Reproductive effects
 - Changes or damage to DNA
 - Impact on learning
- Carcinogenic
 - Lymphoma
 - Breast

Shutdown and Cleaning:

- Gas wash, Rinse
- Hot water rinse
- Citric acid cleansing
- Waste EO is sent to a body of water
- Low flow or high temperature safety shut down on reflux pumps

Environmental Impact:

- 5,000 ppm or 0.5% of CO₂ can be admitted into the air (Permissible Exposure Limit PEL) for 8-hour exposure
- Methane NIOSH permissible amounts released in the air 1,000ppm (.1%)
- Ethylene is not harmful or toxic to humans, but at or above 27,000ppm it is combustible

Exothermic Reaction Safety Measures:

- Safety control systems
- Shatter resistant glass and safe distance monitoring
- Safety shut down system and alarms
- Leak detection systems sensitive to 1 ppm

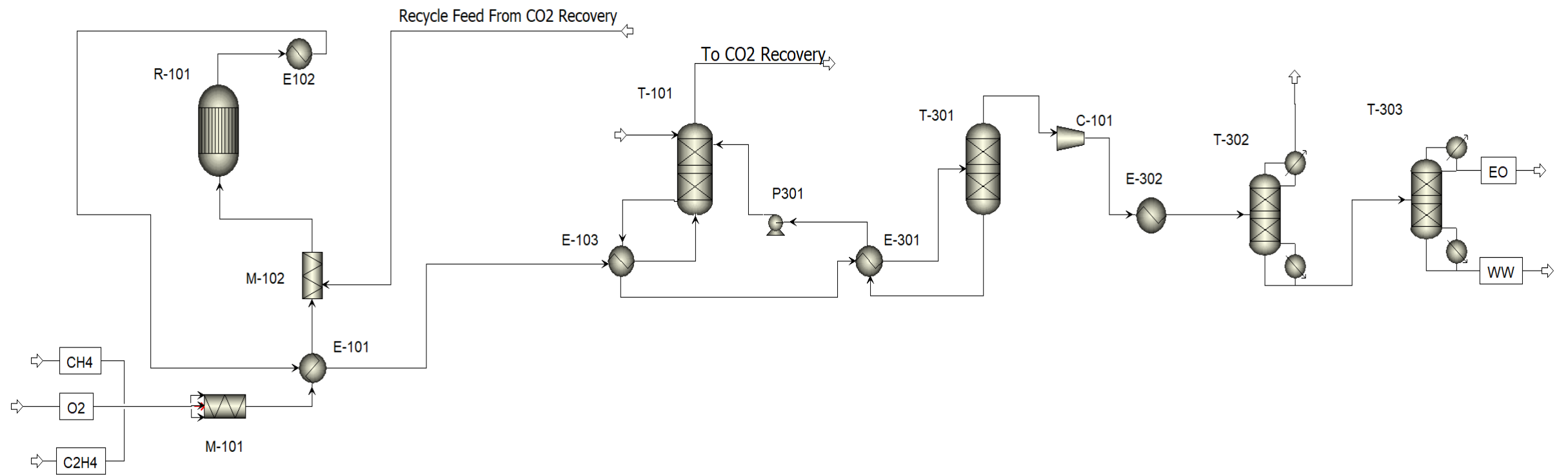
Storage:

- Horizontal Tanks
 - Corrosion resistant material clad to pressure containment material (ss clad to carbon steel)
 - Temperature and Pressure Controlled
 - 1000 feet away from any heated processes
 - Deionized water
 - Inert gas cooling
 - Continuous analyzers



Aspen Plus Simulation

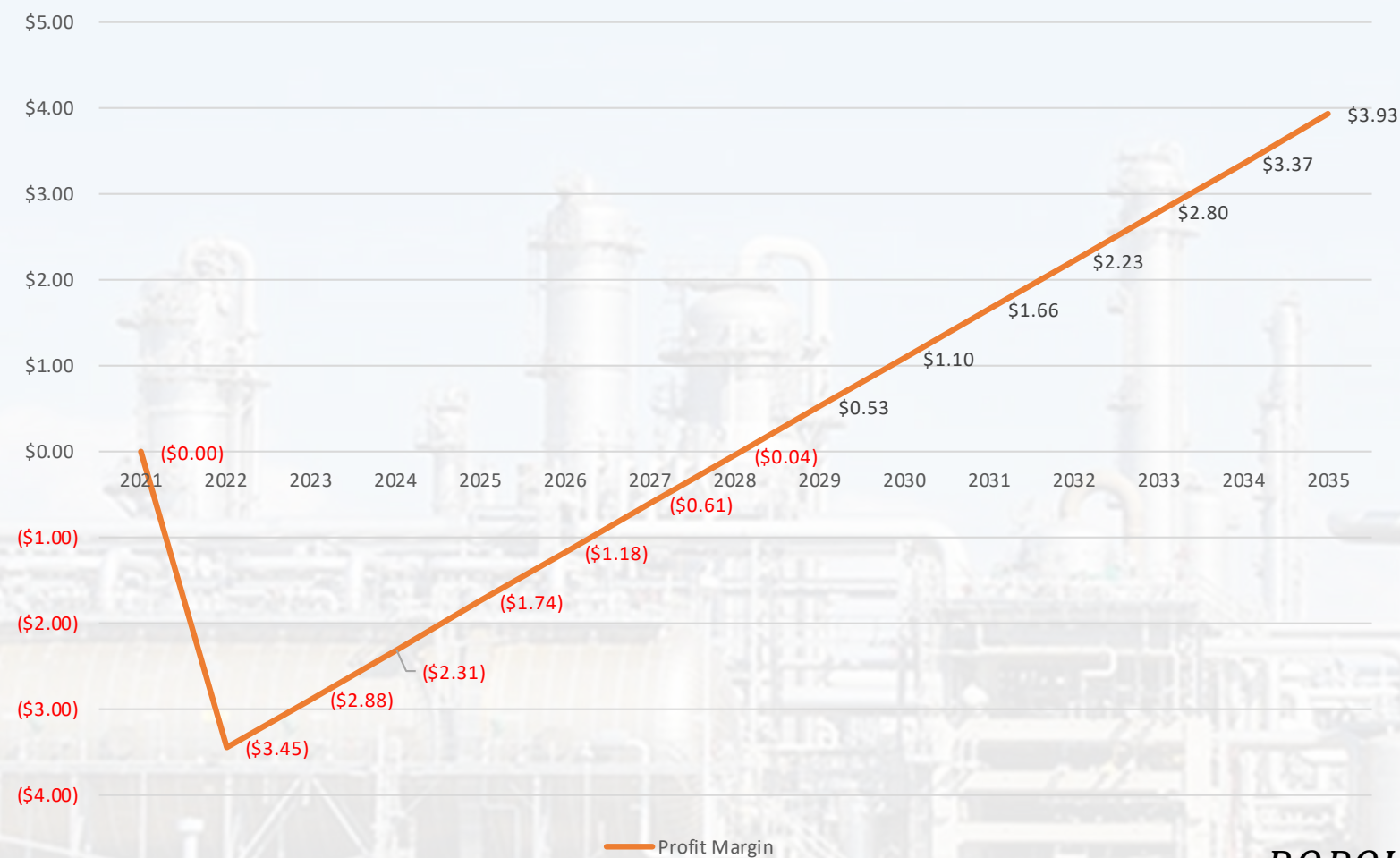




Economic Analysis



PROFIT ANALYSIS BILLION DOLLARS



Land:	\$1,600,000
FCI:	\$1,500,000,000
WC:	\$2,261,950.34
Salvage:	\$0.00
Equip. & RM	\$1,941,601,419.36
Profit:	\$567,560,247

$$ROROI = \frac{\text{Profit per year}}{FCI}$$
$$ROROI = \frac{567,560,247}{1,500,000,000} = 38\%$$



Thank You!



AVERAGE
PROJECT PRESENTATION



Tominisha
Johnson



Joshua
Livingston



Olumide
Longe (Olu)



Collins
Ogogor



Kinza
Rizwan



PRAIRIE VIEW
A&M UNIVERSITY

The Production of Citric Acid by Fermentation

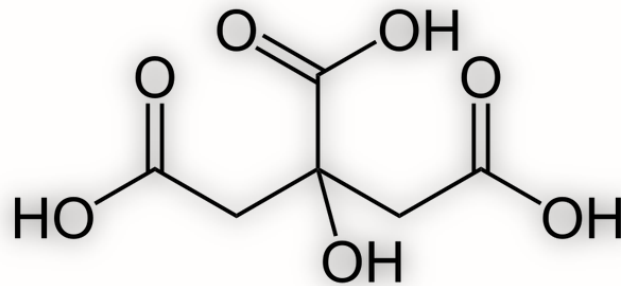
Bioengineering Concentration Group I



What is Citric Acid?

- Weak organic acid found in citrus fruits, plants, and animal tissues
- Common uses are:
 - Flavoring agent – acidic tastes masks unpleasant tastes
 - Blood anticoagulant – citrate chelates calcium
 - Pharmaceuticals – used for effective buffering systems
 - Beverage and food – Acidulant and pH stabilizer

Molecular
Structure of
Citric Acid



Project Overview

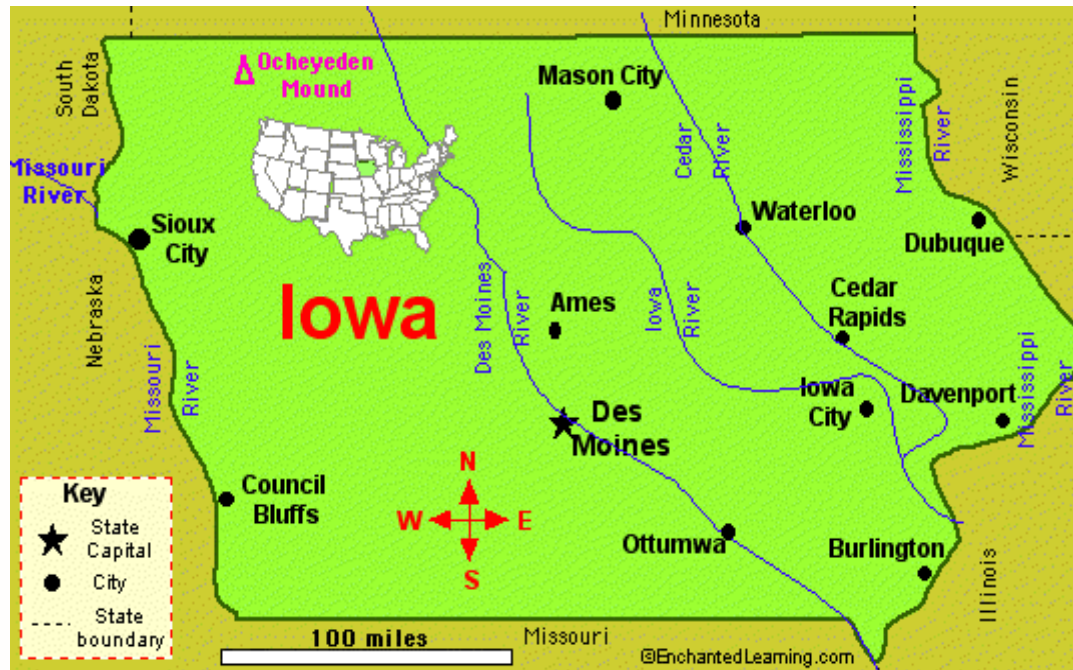
Location: Cedar Rapids, IA

Plant Capacity: 100 kilotons per year

Days of Operation: 334 days (8000 hours per year)

Plant Life: 20 Years

Location Selection

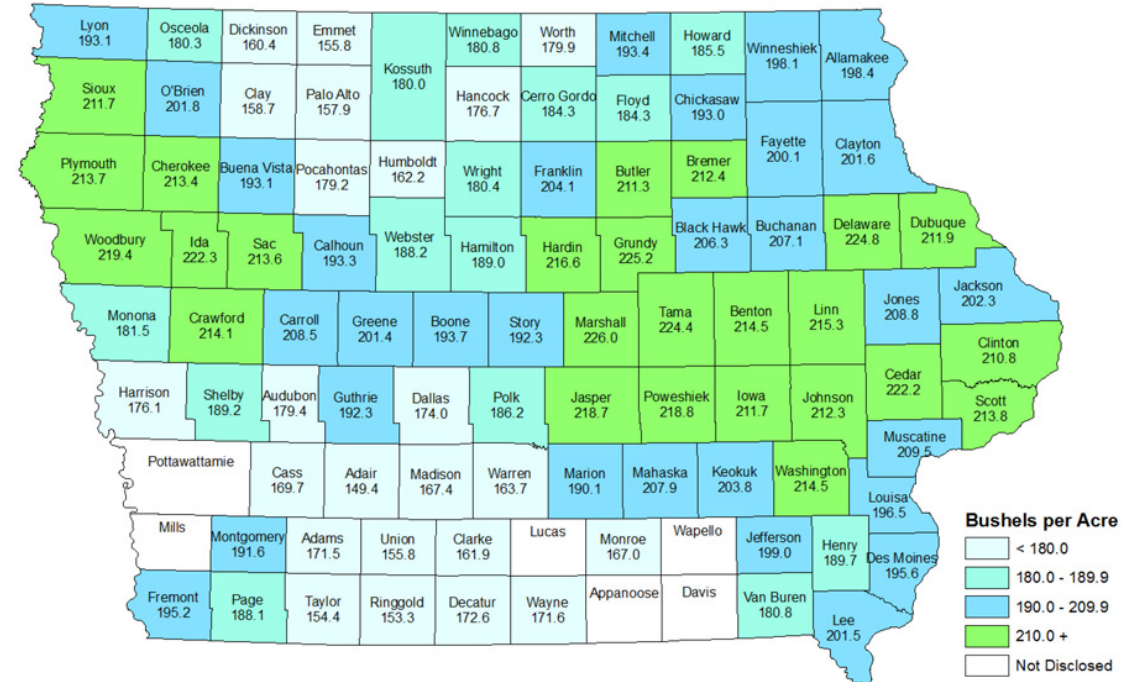


Why Cedar Rapids?

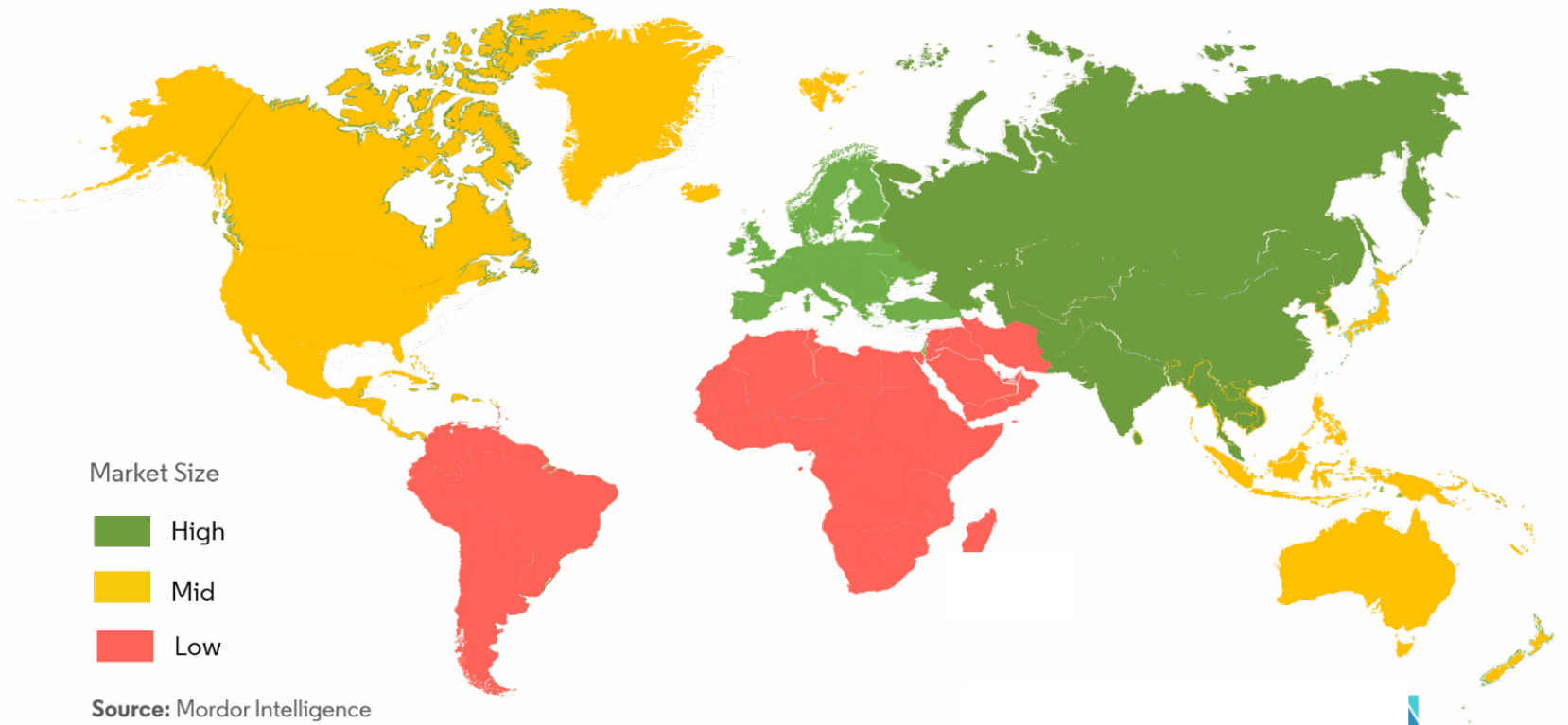
Cedar Rapids, Iowa produces more than 210 Bushels of Corn per acre and is home to Cargill, which processes 100,000+ bushels of corn per day.

Corn for Grain Yield – Iowa: 2018

State Average: 196.0 Bushels per Acre

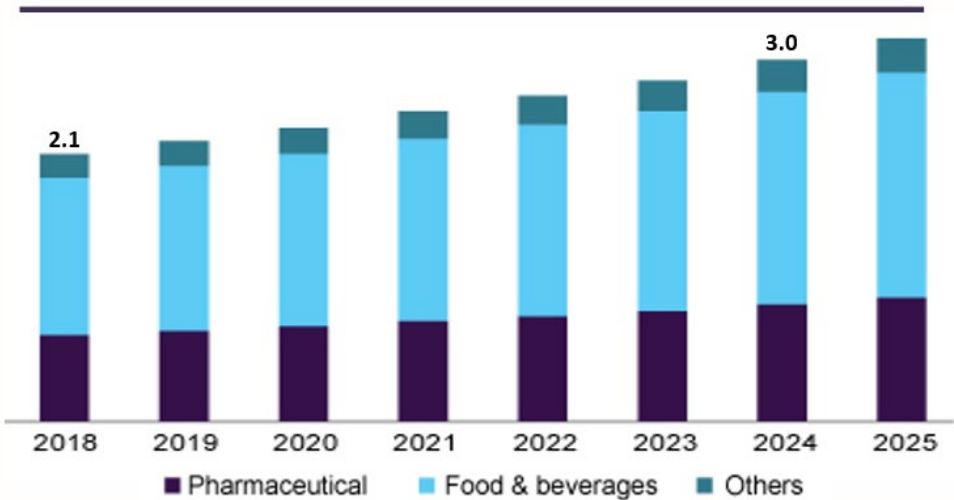


Citric Acid Market - Market Size, by Region, Global, 2018



- Fastest Growing Market: Asia Pacific
- Largest Market: Europe
- **United States is the leading importer of Citric Acid**
- China is the leading exporter of Citric Acid

Global Citric Acid Market Demand, by Industry 2014 - 2025 (million tons)

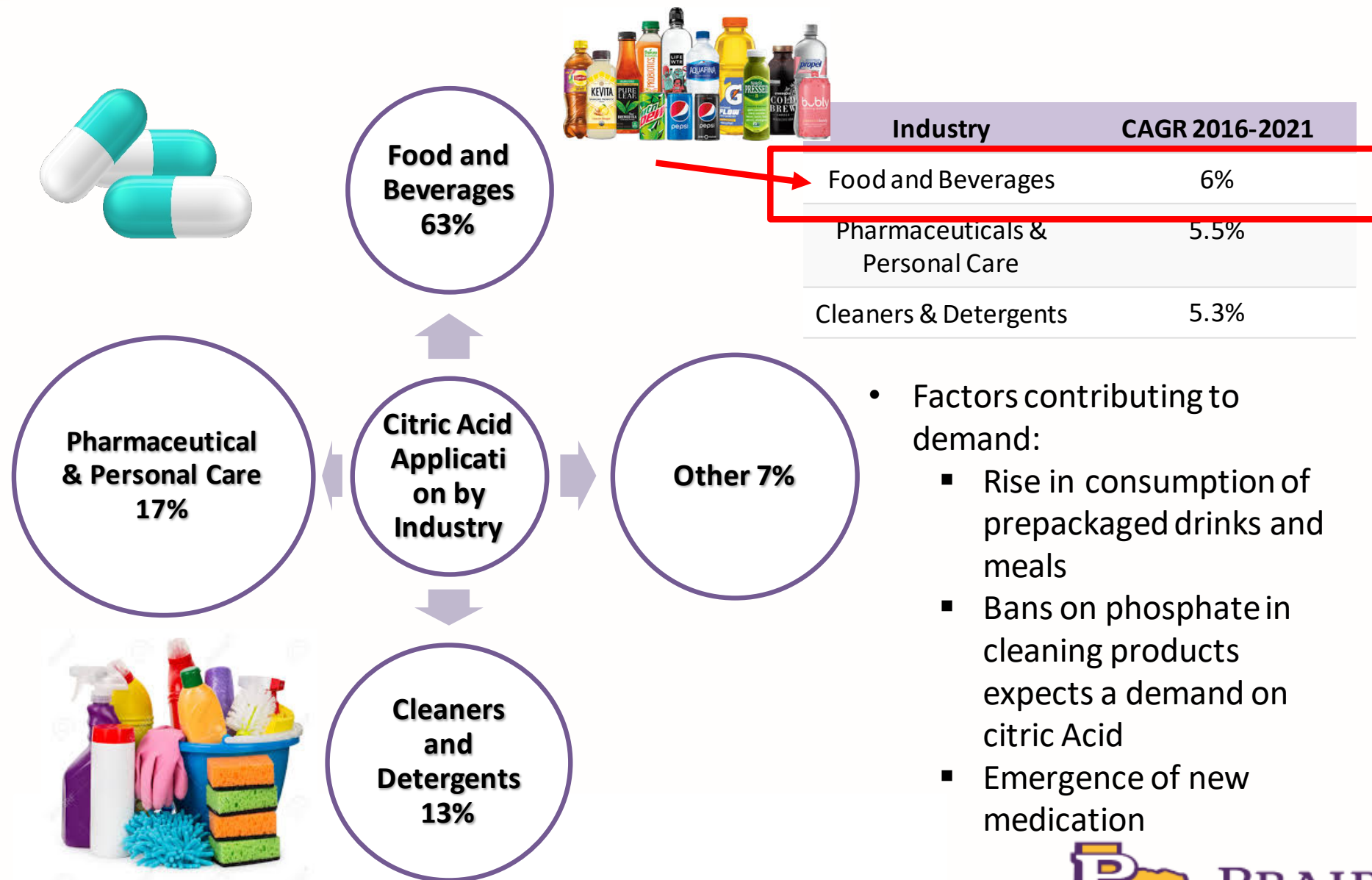


Source: Grand View Research

- Gap in demand: 900 kilotons by 2024
- Based on demand and current capacity
 - Plant Capacity: 100 kilotons per year
 - Satisfy 11% of demand by 2024

Major Global Citric Acid Producers (Kiloton per year); Plant capacity (100% Anhydrous)

Company	Location	Capacity
Jungbunzlauer	Austria	136
Archer Daniels	United States	98
Midland	Ireland	45
Hoffmann-La Roche	Belgium	73
Average		88



Citric Acid (Anhydrous, Food Grade) - $C_6H_8O_7$

Purity:

>99.5% Citric Acid Anhydrous

pH: 1.8



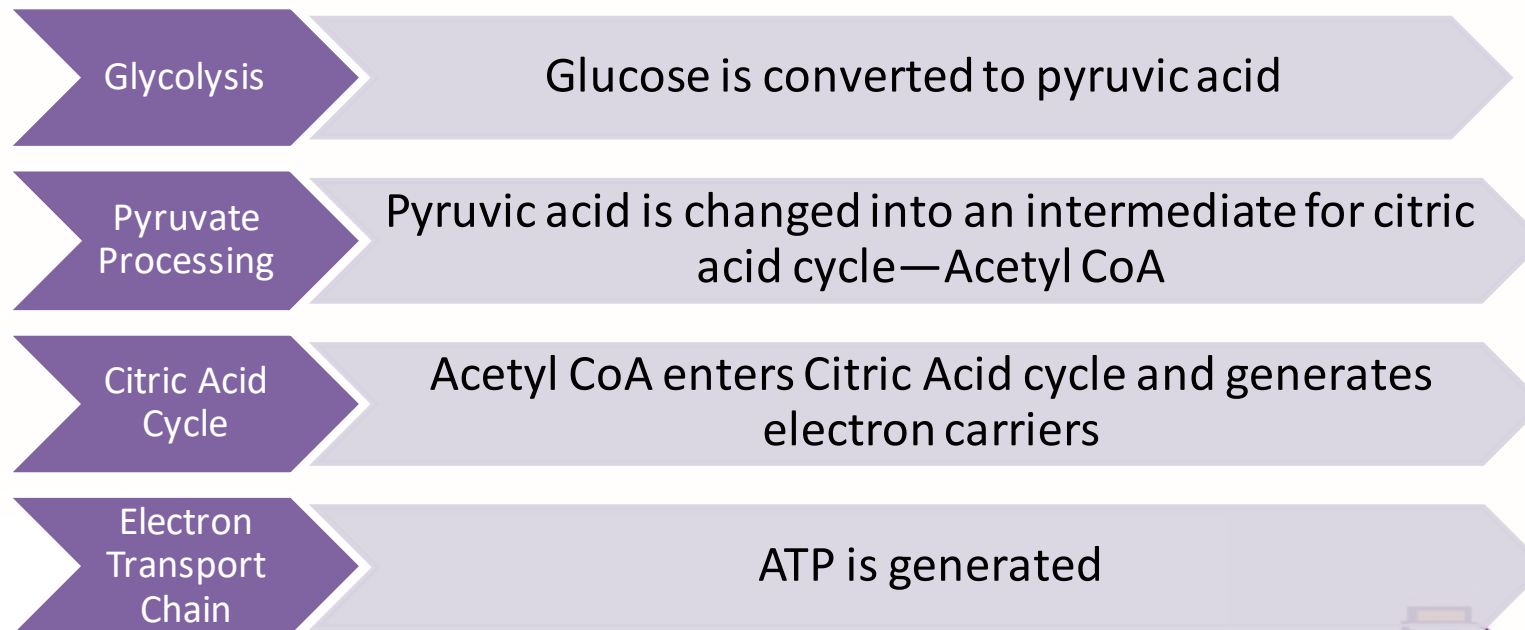
Particle size

> 1.25 mm	max. 5%
< 0.40 mm	max. 10%

Parameters for Ingestible Citric Acid

Heavy metals	5 ppm max
Sulphated Ash	0.05% max

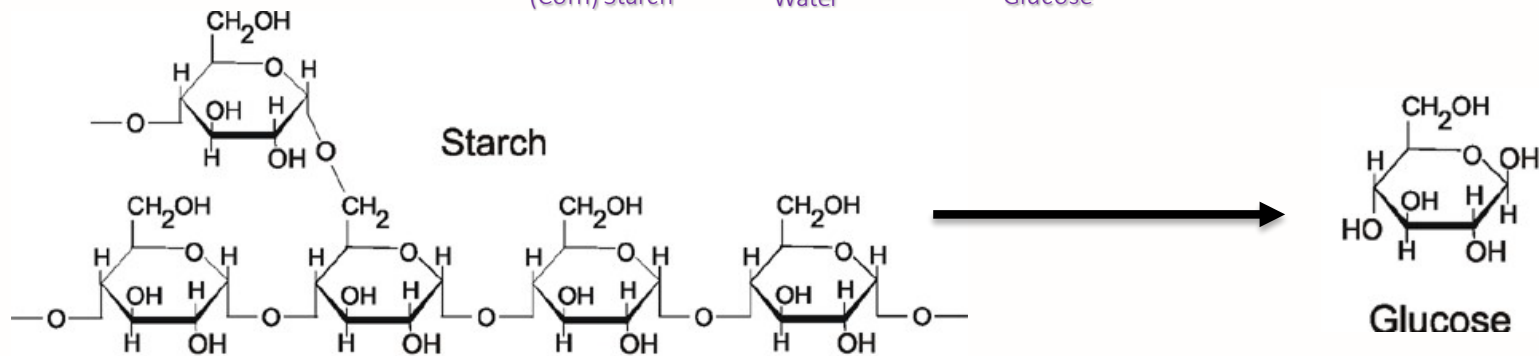
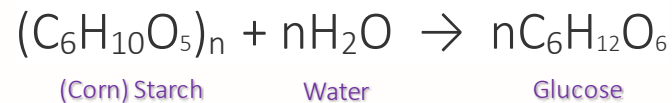
- Aerobic Fermentation: Conversion of carbohydrates such as glucose to CO_2 , alcohols, and organic acids using yeast, bacteria or combination of both
- Living organism need **ATP**
 - **ATP: Energy currency of the cell**
- Main biological pathway to generate ATP is by the means of cellular respiration
 - Consist of 4 stages



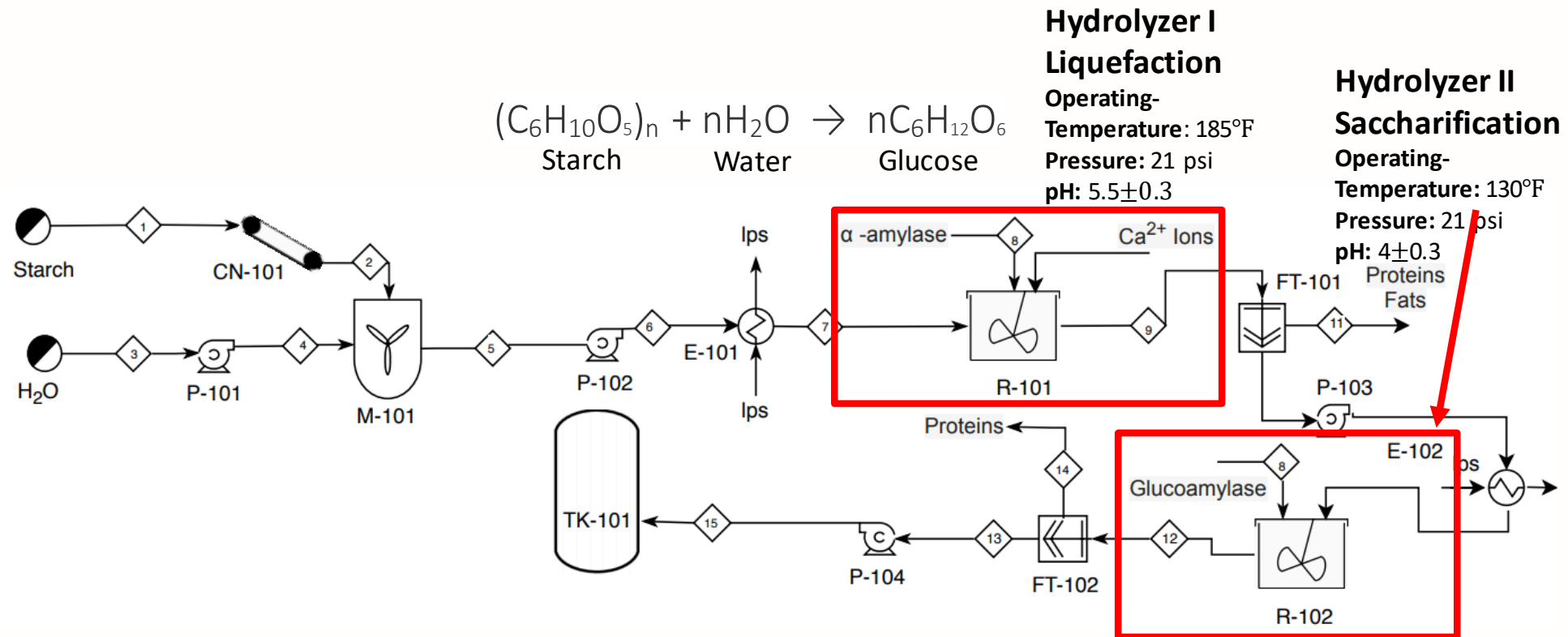
Raw Material Treatment Chemistry Overview

1. Upstream Processing

- Breaking down Corn Starch to Glucose by Hydrolysis reaction
 - Liquefaction + Saccharification

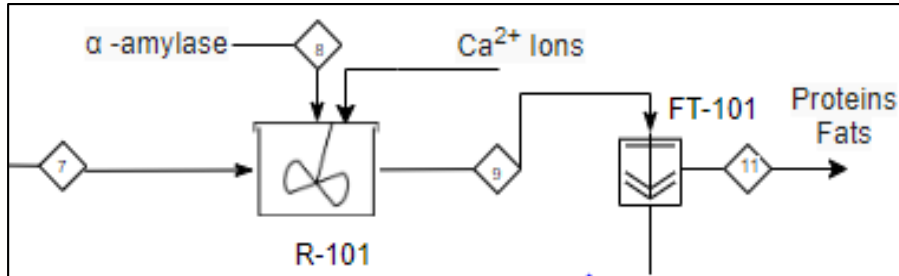


Upstream Processing



P-101	CN-101	M-101	P-102	E-101	R-101	FT-101	P-103	E102	R-102	FT-102	P-103	TK-101
Water Feed Pump	Starch Conveyor	Feed Mixer	Starch Slurry Feed Pump	Starch Slurry Feed Heater	Starch Hydrolyzer 1	Centrifuge-1	Filtrate Pump	Heat exchanger	Starch Hydrolyzer 2	Centrifuge-2	Glucose Slurry Pump	Glucose Slurry Storage Tank

Liquefaction



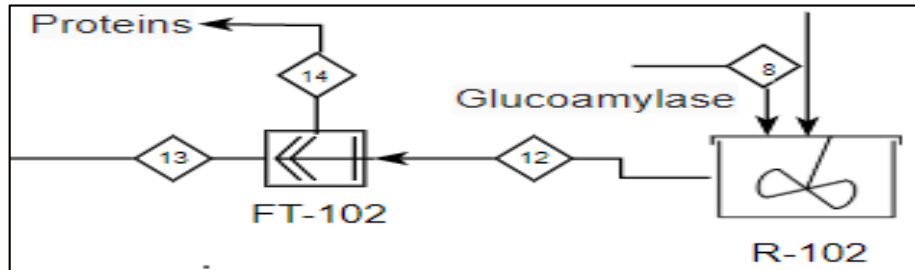
- Temperature: 185°F
- Pressure: 21 psi
- pH: 5.5

Assumptions

- 25% of starch converted to glucose
- Free Enzyme
- 99% of Enzyme Filtered out

- **Alpha amylase**- an enzyme that hydrolyses bonds of starch and glycogen, yielding glucose.
 - Added to catalyze the hydrolysis of corn starch
 - Optimal pH range 5.5-5.8
- Controlling pH by adding using HCl

Saccharification



- Temperature: 130°F
- Pressure: 21 psi
- pH: 4

Assumptions

- 75% of starch converted to glucose
- Free Enzyme
- 99% of Enzyme Filtered out

- **Glucoamylase**- biocatalyst that is utilized in the mass production of glucose from raw starch.
 - Added to catalyze the hydrolysis of corn starch
 - works best under 140°F
 - Acidic condition, pH is at or below 5
- Controlling pH by adding HCl

Hydrolyzer I			
Identification:	Item:	Jacketed Hydrolyzer	
	Item No:	R-101A	
	No. Required:	66	
	C _{TPI} (\$)		
Function: To undergo liquefaction of corn starch slurry, partially hydrolyzing it into glucose			
Operation: Batch			
Materials Handled:	Feed (lb/hr)	Product Stream (lb/hr)	
Cornstarch	36,500	27,500	
Water	263,000	264,000	
Alpha-Amylase	20	20	
Ca+	10	10	
Glucose	0	10,100	
Operating Conditions			
Temperature (°F): 185			
Pressure (psia): 21			
pH: 5.5			

Summary

Operation: Batch (4 hrs/batch)

No. Required: 66

Exothermic Reaction

Isothermal Conditions Maintained by Cooling Jacket

High Enzyme Costs

Relevant Equations

$$\text{Total Reactor volume: } V_r = \frac{m'_1 t_B}{\rho'}$$

V_r = Volume of Reactor

t_B = Batch Time

ρ' = Density of Batch

$$\text{Batch Time: } t_B = t'_F + t'_H + t_R + t'_C + t'_E$$

t'_F = Filling Time

t'_H = Heating Time

t_R = Reaction Time

t'_C = Cooling Time

t'_E = Emptying/Cleaning Time

Hydrolyzer II			
Identification:	Item:	Jacketed Hydrolyzer	
	Item No:	R-101A	
	No. Required:	38	
	C _{TRI} (\$)		
Function: To undergo sacchrification of corn starch slurry, hydrolyzing remaining starch into glucose			
Operation: Batch			
Materials Handled:	Feed (lb/hr)	Product Stream (lb/hr)	
Cornstarch	27,500	0	
Water	264,000	267,000	
Glucose	10100	40500	
Glucomaylase	15	15	
Ca ²⁺	10	10	
Operating Conditions			
Temperature (°F): 130			
Pressure (psia): 21			
pH: 4			

Summary

Operation: Batch (60 hrs/batch)

No. Required: 38

Exothermic Reaction

Isothermal Conditions Maintained by Cooling Jacket

High Enzyme Costs

High Agitation Costs

Relevant Equations

$$\text{Total Reactor volume: } V_r = \frac{m'_1 t_B}{\rho'}$$

V_r = Volume of Reactor

t_B = Batch Time

ρ' = Density of Batch

$$\text{Batch Time: } t_B = t'_F + t'_H + t_R + t'_C + t'_E$$

t'_F = Filling Time

t'_H = Heating Time

t_R = Reaction Time

t'_C = Cooling Time

t'_E = Emptying/Cleaning Time

Aspergillus niger

❖ Organisms evaluated for the production of Citric Acid:

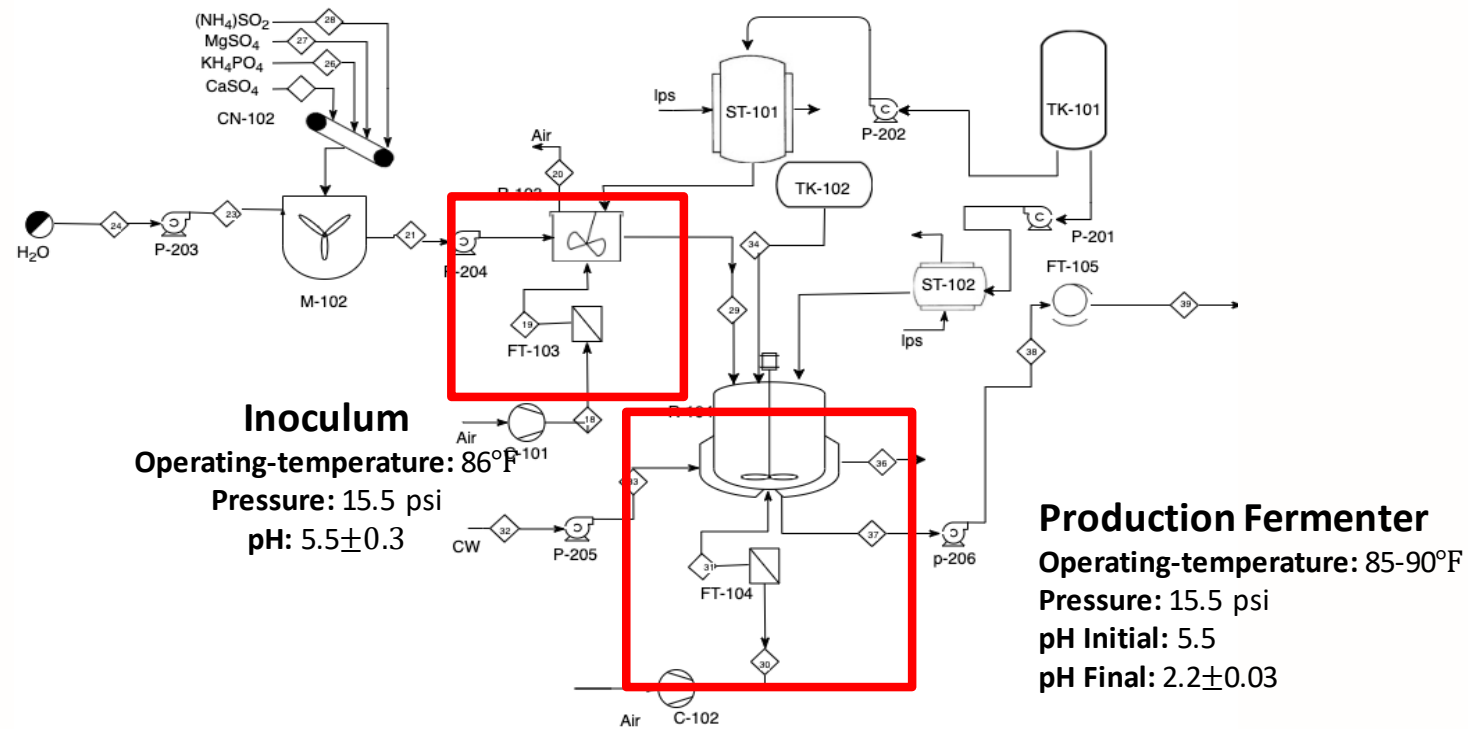
Bacteria	Bacillus licheniformis, B. subtilis, Corynebacterium spp
Fungi	<i>Aspergillus niger</i> , A. awamori, Penicillium restrictum
Yeast	Candida lipolytica, Sacchromyces cerevisiae

Organism of choice: *Aspergillus niger*

1. Ease of handling
2. Ability to ferment a variety of cheap raw materials
3. High yields of citric acid
4. Most commonly used species for fermentation processes

Fermentation

Purpose: Grow *Aspergillus niger* in the inoculum, which will convert glucose to Citric acid



TK-101	P-201	P-202	ST-101	ST-102	CN-102	R-103	FT-103	FT-104	C-101	R-103	R-104	P-205	TK-102	C-102
Glucose Slurry Storage Tank	Pump to Inoculum Sterilizer	Pump to production fermenter Sterilizer	Inoculum Fermenter Feed Sterilizer	Production Fermenter Feed Sterilizer	Nutrient Conveyor	Inoculum Fermenter	Inoculum Air Filter	Production Fermenter Air Filter	Air Compressor	Inoculum tank	Production Fermenter	Cooling Water Pump	Anti-Freeze Storage Tank	Air Compressor

Inoculum Fermenter			
Identification:	Item:	Seed Fermenter	
	Item No:	T-401	
	No. Required:	60	
Function: To grow <i>Aspergillus niger</i> to desired concentration			
Operation: Batch			
Materials Handled	Feed (lb/hr)	Off Gas (lb/hr)	Product Stream (lb/hr)
Glucose Slurry	31,150	0	31,150
Glucose	4050	0	4,050
Water	243,500	0	27,000
Citric Acid	0	0	0
Aspergillus Niger	0.5	0	500
Ammonium Sulfate	1250	0	1,130
Magnesium Sulfate	80	0	70
Potassium Phosphate	32	0	30
Calcium Sulfate	940	0	840
Carbon Dioxide	0	1,400	0
Air	7,600	6,000	0
Operating Conditions:			
Temperature (°F): 86			
Pressure (psia): 15.5			
pH: 5.5			

Purpose of Inoculum

Grow *Aspergillus niger* (fungus that goes through Citric acid cycle to produce Citric acid) to the desired concentration (10% of Final Production Fermenter Volume).

Summary

Operation: Batch (20 hrs/batch)

No. Required: 60

Sparged with Air

Isothermal Conditions Maintained by Cooling Jacket

Production Fermenter				
Identification:	Item:	Jacketed Stirred Tank Bioreactor		
	Item No:	R-401		
	No. Required:	71		
Function: To mix glucose slurry feed and contents of inoculum, producing Citric acid				
Operation: Batch				
Materials Handled	Feed (lb/hr)	Inoculum Feed (lb/hr)	Off Gas (lb/hr)	Product Stream (lb/hr)
Glucose Slurry	280,000	31,150	0	0
Glucose	36,500	4,050	0	200
Water	243,500	27,000	0	294,000
Citric Acid	0	0	0	26,500
Aspergillus Niger	0	500	0	5,000
Ammonium Sulfate	0	1,130	0	0
Magnesium Sulfate	0	70	0	0
Potassium Phosphate	0	30	0	0
Calcium Sulfate	0	840	0	0
Carbon Dioxide	0	0	14,000	0
Air	76,000	0	60,000	0
Sulfate	0	0	0	1,180
Phosphate	0	0	0	15
H+	0	0	0	70
Operating Conditions:				
Temperature (°F): 85 - 90				
Pressure (psia): 15.5				
pH (Initial): 5.5				
pH (Final): 2.2				

Summary

Operation: Batch (192 hrs/batch)

Volume: 20,000 ft³

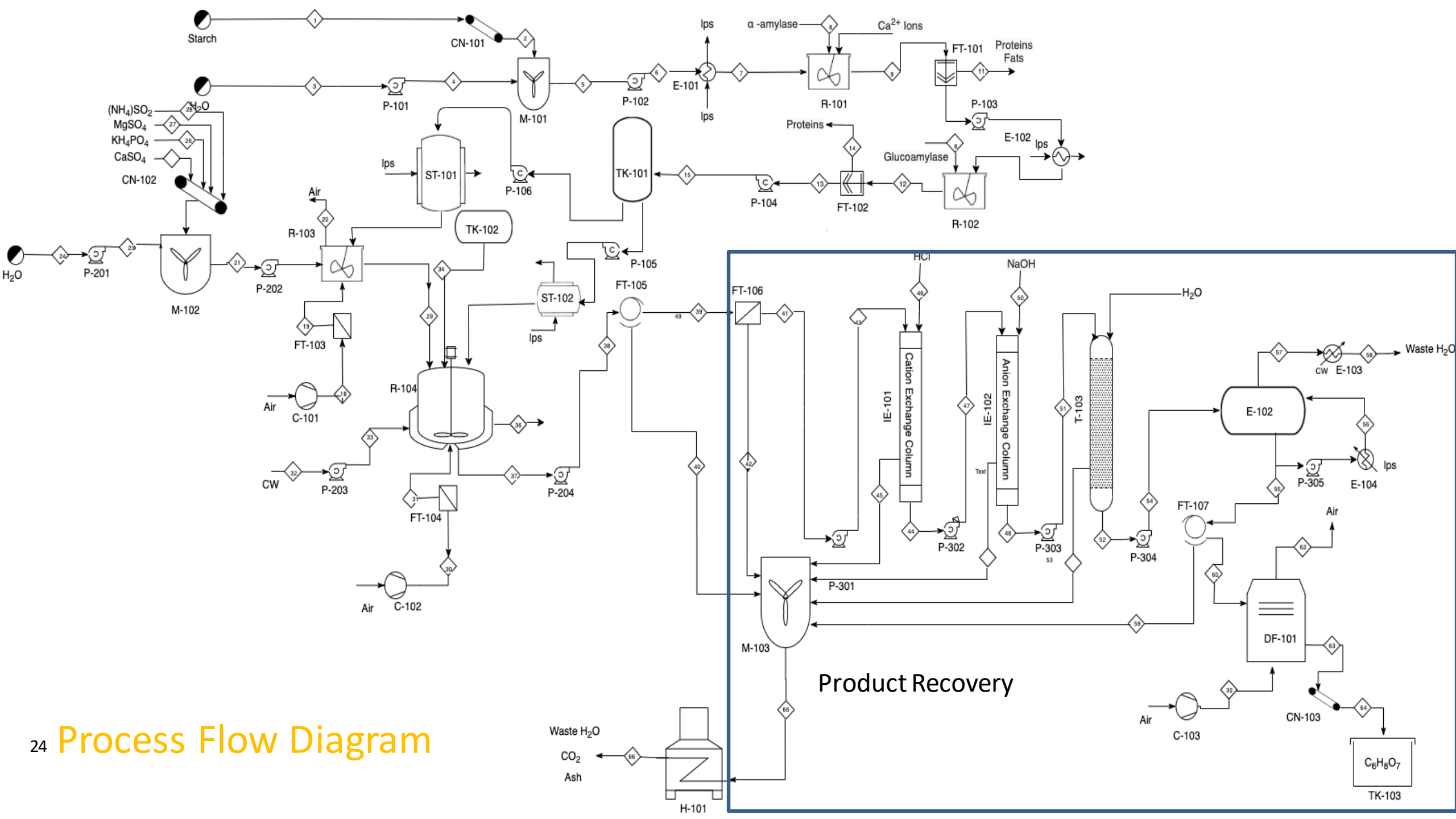
No. Required: 71

Exothermic Reaction

Isothermal Conditions Maintained by Cooling Jacket

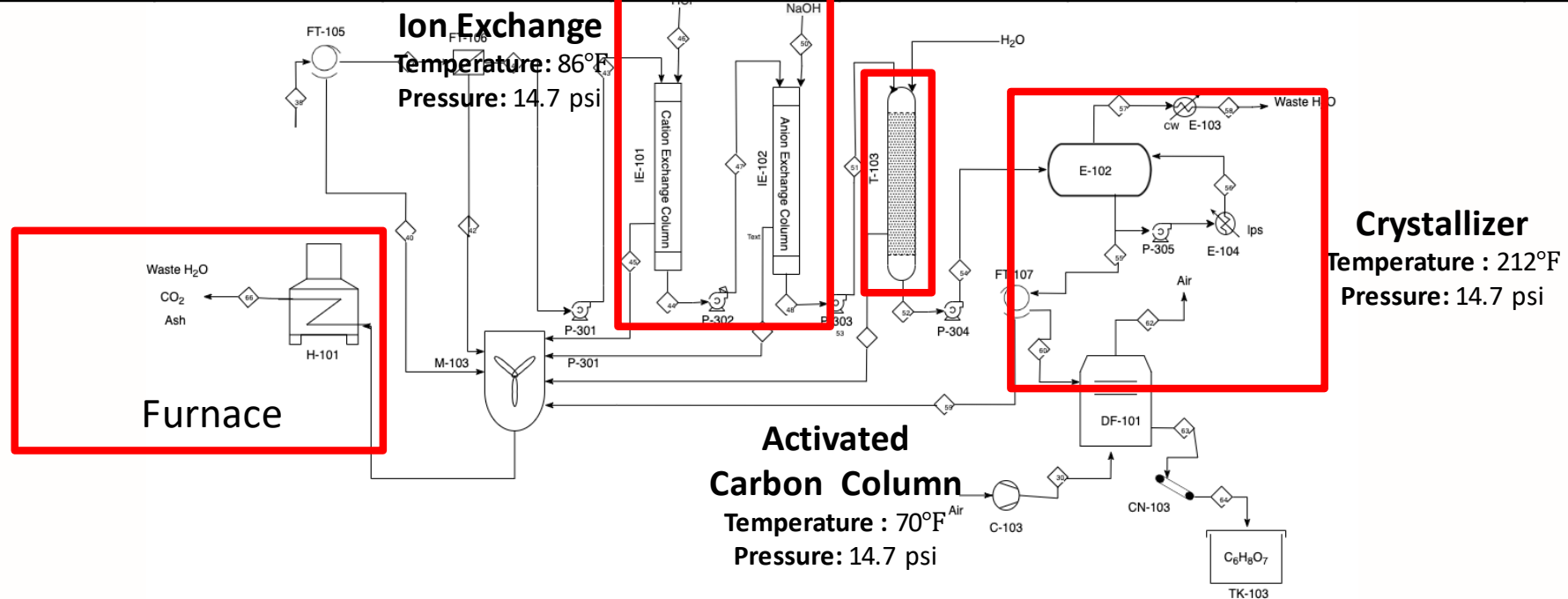
High Agitation Costs (\$14.8M/yr)

High Cooling Water Costs (\$12.7M/yr)



Downstream Processing—Product Recovery/Purification

FT-105	FT-106	P-301	IE-101	P-302	IE-102	P-303	T-103	P-304
Rotary Vacuum Filter	Ultrafiltration Unit	Citric Acid Slurry Pump-2	Cation Exchanger Column	Cation Exchanger Filtrate Pump	Anion Exchanger Column	Anion Exchanger Filtrate Pump	Activated Carbon Packed Bed Column	Decolorized Product Pump



E-102	P-305	E-104	E-103	FT-107	DF-101	C-103	CN-103	TK-103
Crystallizer	Crystallization Cycle Pump	Citric Acid Heater	Partial Condenser	Citric Acid Anhydrous Pump	Fluidized Air Dryer	Air Compressor	Citric Acid Anhydrous Conveyer	Citric Acid Anhydrous Storage Tank

Ion Exchange Column- Design

Cation Exchange Column					
Identification:	Item:	Resin based Ion Exchange Column			
	Item No:	E-101			
	No. Required:	3			
Function: Cation exchange column uses a negatively charged ion resin to remove cations like Na^+ , K^+ , and Mg^{2+} etc in order to obtain a product with higher purity.					
Operation: Continuous					
Materials Handled:	Citric Acid Monohydrate	Water	Glucose	Resin (CG8-C by ResinTech)	Cations to be removed (Na^+ , K^+ , Ca^{2+} , Mg^{2+} etc)
Total Flow (lb/hr):	29,000	280,000	200		Trace amounts
Volumetric Flow (ft ³ /min):	275	4,500	2	4 bed volume (1080 ft ³ of resin)	Hydrogen Ion (H^+) = 68.5 lb/hr
Temperature (°F): 86					
Pressure (psi): 14.7					
Design Data					
Residence Time (hr):	2.5	Material:		Rubber-lined Carbon Steel	
Height (ft): *Not including Resin Bed	17.25	Pressure (psi):		14.7	
Diameter (ft):	11.5	Regenerant:		HCl	
H/D	3/2	Regenerant needed:		2.5 lb/ ft ³ of resin = 2700 ft ³	
Total Volume (ft ³):	1,800	Backwash Flowrate (ft ³ /h):		30 - 80	

Anion Exchange Column					
Identification:	Item:	Resin based Ion Exchange Column			
	Item No:	E-102			
	No. Required:	3			
Function: Anion exchange column uses a positively charged ion exchange resin like Cl^- and OH^- etc in order to obtain a product with higher purity.					
Operation: Continuous					
Materials Handled:	Citric Acid Monohydrate	Water	Glucose	Resin (CG8-C by ResinTech)	Cations to be removed (Na^+ , K^+ , Ca^{2+} , Mg^{2+} etc)
Total Flow (lb/hr):	29,000	280,000	200		Trace amounts
Volumetric Flow (ft ³ /min):	275	4,500	2	3 bed volume (810 ft ³ of resin)	Sulfate (SO_4^{2-}) = 1180 lb/hr Phosphate (PO_4^{2-}) = 13.5 lb/hr
Temperature (°F): 86					
Pressure (psi): 14.7					
Design Data					
Residence Time (hr):	2.5	Material:		Rubber-lined Carbon Steel	
Height (ft):	17.25	Pressure (psi):		14.7	
Diameter (ft):	11.5	Regenerant:		NaOH	
H/D	3/2	Regenerant needed:		2.5 lb/ ft ³ of resin = 2025 ft ³	
Total Volume (ft ³):	1,800	Backwash Flowrate (ft ³ /h):		10 - 30	

Utilities					
Pump specification:	q (flow, ft ³ /h)	ρ - <u>density of</u> fluid (lb/ft ³)	g - gravity (ft/s ²)	h - differential head (ft)	η - pump efficiency
	4,800	104	62.3	17.25	0.6
Hydraulic Power (hp)	4.3		Shaft Power (hp)	7.1	

Relevant Design Equations

$$\text{Hydraulic Power (P)} = \frac{Q \times H \times \rho}{367 \times \eta}$$

P = Power

Q = Flow rate

H=Total developed head

ρ = Density in kg/dm³

η = Efficiency between 0 and <1 (not in %)

$$\text{Shaft Power} = \frac{\text{Hydraulic Power}}{\text{Efficiency}}$$

Activated Carbon Column- Design

Identification :	Materials Handled	Citric Acid Monohydrate, Water	
	Item no	T-103	
	No required	3	
Function:	Remove color from citric acid monohydrate		
Operation:	Batch		
Materials Handles:	Citric Acid Monohydrate	Water	
Flow (lb/hr)	28,000	282,300	
Design Data :		Adsorbent Data:	
Batch Time (hour(s))	2	Amount of AC per column (ft^3)	3500
Height (ft)	30	Void fraction	0.6
Diameter (ft)	15		
Height to Diameter ratio	2		
Material	Alloy Steel		
Bulk Volume (ft ³)	5,300		
Operating Temperature(F)	70		
Working Pressure(psia)	14.7		
Residence Time (hour)	0.5		

Relevant Equations

Empty Bed Contact Time (EBCT) = $\frac{V_B}{Q}$; where V_B is volume of carbon bed and Q is flowrate of input stream.

Column Bulk Volume = $\pi r^2 h$

Crystallizer – Unit Description

A solid separations unit in which mass transfer occurs from liquid to solid phase in the form of pure crystals. Crystallization acts as both a separation and purification step.



Industrial Crystallizer Unit



Molecules undergoing crystallization

Crystallizer Design

Crystallizer		
Identification:	Item:	Forced Circulation Crystallizer
	Item No:	E-102
	No. Required:	1
Function: To achieve solid separation of citric acid from slurry by means of crystal growth		
Operation: Continuous or Batch		
Materials Handled:	Citric Acid (lb/hr)	Water (lb/hr)
Total Flow (lb/hr):	26,000	283,000
Entering Temperature (°F)	68	68
Operating Temperature (°F):	212	
Operating Pressure (psia):	14.7	

Assumptions

- Heat Transfer Coefficient: 300 Btu/hr ft² °F
- Max Temperature Increase through the heat exchanger: $\Delta 144$ °F
- 84% wt/wt solubility of Citric acid in water at 212 °F
- Mother liquor is well mixed
- Inlet feed is at ambient temperature and pressure

Key Parameters	
Steam Temperature (°F):	250
Specific Volume (ft ³ /lbs):	0.016
Heat of Vaporization (Btu/lbs):	970
Crystal Production (lbs/h):	25,100
Heat Transfer Coefficient (Btu/h*ft ² *°F)	300
Heating Surface (ft ²):	2,100
Circulation Rate (ft ² /h):	4,000,000
Temp Rise (°F):	144
Tube Velocity (ft/s):	51
Steam Flow: (lbs/hr):	329,000
Slurry Density (ft ³)	64.7

Crystallizer Design Data:		Crystallizer Mechanical Design:	
Batch Time (hr):	3	Crystallizer Type:	Forced Circulation
Height (ft):	28	Material:	Stainless Steel
Diameter (ft):	14		
Height to Diameter Ratio:	2		
Total Volume (ft ³):	5,750		
Operating temperature (°F):	212		
Liquid Temperature (°F):	68		
Evaporation (lb/hr):	279,500		
Crystal Production (lb/hr):	26,000		
Feed (lb/hr):	311,000		
Purge: (lb/hr):	200		
Circulation Rate (ft ² /h):	39,000		
Temp Rise (°F):	144		
Operating Pressure (psia):	14.7		
Heat Exchanger Data:		Condenser Data:	
Heat of Vaporization (Btu/lb)	212	Area (ft ²):	2,200
Steam Temperature (°F)	250	Diameter (ft):	53
Heat Transfer Coefficient (Btu/h*ft ² *°F)	300	Water Flow ft ³ /hr:	915,000
Heating Surface (ft ²):	2,800		
Tube Velocity (ft/s):	7,500		
Number of tubes	184		
Pump Data		Utility: Pump power	
Flowrate (lb/hr):		Power (Hp):	5
Inlet pressure (psig):	14.7		
Outlet Pressure (psig):	45		
Efficiency:	0.7		
Power Required (hp):	0.78		
Total Head (ft):	35		

Relevant Equations

Heat Energy from slurry: $Q = mC_p\Delta T$

Q = Energy required to change slurry temperature

M = Mass of slurry

C_p = Specific heat of slurry

ΔT = Change in temperature

Heat Transfer Area Required: $A = Q/U \cdot \text{LMTD}$

A = Surface area required for heat transfer

Q = amount of heat energy required

U = Heat transfer coefficient

LMTD = log mean temperature difference

Crystallizer volume: $\frac{1}{3}\pi r^2 h + \pi r^2 h$

r = radius of crystallizer body

h = height of crystallizer body

Economic Analysis



Classification of Cost Estimates

Class	Type of Estimate	Description	Accuracy Ranges
5	Order-of-magnitude estimate (also Ratio/Feasibility)	Based on limited information. Concept screening.	Low: -20% to -50% High: +30% to +100%
4	Study estimate (also Major Equipment/Factored)	List of major equipment. Project screening, feasibility assessment, concept evaluation, and preliminary budget approval.	Low: -15% to -30% High: +20% to +50%
3	Preliminary design estimate (also Scope)	More detailed sizing of equipment. Budget authorization, appropriation, and/or funding.	Low: -10% to -20% High: +10% to +30%
2	Definitive estimate (also Project Control)	Preliminary specification of all the equipment, utilities, instrumentation, electrical and off-sites. Control or Bid/Tender.	Low: -5% to -15% High: +5% to +20%
1	Detailed estimate (also Firm/Contractor's)	Complete engineering of process and related off-sites and utilities required. Check Estimate or Bid/Tender.	Low: -3% to -10% High: +3% to +15%

Step 1: Plant Direct Cost

Direct Costs:

1. Purchased equipment: Columns, Heat Exchangers, pumps, tanks, etc.
2. Equipment Installation
3. Piping (includes insulation)
4. Instruments and Control
5. Electrical Equipment.
6. Buildings: Process, Administration, Maintenance shops, etc.
7. Auxiliary Services : steam, water, etc.

Step 1: Plant Direct Cost

Direct Costs:

1. Purchased equipment: Columns, Heat Exangers, pumps, tanks, etc.
2. Equipment Installation
3. Piping (includes insulation)
4. Instruments and Control
5. Electrical Equipment.
6. Buildings: Process, Administration, Maintenance shops, etc.
7. Auxiliary Services : steam, water, etc.

Purchased Equipment for Citric Acid Plant					
Unit	Description	Cost Exponent Factor, n^*	No. of Units Requires	Cost Estimate for Desired Volume (\$)	Total Cost of Equipment (\$)
T-103	Activated Carbon Column	0.63	3	1,500,000	4,400,000
R-101	Starch Hydrolyzer 1	0.6	66	17,000	1,100,000
R-102	Starch Hydrolyzer 2	0.6	38	116,000	4,430,000
FT-103	Inoculum Air Filter	0.58	58	1,350,000	78,400,000
ST-101	Inoculum Feed Sterilizer	0.68	1	1,300,000	1,300,000
ST-102	Fermenter Feed Sterilizer	0.68	1	3,320,000	3,320,000
FT-104	Fermenter Air Filter	0.58	71	9,000	600,000
R-104	Production Fermenter	0.74	71	1,900,000	134,000,000
FT-106	Ultrafiltration Unit	0.58	3	340,000	1,000,000
IE-101	Cation Exchange Column	0.65**	3	810,000	2,430,000
IE-102	Anion Exchange Column	0.65**	3	810,000	2,430,000
E-102	Crystallizer	0.70	1	780,000	780,000
DF-101	Fluidized Air Dryer	0.71	4	220,000	880,000
Total Equipment Cost					\$ 236,000,000

Cost-Estimating Relationship

Uses design variables to estimate cost. (Effect of size variation)

- **Cost-capacity equation:**

$$C_2 = C_1 \left(\frac{Q_2}{Q_1} \right)^x$$

- C_1 = cost at capacity Q_1
- C_2 = cost at capacity Q_2
- x = correlating exponent



Table 6-9 Ratio factors for estimating capital investment items based on delivered-equipment cost

Values presented are applicable for major process plant additions to an existing site where the necessary land is available through purchase or present ownership.[†] The values are based on fixed-capital investments ranging from under \$1 million to over \$100 million.

	Percent of delivered-equipment cost for		
	Solid processing plant [†]	Solid-fluid processing plant [†]	Fluid processing plant [†]
Direct costs			
Purchased equipment delivered (including fabricated equipment, process machinery, pumps, and compressors)	100	100	100
Purchased-equipment installation	45	39	47
Instrumentation and controls (installed)	18	26	36
Piping (installed)	16	31	68
Electrical systems (installed)	10	10	11
Buildings (including services)	25	29	18
Yard improvements	15	12	10
Service facilities (installed)	40	55	70
Total direct plant cost	269	302	360
Indirect costs			
Engineering and supervision	33	32	33
Construction expenses	39	34	41
Legal expenses	4	4	4
Contractor's fee	17	19	22
Contingency	35	37	44
Total indirect plant cost	128	126	144
Fixed-capital investment	397	428	504
Working capital (15% of total capital investment)	70	75	89
Total capital investment	467	503	593

Step 1: Plant Direct Cost

Direct Plant Cost for Production of Citric Acid		
Direct Costs	Ratio Factor, (Percent of delivered-equipment cost) **	Capital Cost (\$)
Purchased Equipment Delivered	100	236,000,000
Purchased Equipment Installation	45	106,000,000
Instrumentation and Controls*	18	43,000,000
Piping*	16	38,000,000
Electrical Systems*	10	24,000,000
Buildings	25	59,000,000
Site Developments	5	12,000,000
Auxiliary Services	20	47,000,000
Total Plant Direct Cost (PDC)		564,000,000

*Installation included

** From Turton et al., 2009

Step 2: Plant Indirect Cost

Indirect Costs:

1. Engineering and Supervision:
Administrative and Design. Supervision and Inspection.
2. Construction Expenses

Indirect Plant Cost for Production of Citric Acid		
Indirect Costs	Ratio Factor, (Percent of delivered-equipment cost) **	Capital Cost (\$)
Engineering and Supervision	33	78,000,000
Construction Expenses	39	92,000,000
Legal Expenses	4	9,000,000
Total		180,000,000

** From Turton et al., 2009

Step 3: Total Capital Investment

- Total capital investment required is comprised of the purchased equipment cost, plant direct capital costs, indirect capital costs, contractors fees and contingency, and finally start up costs

Summary of Total Capital Investment for Citric Acid Plant	
	Capital Cost (\$)
Plant Direct Cost (PDC)	564,000,000
Plant Indirect Cost (PIC)	180,000,000
Total Plant Cost (TPC = PDC + PIC)	745,000,000
Contractors Fees and Contingency (CFC)	20,000,000
Direct Fixed Capital Cost (DFC = TPC + CFC)	637,000,000
Plant Start Up Cost	38,000,000
Total Capital Investment	802,000,000

Step 3: Total Operating cost

Total Operating Costs:

1. Raw
2. Labor
3. Disposal
4. Waste Treatment
5. Utilities

Step 3: Total Operating cost

Table 3.1

Raw Material	Major Raw Material Input Cost		
	Unit Cost (\$/lb)	Consumption (lb/ year)	Cost
α - Amylase	8.62	160,000	\$1,380,000
Glucoamylase	22	120,000	\$2,700,000
Ammonium Nitrate	0.33	530,000	\$1745,000
Hydrogen Chloride	0.33	112,500	\$37,000
Nitrogen	0	48,000,000	\$0
Oxygen	0	13,000,000	\$0
Potassium Phosphate	0.75	248,000	\$186,000
Sodium Hydroxide	0.35	84,375	\$30,000
Starch	0.11	292,000,000	\$32,000,000
Water	0.001	325,000,000	\$325,000
<i>Aspergillus Niger</i>	2.3	Negligible	Negligible
Total			\$40,000,000

Table 3.2

Labor Demand and Cost				
Demand (Days)	Operators Needed per Shift	Number of Shifts	Labor Rate (\$/hr)	Cost (\$/year)
334	15	2 (12 hrs)	33	7,940,000

Step 3: Total Operating cost

Table 3.3

Waste Treatment Demand and Cost for Citric Acid Production			
Waste Material	Disposal Cost (\$/lb)	Disposal (lb/ year)	Cost (\$/year)
α - Amylase	0.02	160000	3,200
Biomass	0.02	4000000	80,000
Carbon Dioxide	0	115,000,000	0
Citric Acid loss	0.001	4,740,000	4,700
Glucoamylase	0.02	120,000	2,400
Potassium (dissolved)	0.001	120,000	100
Sodium (dissolved)	0.001	250,000	250
Water	0.02	251,000	3,200
Total			97,000

Table 3.4

Waste Treatment Demand and Cost for Citric Acid Production			
Utilities	Cost per Unit (\$/Unit)	Consumption (Units/year)	Cost (\$/year)
Electricity (kWh)	0.07	8,210,000,000	575,000,000
Cooling Water (ft ³)	0.006	2,200,000,000	13,000,000
Total			600,000,000

Step 3: Total Operating cost

Annual Operating costs for citric acid production	
Operating Costs Type	Cost (\$)
Raw Materials	40,000,000
Labor	7,940,000
Waste Treatment	97,000
Utilities	600,000,000
Miscellaneous (Laboratory, Plant Tax, Insurance)	6,000,000
Total Operating Cost (OC)	654,000,000

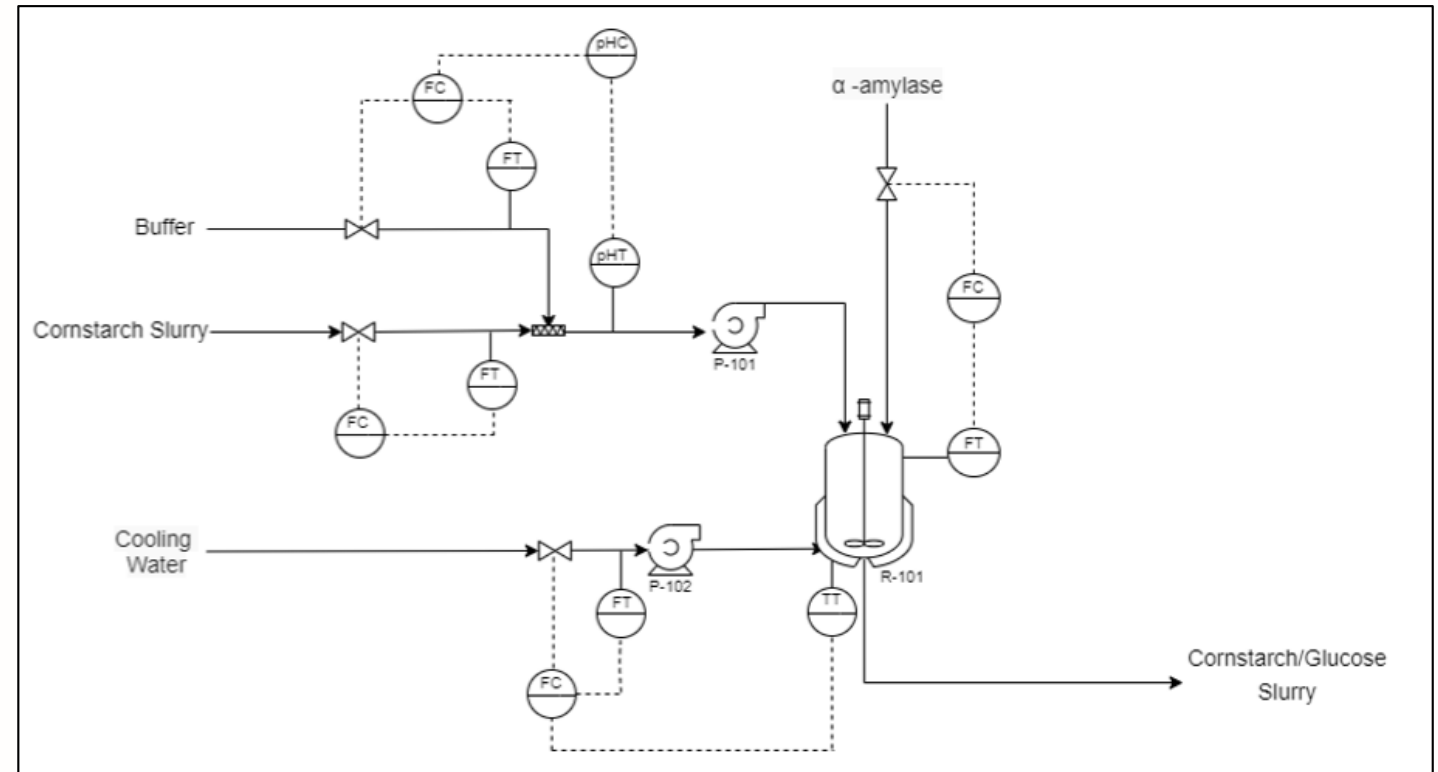
Profitability Analysis

Profitability Analysis		
Operating Costs Type	Units	Cost (\$/year)
Revenue	\$/yr	220,000,000
Operating Cost	\$/yr	654,000,000
Gross Profit	\$/yr	-434,000,000
Payback Period	Years	7

Profitability measures including time value of money, with CONTINUOUS cash flows and discounting					
29. Net present worth, 10 ⁶ \$	=	-420.07			

HAZOP Factors to Consider

Incoming Flow Rate
Temperature
Enzyme Amount
Agitation
pH
Fluid Level



HAZOP Analysis on Hydrolyzer I

Property word or Keyword	Guideword	Cause	Consequence	Action
Flow of Cornstarch Slurry	More	1. Flow controller fault	Sufficient amount of conversion will not be achieved Damage to the agitator Temperature increase	Install an independent high flow alarm and perform maintenance on a regular basis
	No	1. Product feed pump failed. 2. Isolating valve jammed	No reaction will occur as there is no raw material	Perform maintenance on a regular basis
	Less	1. Product feed pump failed. 2. Isolating valve jammed	conversion will occur at the highest possible rate but it will not be economically efficient	Install an independent low flow alarm and perform maintenance on a regular basis
Amount of alpha amylase	More	1. Additional enzyme is added to the tank	Reaction will occur at the highest possible rate but it will not be economically efficient	Ensure correct amount is added before each liquefaction cycle begins
	None present	1. Enzyme was not added or it was not activated	Reaction will not proceed without the enzyme at the conditions determined for the tank	Ensure correct amount is added before each liquefaction cycle begins
	Less	1. Inactivation of enzyme if tank conditions are not optimal	Reaction will occur at a much slower rate	Ensure correct amount is added before each liquefaction cycle begins
Temperature of Reactor	High	1. Enzyme (α amylase) may be masked, poisoned, or fouled 2. Faulty Control valve	Overheating of enzyme in the liquefaction tank	Perform maintenance on a regular basis and perform regular tests to

	3. Temperature of the cooling water might is not low enough	might cause permanent damage to the enzyme There is also a slight possibility of a runaway reaction occurring	check the accuracy of the control valve Make sure the conditions of the cooling are correct
Low	1. Cooling system may not be operating optimally 2. Ambient temperature around the plant may be very low 3. Faulty control valve	At low temperatures the oligosaccharides will not be broken down into smaller glucose polymer chains	Perform maintenance on a regular basis and perform regular tests to check the accuracy of the control valve Make sure the conditions of the cooling are correct

Pressure of Reactor	High	1. Faulty Control Valve	Possibility of having an explosion increases May also damage enzyme	Perform maintenance on a regular basis
	Low	1. Pressure leak from control valve	Low pressures can affect the rate at which the enzymes can carry out the reaction	Perform maintenance on a regular basis
Level	More	1. Malfunction of flow valve	Overflow, spillage, breakdown the agitator, corrosion	Install a high level indicator
	Less	LIC (liquid indicator controller) in the liquefaction tank fails to open, causing liquid drainage	Can cause corn starch slurry to flow through the bottom exit to the next tank causing hammering	Install a low level trip in the tank to prevent slurry entering

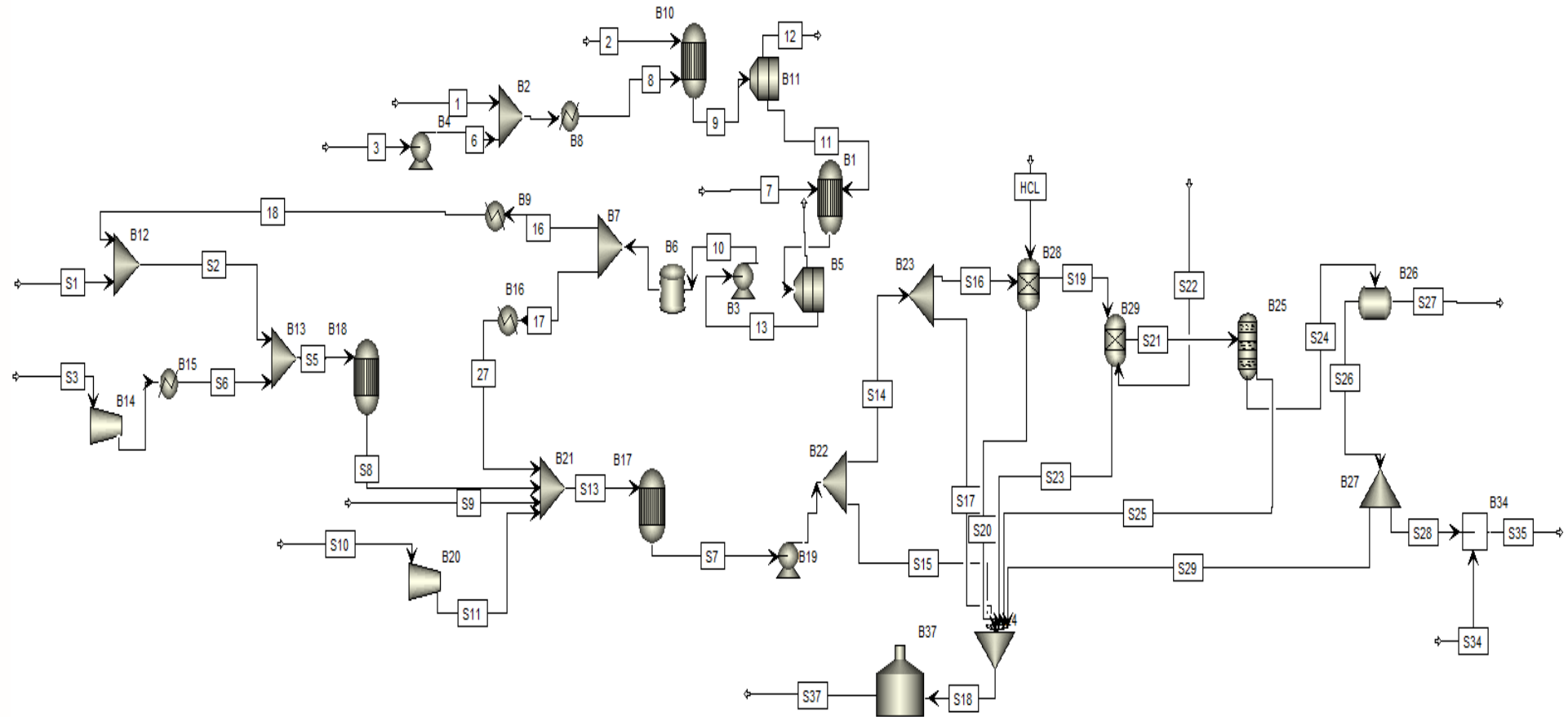
<i>pH</i>	High	1. Too much buffer being added	The reaction will not proceed. Damage to enzyme	Installation of pH meter
	Low	1. Not sufficient amount of buffer	Tank material corrosion, Leakage Damage to enzyme	Monitoring system of corrosion Installation of pH meter
<i>Agitation</i>	No mixing	1. Agitator motor failure 2. Shaft seal failure	Slurry gets thicken inside the reactor	Motor to be checked Proper lubrication of motor
	Slow mixing	1. Corrosion in the impeller 2. Wear or tear on motor 3. Gear reducer, belt or shaft damage	Proper mixing does not takes place	Proper lubrication of motor
	More mixing	1. Gear reducer failure	Impeller runs with high rpm	Proper inspection and maintenance

Biological Safety of Aspergillus Niger

- Relatively safe
- Exposure to intense spore dust may cause hyper-sensitivity (rare)
- Non-pathogenic (colonize the human body as an opportunistic invader)

HANDLING AND STORAGE

- **SPILLS:** Allow aerosols to settle, then, wearing protective clothing, gently cover the spill with absorbent paper towel and apply appropriate disinfectant, starting at the perimeter and working towards the center. Allow sufficient contact time before clean up.
- **DISPOSAL:** Decontaminate all wastes that contain or have come in contact with the organism by autoclave, chemical disinfection, gamma irradiation, or incineration before disposing.
- **STORAGE:** Should be stored in leak-proof containers that are appropriately labeled



- Thermodynamic Analysis:

$$\Delta S_{total} = -\frac{\Delta H}{T} + \Delta S_{system}$$

$$T\Delta S_{total} = -\Delta H + T\Delta S_{system}$$

$$-T\Delta S_{total} = \Delta H - T\Delta S_{system}$$

Production Fermenter		
Mass Enthalpy	(Btu/lb)	-6195
Mass Entropy	(Btu/lb-R)	-2
Temperature	(°R)	200
Total Entropy	(Btu/lb-R)	-29

Hydrolizer I		
Mass Enthalpy	(Btu/lb)	-6820.43
Mass Entropy	(Btu/lb-R)	-2.1629
Temperature	(°R)	77
Total Entropy	(Btu/lb-R)	-86

Hydrolizer II		
Mass Enthalpy	(Btu/lb)	-6195
Mass Entropy	(Btu/lb-R)	-2
Temperature	(°R)	200
Total Entropy	(Btu/lb-R)	-29

```
->Processing input specifications ...

->Finished processing new specifications

->Calculations begin ...

->Simulation calculations completed ...

*** Warning(s) were issued during Input Translation ***
*** Check the Run Status Results for more Information ***

*** Summary of Simulation Errors ***
```

	Physical Property	System	Simulation
Terminal Errors	0	0	0
Severe Errors	0	0	0
Errors	0	0	0
Warnings	1	0	0

Without Crystallizer

The following Unit Operation blocks were completed with errors:

[B1](#)

The following messages were issued during Input Translation:

```
* WARNING WHILE CHECKING INPUT SPECIFICATIONS
  BLOCK NAME: B1    MODEL NAME: CRYSTALLIZER
  REACTION NUMBER '1' DOES NOT SATISFY ATOM BALANCE.
  CHECK STOICHIOMETRY.

* WARNING WHILE CHECKING INPUT SPECIFICATIONS
  BLOCK NAME: B1    MODEL NAME: CRYSTALLIZER
  PHYSICAL PROPERTY PARAMETER DHFORM OR DHAQFM IS MISSING
  FOR THE FOLLOWING COMPONENTS:
    CITRI-02
  ABSENCE OF THIS PARAMETER WILL RESULT IN INCORRECT ENTHALPY RESULTS.
```

With Crystallizer

Plant is not profitable due to:

- High Equipment Costs
- High Utility Costs

Must Consider a multitude of changes to ensure plant will be profitable, including:

- Optimize Mechanical Designs
- Consider Alternative Cooling Options
- Consider Enzyme Encapsulation to Reduce Expenditures
- Recycle Cooling Water
- Downsize Plant

- Dr. Martin
- Dr. Gyamerah
- Dr. Dada
- Dr. Antoine
- Fellow Students
- Department of Chemical Engineering



PRAIRIE VIEW
A&M UNIVERSITY

Supplementary Slides

Comparison of Profitability Analysis

Source: University of Capetown, 2011

	Units	Starch ^a
Revenue	\$/yr	\$22,670,000
Operating Cost	\$/yr	\$26,160,000
Gross Profit	\$/yr	-\$3,493,000
Taxes	\$/yr	0.00
Net Profit	\$/yr	-\$3,493,000
Gross Margin	%	-15.41
Return on Investment	%	-0.03
Payback Period	years	NA (> 50 Years)
NPV	\$	-\$75,648,000
IRR	%	NA (< 0-100%)

^aGeneric flowsheet simulation with Biwer *et al.* (2006) input data

University of
Capetown spent
\$1.05/lb of citric acid
for production

Pvamu spends
\$0.9/lb of citric acid
for production

Ion Exchange Chromatography

- Principle: Reversible exchange of ions between the ions present in the solution and those present in the ion exchange resin

Cation Exchange	Anion Exchange
$S-X-C^+ + M^+ \leftrightarrow S-X-M^+ + C^+$	$S-X+A^- + B^- \leftrightarrow S-X+B^- + A^-$
In this process the cation M^+ of the eluent replaced with the analyte cation C^+ bound to the anion X^- which is fixed on the surface of the chromatographic support (S).	The anion B^- of the eluent replaced with the analyte cation A^- bound to the positively charged ion X^+ on the surface of the stationary phase. Separation occurs by the adsorption of the analyte to the stationary phase



Common Ion exchange resins

Class of resin	Nature	pH range	Application
Strong Cation Exchange resin	Sulfonated polystyrene	1-14	Fractionation of cation, peptides, amino acids & vitamins
Weak Cation Exchange resin	Carboxylic methacrylate	5-14	Biochemical separation, Organic bases, antibiotics
Strong Anion Exchange resin	Quaternary ammonium polystyrene	0-12	Alkaloids, Vitamins, Fatty Acids
Weak Anion Exchange resin	Polyamine polystyrene Or phenol	0-9	Anions of different valency, vitamins, amino acids



Strong Anion Exchange Resin Specification

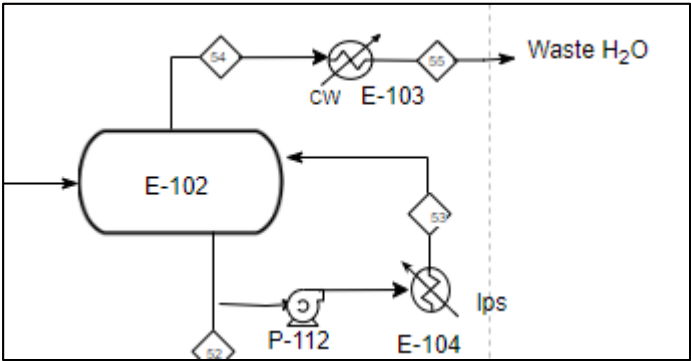
Polymer Structure	Acrylic/DVB
Functional Group	Tertiary Amine
Physical Form	Spherical Beads
Ionic Form (as shipped)	Free Base
Total capacity	> 1.4 meq/mL (Free base Form)
Water Retention	56 to 64 percent (Free base Form)
Approximate Shipping Weight	44 lbs/cu.ft. (Free base Form)
Swelling	10 to 15 percent Free base to Cl
Screen Size Distribution	16 to 50 (U.S. Mesh)
Minimum Sphericity	93 percent
Uniformity Coefficient	1.6 (Approximate)
Resin Color	Off white



Strong Cation Exchange Resin Specification

Polymer Structure	Styrene/DVB
Functional Group	Sulfonic Acid
Physical Form	Spherical Beads
Ionic Form (as shipped)	Sodium
Total capacity	> 2 meq/mL (Na Form)
Water Retention	42 to 49 percent (Na Form)
Approximate Shipping Weight	51 lbs/cu.ft. (Na Form)
Screen Size Distribution	16 to 30 (U.S. Mesh)
Maximum Fines Content	1 percent (less than 50 Mesh)
Minimum Sphericity	93 percent
Uniformity Coefficient	1.4 (Approximate)
Resin Color	Amber





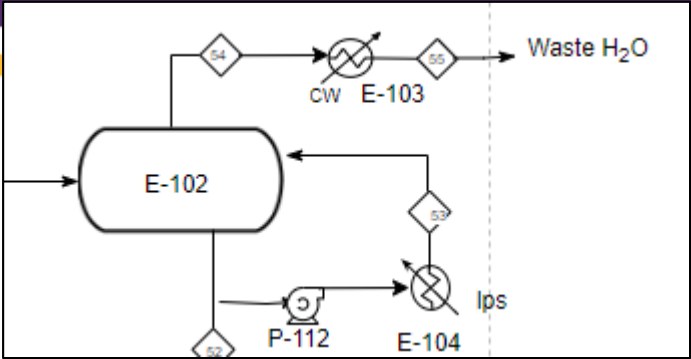
Assumptions

- 99% of Water introduced is Converted to Steam

Type of Heat	
Heat of Evaporation (Btu/hr):	271165310
Sensible Heat (Btu/hr):	44784000
Heat of Crystallization (Btu/hr):	89820096
Total Heat Required from steam (Btu/hr):	-136561214
Steam Flow (lbs/h):	140759

Design Equations:	
Heat Energy from slurry (Btu/hr) ($Q = mCp\Delta T$):	45,000,000
Heat Transfer Area Required (ft ²) ($A = Q/U \cdot \text{LMTD}$):	2,800
Heat in Vapor (Btu/hr) (Evaporation * LHV):	272,000,000
Sensible Heat (Btu/hr) (Feed * $\Delta T \cdot Cp$):	-44,800,000
Heat of crystallization (Btu/hr) (Desired mass * ΔH of formation):	-90,000,000
Steam Flow (lbs/h) (Heat required from steam / LHV):	141,000
Volume Required (ft ³) ((Desired mass * Batch time) / Slurry Density):	1,200
Crystallizer volume (ft ³) (cone volume + cylinder volume):	5,800
Circulation rate through heater (ft ³ /hr) (Total Heat from steam / $\Delta T \cdot Cp \cdot \rho$):	388,000
Number of Tubes (Heat Transfer Area / tube Surface area):	184
Tube velocity (ft/s) (circulation rate / No. of Tubes * crosssectional area of pipe * time elapse):	7,500
Pump Power (hp):	4
Condenser Area required (ft ²):	0.01
Condenser Diameter (ft)	0.1
Condensor Water Flow (gal/min):	9,150,000

Crystallizer - MEB



Assumptions

- 99% of Water introduced is Converted to Steam

Type of Heat	
Heat of Evaporation (Btu/hr):	271165310
Sensible Heat (Btu/hr):	44784000
Heat of Crystallization (Btu/hr):	89820096
Total Heat Required from steam (Btu/hr):	-136561214
Steam Flow (lbs/h):	140759

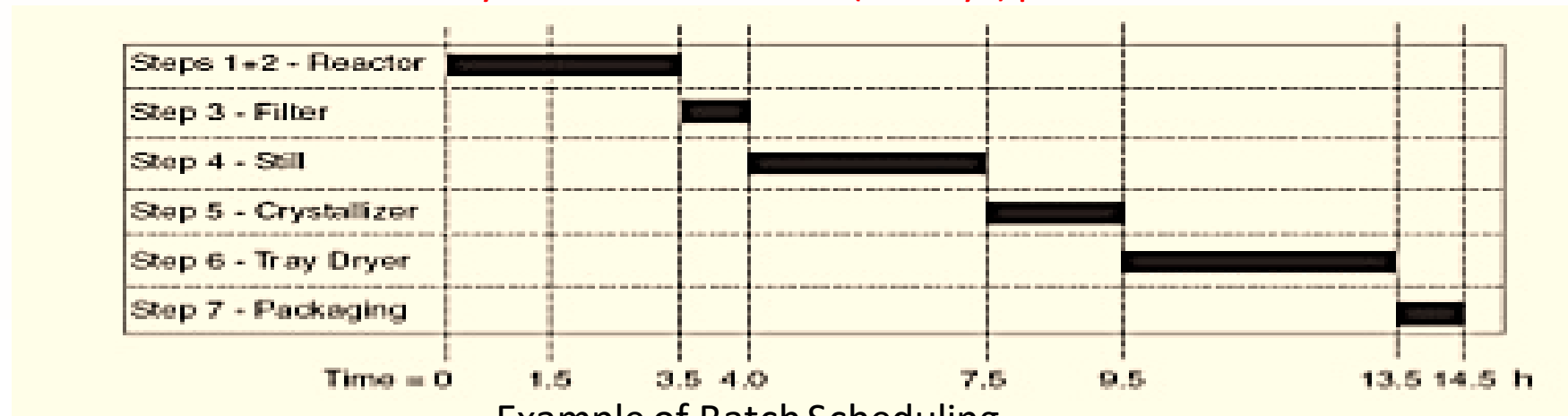
Design Equations:	
Heat Energy from slurry (Btu/hr) ($Q = mC_p\Delta T$):	45,000,000
Heat Transfer Area Required (ft ²) ($A = Q/U\Delta T_{LMTD}$):	2,800
Heat in Vapor (Btu/hr) (Evaporation*LHV):	272,000,000
Sensible Heat (Btu/hr) (Feed* ΔT * C_p):	-44,800,000
Heat of crystallization (Btu/hr) (Desired mass* ΔH of formation):	-90,000,000
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Tube velocity (ft/s) (circulation rate /No. of Tubes*crossectional area of pipe*time elapse):	7,500
Pump Power (hp):	4
Condenser Area required (ft ²):	0.01
Condenser Diameter (ft)	0.1
Condensor Water Flow (gal/min):	9,150,000

Batch Process Timing

Batch Process

Process	Liquefaction	Sacchrification	Inoculum Preparation	Fermentation	Filtration and purification	Crystallization	Drying
Duration	2 hrs	48 to 72 hrs	30 hrs	192 hrs	4 to 6 hrs	48 hrs	5 hrs
Conditions	176 to 194 °F pH 5.5 to 7	130 to 140°F pH 4 – 4.5	85 °F Initial pH 5.5 Final pH 2	85 °F pH 2.2 to 2.6	Cool to Ambient conditions	77°F to 210 °F Then 210 to 60 °F	Ambient conditions pH 1.8

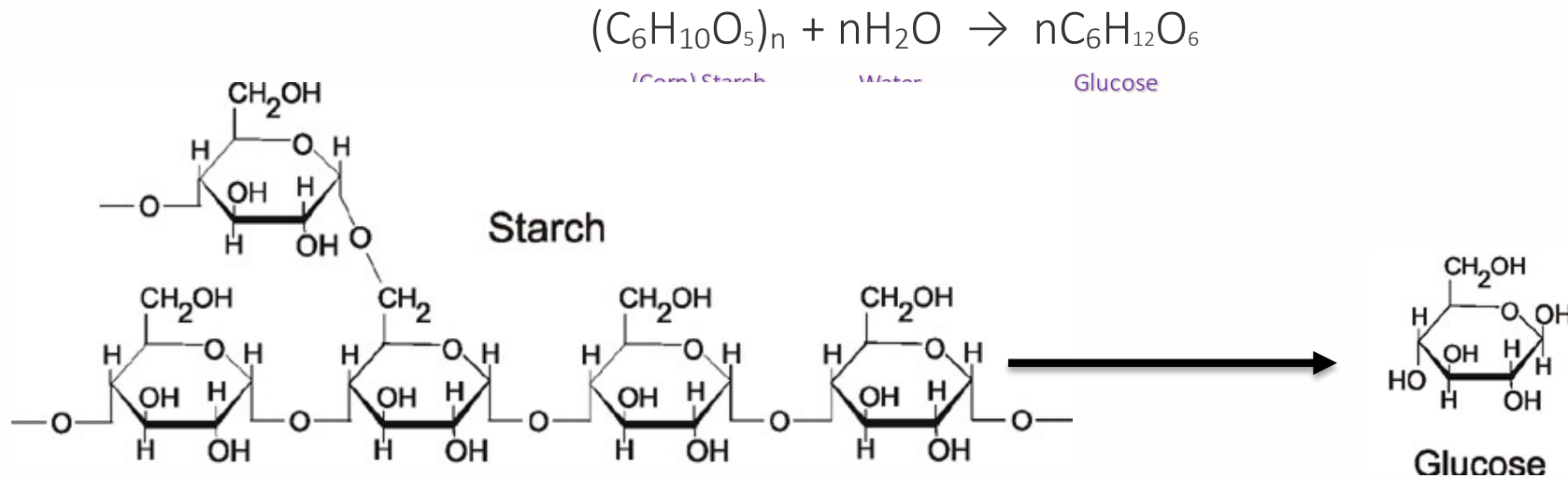
Cycle Time: 342 hours (14 days) per batch



Example of Batch Scheduling

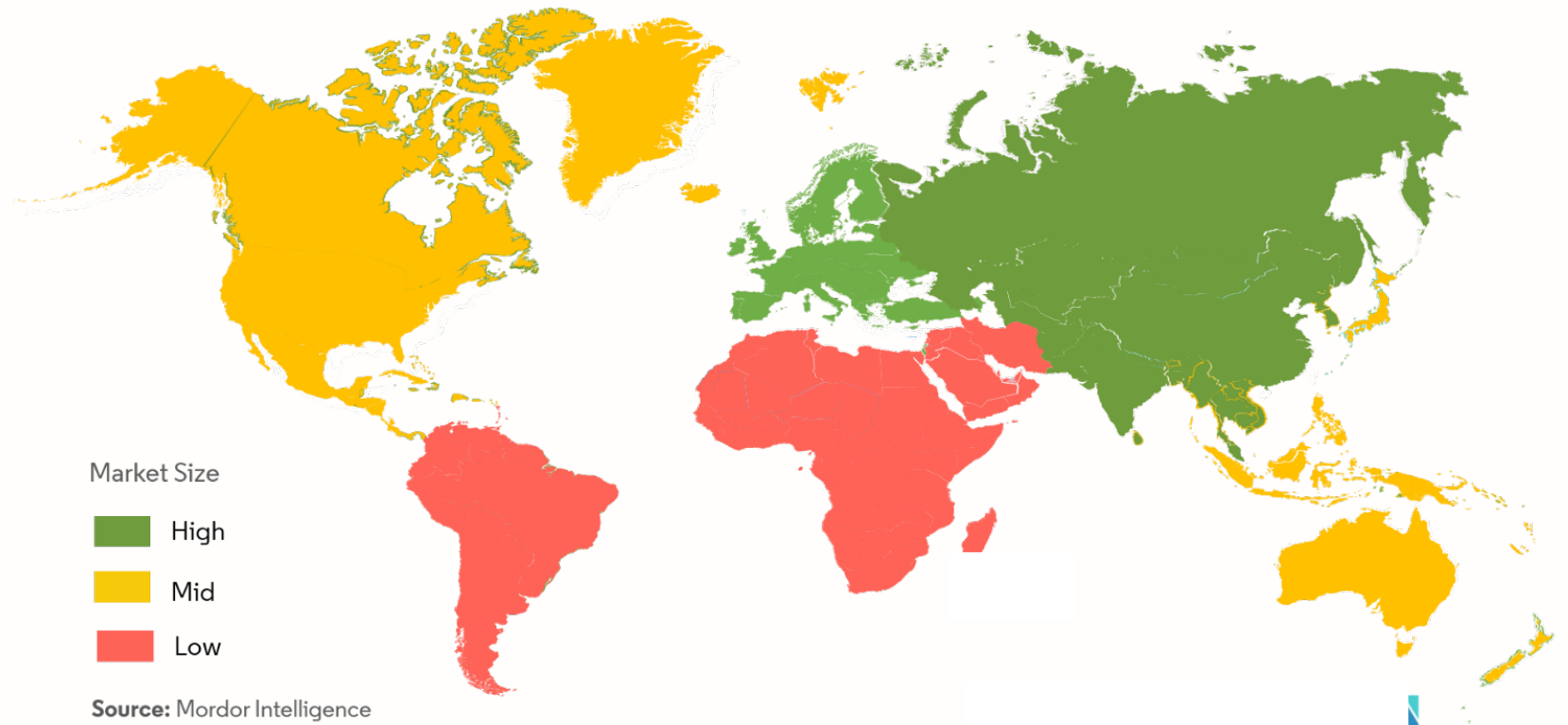
1. Upstream Processing

- Breaking down Starch to Glucose
- Hydrolysis reaction
 - Liquefaction + Saccharification



Market Analysis

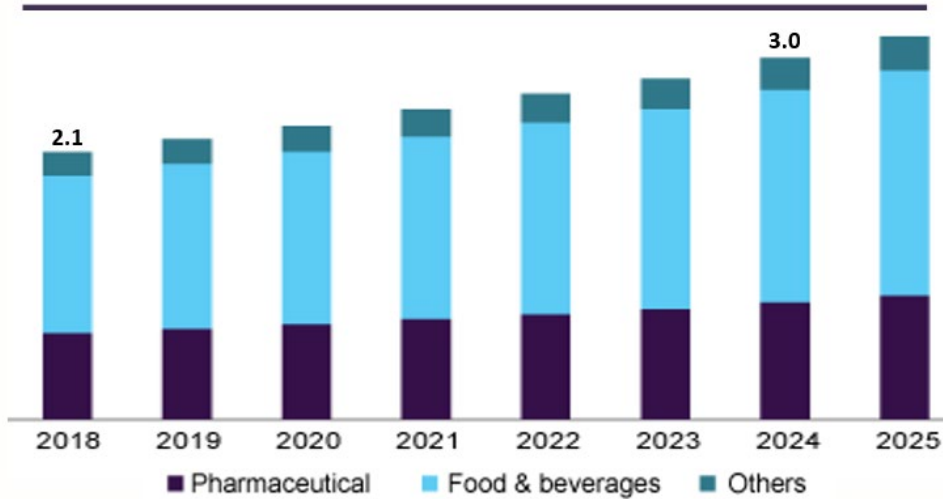
Citric Acid Market - Market Size, by Region, Global, 2018



- Fastest Growing Market: Asia Pacific
- Largest Market: Europe
- **United States is the leading importer of Citric Acid**
- China is the leading exporter of Citric Acid

Market Analysis

Global Citric Acid Market Demand, by Industry 2014 - 2025 (million tons)



Source: Grand View Research

- Gap in demand: 900 kilotons by 2024
- Based on demand and current capacity
 - **Plant Capacity: 100 kilotons per year**
 - Satisfy 11% of demand by 2024

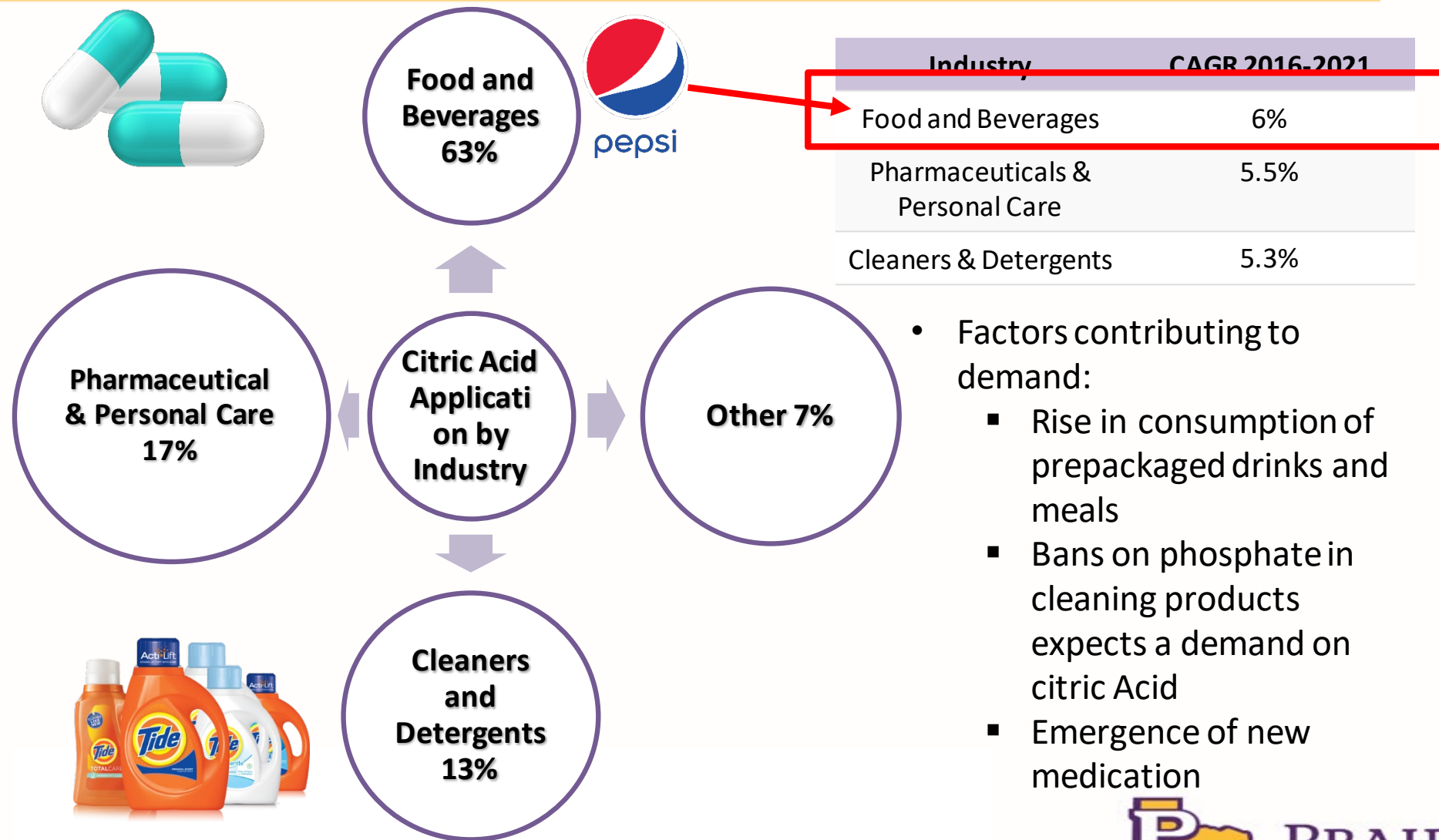
Major Global Citric Acid Producers (Kiloton per year); Plant capacity (100% Anhydrous)

Company	Location	Capacity
Jungbunzlauer	Austria	136
Archer Daniels	United States	98
Midland	Ireland	45
Hoffmann-La Roche	Belgium	73

Average

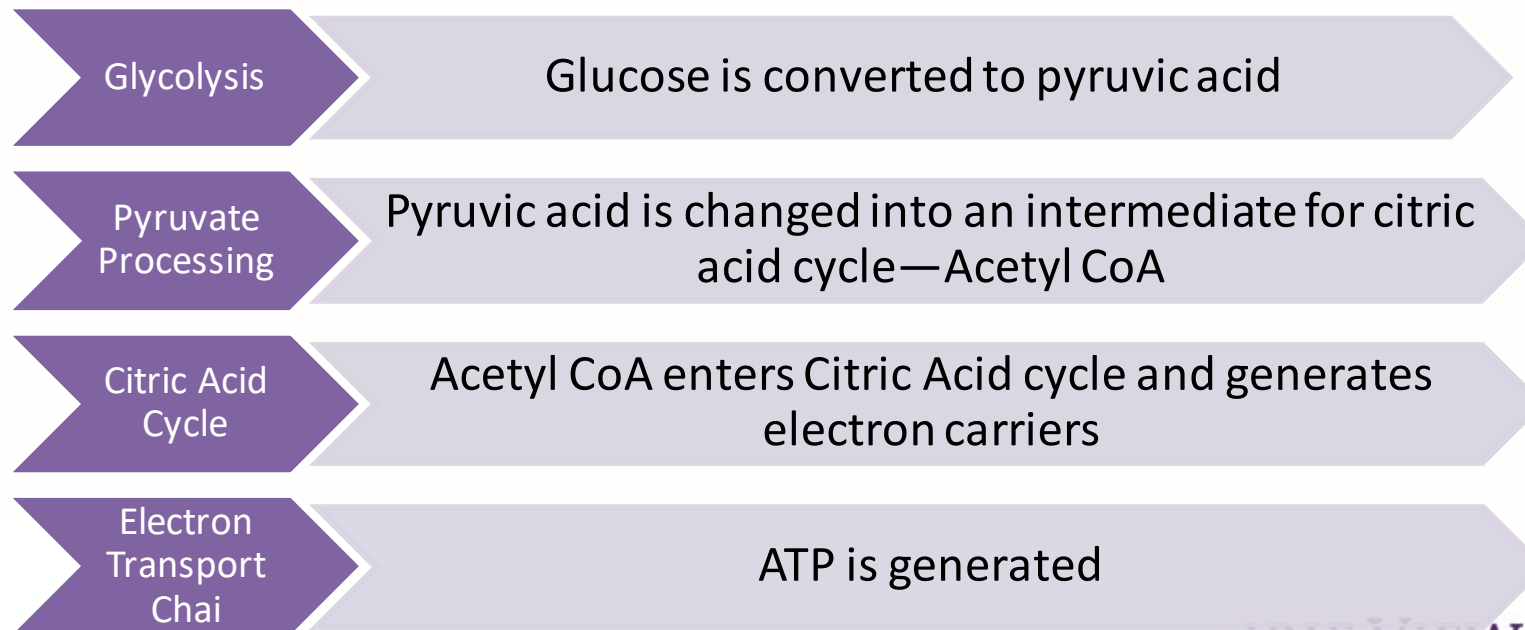
Source: ICIS

Client Identification

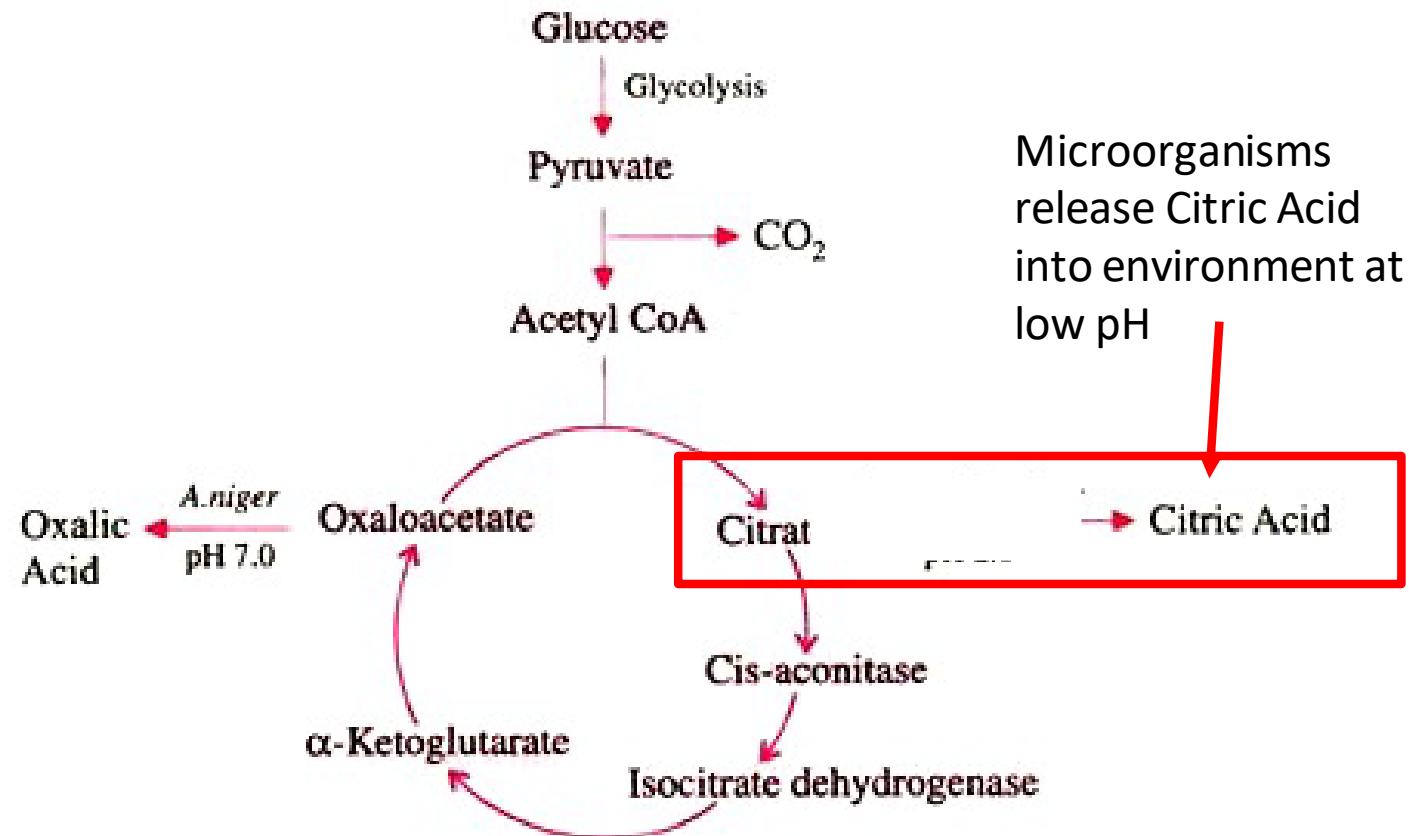


Process Biochemistry

- Aerobic Fermentation: Conversion of carbohydrates such as glucose to CO₂, alcohols, and organic acids using yeast, bacteria or combination of both.
- Living organism need **ATP**
 - **ATP: Energy currency of the cell**
- Main biological pathway to generate ATP is by the means of cellular respiration
 - Consist of 4 stages



Biochemical Pathway for Citric Acid Production



Selection of Microorganisms

❖ Organisms evaluated for the production of Citric Acid:

Bacteria	Bacillus licheniformis, B. subtilis, Corynebacterium spp
Fungi	<i>Aspergillus niger</i> , A. awamori, Penicillium restrictum
Yeast	Candida lipolytica, Sacchromyces cerevisiae

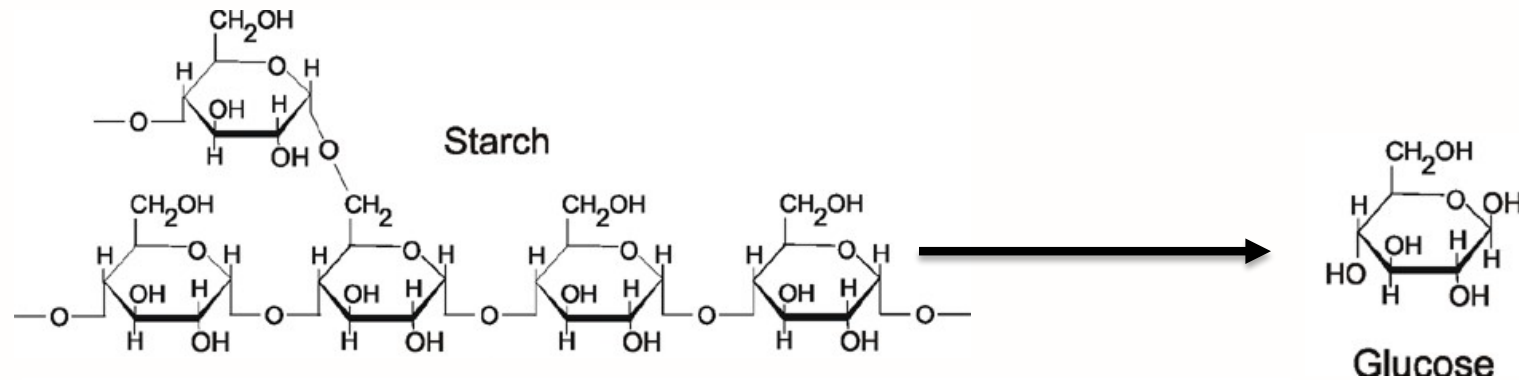
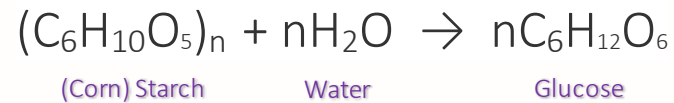
Organism of choice: *Aspergillus niger*

1. Ease of handling
2. Ability to ferment a variety of cheap raw materials
3. High yields of citric acid
4. Most commonly used species for fermentation processes

Overview: Process Chemistry

1. Upstream Processing

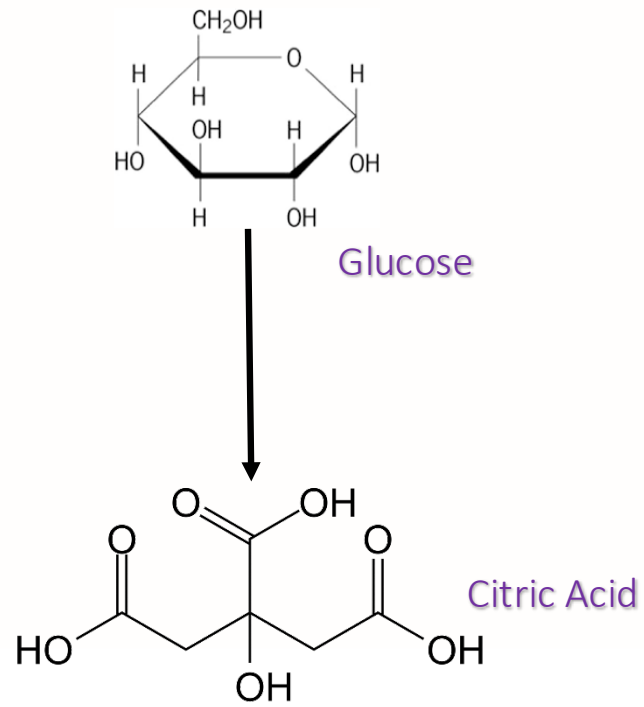
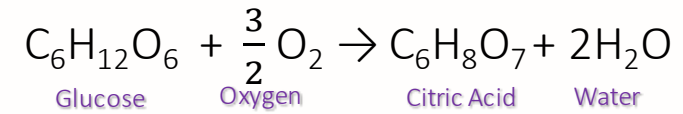
- Breaking down Starch to Glucose
- Hydrolysis reaction
 - Liquefaction + Saccharification



Overview: Process Chemistry

2. Fermentation

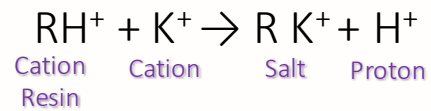
- Glucose metabolized to Citric Acid



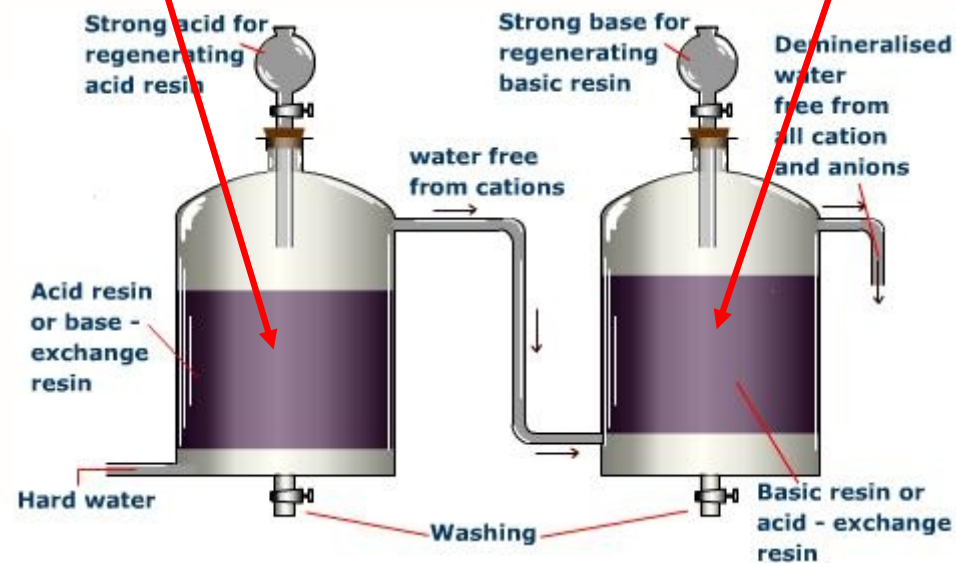
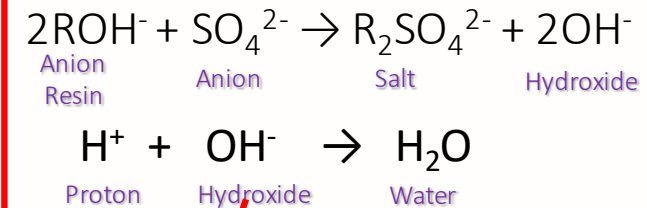
Overview: Process Chemistry

3. Ion Exchange Column

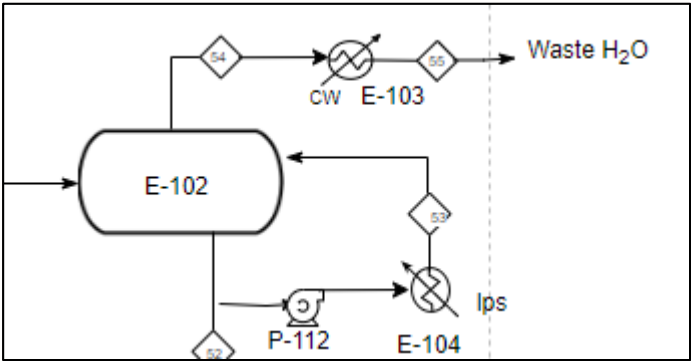
- Cation Exchange Column



- Anion Exchange Column



Crystallizer - MEB



Assumptions

- 99% of Water introduced is Converted to Steam

Type of Heat	
Heat of Evaporation (Btu/hr):	271165310
Sensible Heat (Btu/hr):	44784000
Heat of Crystallization (Btu/hr):	89820096
Total Heat Required from steam (Btu/hr):	-136561214
Steam Flow (lbs/h):	140759

Design Parameters to be Considered:

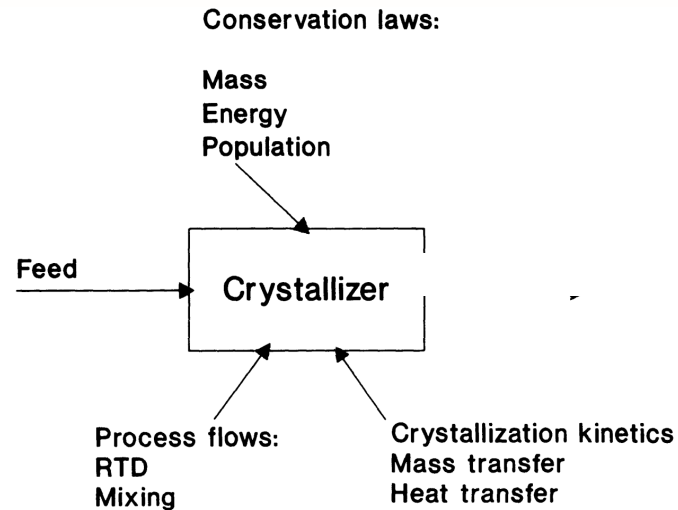
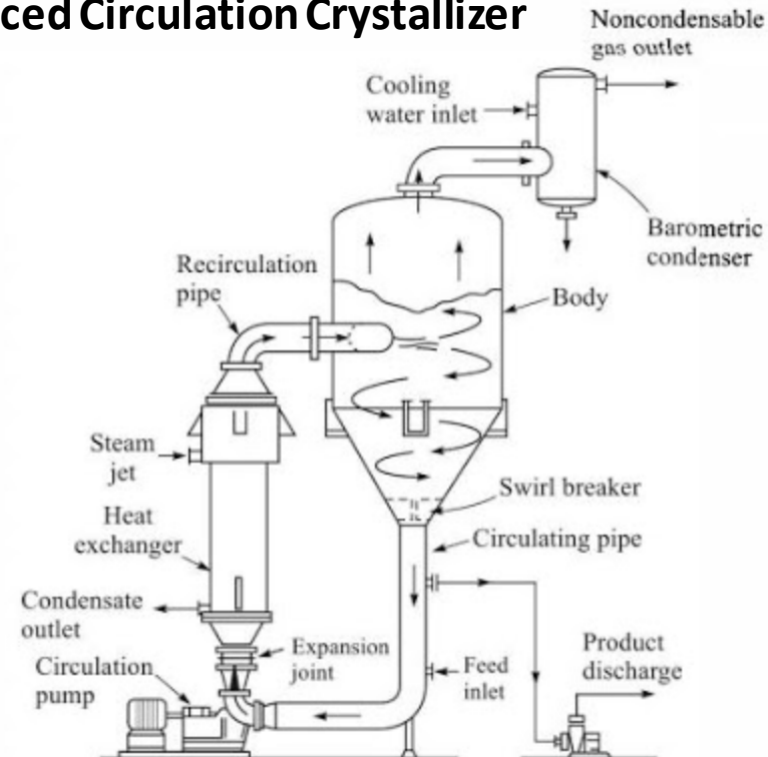


Figure 1. Algorithm for performance evaluation.

Forced Circulation Crystallizer



Pump Specifications

Water Feed Pump		
Item:	Centrifugal Pump	
Item No:	P-101	
No. Required:	1	
Function: To pump water from source to cornstarch-water mixer		
Operation: Continuous		
Materials Handled	Inlet (lb/hr)	Outlet (lb/hr)
Water	265,000	265,500
Cornstarch		
Glucose		
Operating Conditions		
Flow Rate (gph)	31,500	
Pressure Rise (psi)	0	
Fluid Density (lb/ft ³)	62.4	
Vapor Pressure of H ₂ O at 70 °F (psia)	0.36	
Inlet Pressure (psia)	14.7	
Outlet Pressure (psia)	14.7	
Pipe Diameter (in)	6	
Pump Head (ft)	3.6	
Pump Efficiency (%)	60	
Shaft Power (hp)	85	
Hydraulic Power (hp)	140	

Hydrolyzer I Feed Pump		
Item:	Centrifugal Pump	
Item No:	P-102	
No. Required:	1	
Function: To pump cornstarch slurry the from mixer to R-101		
Operation: Continuous		
Materials Handled	Inlet (lb/hr)	Outlet (lb/hr)
Water	265,000	265,500
Cornstarch	36,500	36,500
Glucose		
Operating Conditions		
Flow Rate (gph)	34,400	
Pressure Rise (psi)	7	
Fluid Density (lb/ft³)	66.7	
Vapor Pressure of H ₂ O at 70 °F (psia)	0.36	
Vapor Pressure of Cornstarch at 70 °F (psia)	0	
Inlet Pressure (psia)	14.7	
Outlet Pressure (psia)	21.7	
Pipe Diameter (in)	6	
Pump Head (ft)	18	
Pump Efficiency (%)	60	
Shaft Power (hp)	165	
Hydraulic Power (hp)	275	

Pump Specifications

Hydrolyzer II Feed Pump		
Item:	Centrifugal Pump	
Item No:	P-103	
No. Required:	1	
Function: To pump cornstarch slurry from FT-101 to R-102		
Operation: Continuous		
Materials Handled	Inlet (lb/hr)	Outlet (lb/hr)
Water	265,000	265,500
Cornstarch	27,400	27,400
Glucose	10,100	10,100
Operating Conditions		
Flow Rate (gph)	34,400	
Pressure Rise (psi)	0	
Fluid Density (lb/ft ³)	66.7	
Vapor Pressure of H ₂ O at 130 °F (psia)	2.2	
Vapor Pressure of Cornstarch at 130 °F (psia)	0	
Vapor Pressure of Glucose at 130 °F (psia)	0	
Inlet Pressure (psia)	21.7	
Outlet Pressure (psia)	21.7	
Pipe Diameter (in)	6	
Pump Head (ft)	0.7	
Pump Efficiency (%)	60	
Shaft Power (hp)	6	
Hydraulic Power (hp)	11	

Filtration to Storage Pump		
Item:	Centrifugal Pump	
Item No:	P-104	
No. Required:	1	
Function: To pump cornstarch slurry from FT-102 to TK-101		
Operation: Continuous		
Materials Handled	Inlet (lb/hr)	Outlet (lb/hr)
Water	265,000	265,500
Glucose	40,500	40,500
Operating Conditions		
Flow Rate (gph)	35,600	
Pressure Rise (psi)	7	
Fluid Density (lb/ft³)	67	
Vapor Pressure of H ₂ O at 130 °F (psia)	2.2	
Vapor Pressure of Cornstarch at 130 °F (psia)	0	
Vapor Pressure of Glucose at 130 °F (psia)	0	
Inlet Pressure (psia)	14.7	
Outlet Pressure (psia)	14.7	
Pipe Diameter (in)	6	
Pump Head (ft)	10.7	
Pump Efficiency (%)	60	
Shaft Power (hp)	105	
Hydraulic Power (hp)	175	

Pump Specifications

Production Sterilizer Pump		
Item:	Centrifugal Pump	
Item No:	P-105	
No. Required:	1	
Function: To pump cornstarch slurry from FT-102 to TK-101		
Operation: Continuous		
Materials Handled	Inlet (lb/hr)	Outlet (lb/hr)
Glucose Slurry	280,000	280,000
Operating Conditions		
Flow Rate (gph)	32,000	
Pressure Rise (psi)	5	
Fluid Density (lb/ft³)	67	
Vapor Pressure of H ₂ O at 160 °F (psia)	4.75	
Vapor Pressure of Cornstarch at 160 °F (psia)	0	
Vapor Pressure of Glucose at 160 °F (psia)	0	
Inlet Pressure (psia)	14.7	
Outlet Pressure (psia)	19.7	
Pipe Diameter (in)	6	
Pump Head (ft)	6	
Pump Efficiency (%)	60	
Shaft Power (hp)	50	
Hydraulic Power (hp)	80	

Inoculum Sterilizer Pump		
Item:	Centrifugal Pump	
Item No:	P-106	
No. Required:	1	
Function: To pump cornstarch slurry from FT-102 to TK-101		
Operation: Continuous		
Materials Handled	Inlet (lb/hr)	Outlet (lb/hr)
Glucose Slurry	280,000	280,000
Operating Conditions		
Flow Rate (gph)	3,600	
Pressure Rise (psi)	5	
Fluid Density (lb/ft³)	67	
Vapor Pressure of H ₂ O at 160 °F (psia)	4.75	
Vapor Pressure of Cornstarch at 160 °F (psia)	0	
Vapor Pressure of Glucose at 160 °F (psia)	0	
Inlet Pressure (psia)	14.7	
Outlet Pressure (psia)	19.7	
Pipe Diameter (in)	6	
Pump Head (ft)	5	
Pump Efficiency (%)	60	
Shaft Power (hp)	3.5	
Hydraulic Power (hp)	6	

General Design		Mechanical Design	
Batch Time (hr):	4	Material:	516-70 Alloy Steel
Height (ft):	10.5	Yield Stress (psi):	48500
Diameter (ft):	7	Internal Radius (ft):	3.5
Height to Diameter Ratio	1.5	Corrosion Allowance(in):	0.08
Total Volume (ft ³)	400	Impeller Diameter(ft):	2.3
Operating Temperature Range (°F)	180 - 190	Impeller Height Above Floor (ft):	2.3
Operating pH Range	5.5 - 7	Length of Impeller Blade (ft):	0.6
Headspace (%)	30	Width of Impeller Blade (ft):	0.5
		Width of Baffle (ft):	0.7
		Number of Impellers:	3
		Number of Impeller Blades:	6
		Distance Between Consecutive Impellers (ft):	2.3
Utility: Agitator Power		Number of Baffles	4
Electricity (kWh)	9300	Height of Baffle (ft)	0.7
Electricity Costs (\$/year)	980,000	Width of Baffle (ft)	10.5
Utility: Cooling Water		Utility: Enzyme	
Inlet Temperature (°F)	65	Name	Alpha-Amylase (powder)
Outlet Temperature (F)	100	Inlet Temperature (F)	70
Flow Rate (lb/hr)	1100	Flow Rate (lb/hr)	20
Cost (\$/yr)	\$54,000	Cost (\$/yr)	\$1,380,000
Comments			

Relevant Equations

$$\text{Impeller Diameter: } D_a = \frac{D_t}{3}$$

$$\text{Impeller Height above Vessel floor: } E = D_a$$

$$\text{Length of Impeller: } L = \frac{D_a}{4}$$

$$\text{Width of Impeller Blade: } W = \frac{D_a}{5}$$

$$\text{Width of Battle: } J = \frac{D_t}{10}$$

$$\text{Agitator Power Requirements: } N_P = \frac{P}{n^3 D_a^5 \rho}$$

Heat of Reaction:

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

Cooling Jacket Heat Transfer Rate:

$$Q_J = U_J A_J (T_J - T'_R) \quad T_J = \frac{T'_{J1} + T'_{J2}}{2}$$

General Design		Mechanical Design	
Batch Time (hr):	60	Material:	516-70 Alloy Steel
Height (ft):	20.5	Yield Stress (psi):	48500
Diameter (ft):	13.5	Internal Radius (ft):	13.5
Height to Diameter Ratio	1.5	Corrosion Allowance (in):	0.08
Total Volume (ft ³)	10,000	Impeller Diameter (ft):	4.6
Operating Temperature Range (°F)	130 - 140	Impeller Height Above Floor (ft):	4.6
Working Pressure (psia)	21	Length of Impeller Blade (ft):	1.15
Headspace (%)	30	Width of Impeller Blade (ft):	0.9
		Width of Baffle (ft):	1.4
		Number of Impellers:	3
		Number of Impeller Blades:	6
		Distance Between Consecutive Impellers (ft):	2.3
Utility: Agitator Power		Number of Baffles	4
Electricity (kWh)	160,000	Height of Baffle (ft)	1.4
Electricity Costs (\$/year)	\$16,800,000	Width of Baffle (ft)	20.5
Utility: Cooling Water		Utility: Enzyme	
Inlet Temperature (F)	65	Name	Glucoamylase (powder)
Outlet Temperature (F)	100	Inlet Temperature (F)	70
Flow Rate (lb/hr)	6100	Flow Rate (lb/hr)	15
Cost (\$/yr)	\$293,000	Cost (\$/yr)	\$3,000,000
Comments			

Relevant Equations

$$\text{Impeller Diameter: } D_a = \frac{D_t}{3}$$

$$\text{Impeller Height above Vessel floor: } E = D_a$$

$$\text{Length of Impeller: } L = \frac{D_a}{4}$$

$$\text{Width of Impeller Blade: } W = \frac{D_a}{5}$$

$$\text{Width of Battle: } J = \frac{D_t}{10}$$

$$\text{Agitator Power Requirements: } N_P = \frac{P}{n^3 D_a^5 \rho}$$

Heat of Reaction:

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

Cooling Jacket Heat Transfer Rate:

$$Q_J = U_J A_J (T_J - T'_R) \quad T_J = \frac{T'_{J1} + T'_{J2}}{2}$$

General Design		Mechanical Design	
Batch Time (hr)	192	Material	Stainless Steel (10.5% Chromium)
Height (ft)	38.5	Yield Stress (psi)	31,000
Diameter (ft)	26	Internal Radius (ft)	13
Height to Diameter Ratio:	1.5	Corrosion Allowance (in)	0.08
Total Volume (ft ³)	20,000	Impeller Diameter (ft)	8.7
Working Volume (ft ³)	14,000	Impeller Height Above Floor (ft)	8.7
Headspace (% of Total Volume)	30	Length of Impeller Blade (ft)	2.2
Operating Temperature (°F)	86	Width of Impeller Blade (ft)	1.7
Working Pressure (psig)	15.5	Number of Impellers	3
pH	2.2-2.6	Number of Impeller Blades	6
		Number of Baffles	4
		Height of Baffle (ft)	38.5
		Width of Baffle (ft)	2.6
Utilities			
Cooling Water		Agitator Power Requirements	
Inlet Temperature (°F)	65	Electricity (kWh)	26,800
Outlet Temperature (°F)	86	Electricity Costs (\$/year)	\$14,780,000
Flow Rate (lb/hr)	265,000	Stirred Speed (rpm)	200
Required Heat Transfer Area per Fermenter (ft ²)	900		
Jacket Heat Transfer Area (ft ²)	3,150		
Overall Heat Transfer Coefficient, U (Btu/h lbm °F)	300		
Cooling Water Cost (\$/yr)	12,700,000		

Relevant Equations

$$\text{Impeller Diameter: } D_a = \frac{D_t}{3}$$

$$\text{Impeller Height above Vessel floor: } E = D_a$$

$$\text{Length of Impeller: } L = \frac{D_a}{4}$$

$$\text{Width of Impeller Blade: } W = \frac{D_a}{5}$$

$$\text{Width of Battle: } J = \frac{D_t}{10}$$

$$\text{Agitator Power Requirements: } N_P = \frac{P}{n^3 D_a^5 \rho}$$

Heat of Reaction:

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

Cooling Jacket Heat Transfer Rate:

$$Q_J = U_J A_J (T_J - T'_R) \quad T_J = \frac{T'_{J1} + T'_{J2}}{2}$$

BELOW AVERAGE
PROJECT PRESENTATION



PRAIRIE VIEW
A&M UNIVERSITY

Manufacturing of Nitric Acid

Group 3

James Fearon
Guty Francisco

Ryan Hooks

Maya Hunter

Robert Jackson II

Nitry, Inc.

- Founded: August 2019
- By: J. Fearon, G. Francisco, R. Hooks, M. Hunter, R. Jackson II
- Location: La Porte, TX
- Producing: Nitric Acid
- Capacity: 400,000 ^{ton}/year

Problem Statement and Goals

- Problem Statement
 - Design a plant which manufacture Nitric Acid
- Project Goals
 - Design and Size Major Units
 - HAZOP and Safety Analysis
 - Economic Analysis

Project Summary

- Plant Capacity = $400,000 \text{ ton/yr}$
 - Operating at $8,000 \text{ hr/yr}$
- Raw Materials: NH_3 and O_2 (Air)
- Product: 60 wt% Nitric Acid ($\text{HNO}_3(\text{aq})$)
 - Equations
 - Via Ostwald Process (3-step process, catalyst – PtRh)
- Utilities
 - Steam
 - Cooling Water
 - Electricity
- Safe Environment



Gantt Chart

i	Task Mode	Task Name	Duration	Start	Finish	Predecessors	Resource Names
	★	Senior Design and Professionalism 2: Production of Nitric Acid	71 days	Mon 1/13/20	Sat 4/18/20		
👤	★	1. Review of Semester 1	26 days	Mon 1/13/20	Mon 2/17/20		Group 3
👤	★	1.1 Group Dynamics	6 days	Mon 1/13/20	Mon 1/20/20		Group 3
	★	1.2 Converge ASPEN Simulation	11 days	Mon 1/20/20	Mon 2/3/20		Ryan, James, Rol
👤	★	1.3 Review Presentation/Repor Semester 1	3 days	Tue 2/4/20	Thu 2/6/20		Maya, Guty
👤	★	2. Design of Major Units	22 days	Tue 2/4/20	Wed 3/4/20		Group 3
	★	2.1 Reactor Design	20 days	Wed 2/5/20	Tue 3/3/20		Rob
	★	2.2 Absorption Colum Design	20 days	Wed 2/5/20	Tue 3/3/20		Ryan
	★	2.3 Stripping Column Design	20 days	Wed 2/5/20	Tue 3/3/20		James
👤	★	2.4 Knockout Drum Design	20 days	Wed 2/5/20	Tue 3/3/20		Maya
👤	★	2.5 Evaportaion Design	20 days	Wed 2/5/20	Tue 3/3/20		Guty
👤	★	3. Economic Cost Analysis	20 days	Wed 3/4/20	Tue 3/31/20		Group 3
👤	★	3.1 Equipment Pricing	6 days	Wed 3/4/20	Wed 3/11/20		Guty,Maya
👤	★	3.2 Raw Materials	11 days	Wed 3/4/20	Wed 3/18/20		James,Maya
	★	3.3 Return on Investment Calculation	6 days	Thu 3/19/20	Thu 3/26/20		Rob,Ryan,Maya
👤	★	4. Safety Analysis	8 days	Wed 4/1/20	Fri 4/10/20		Group 3
👤	★	4.1 EHS, EPA and OSHA Requirements	4 days	Wed 4/1/20	Sat 4/4/20		Maya, James, Gu
👤	★	4.2 Safety Considerations	4 days	Sun 4/5/20	Wed 4/8/20		Ryan, Rob
👤	★	4.3 Chemical Safety	3 days	Wed 4/8/20	Fri 4/10/20		James,Ryan
👤	★	5. Project Presentation and Report	15 days	Fri 4/10/20	Thu 4/30/20		Group 3
👤	★	5.1 Powerpoint Presentation and Report	7 days	Fri 4/10/20	Sat 4/18/20		Group 3
👤	★	5.2 Draft Detailed Report	7 days	Sat 4/18/20	Sat 4/25/20		Group 3
👤	★	5.3 Complete Final Detailed Report	1 day	Sat 4/25/20	Sat 4/25/20		Group 3



General Information

- Compound IUPAC Name: Nitric Acid
- Chemical Formula: HNO_3
- Molecular Weight: 63.01 g/mol
- Appearance: Colorless, yellow or red fuming liquid
- Odor: Irritating and suffocating
- Raw Materials: NH_3 and O_2
- Desired Product: 60 wt% HNO_3 (aq)
- Boiling Point: 181°F
- Freezing Point: -44°F

Uses



Fertilizer



Rocket Fuel



Explosives



Plastics



Dyes

Customers

Companies	Locations
Ouachita Fertilizer	Monroe, LA
Gavilon Fertilizer LLC	Shreveport, LA
CF Industries	Donaldsonville, LA
Gavilon Fertilizer	Greenville, MS
Helena Chemical Co.	Guntown, MS
Mosaic Faustina A	Hockley, TX
Nelson Plan Food	Bellville, TX
Southwest Fertilizer	Houston, TX
Lavaca Feed & Fertilizer	Hallettsville, TX
Helena Chemical Co.	Garwood, TX
Abilene AG Services & Supply Inc	Abilene, TX

Plant Location

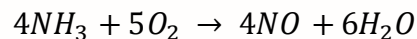


- Baytown, TX
 - Proximity to water source
 - Easy access for raw material and product transportation
 - Piping present for importing of NH_3
 - Provides for cooling process
 - Located in industrial area

Ostwald Process

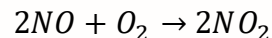
1

Oxidation of
Ammonia



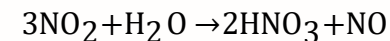
2

Oxidation of
Nitrogen Monoxide



3

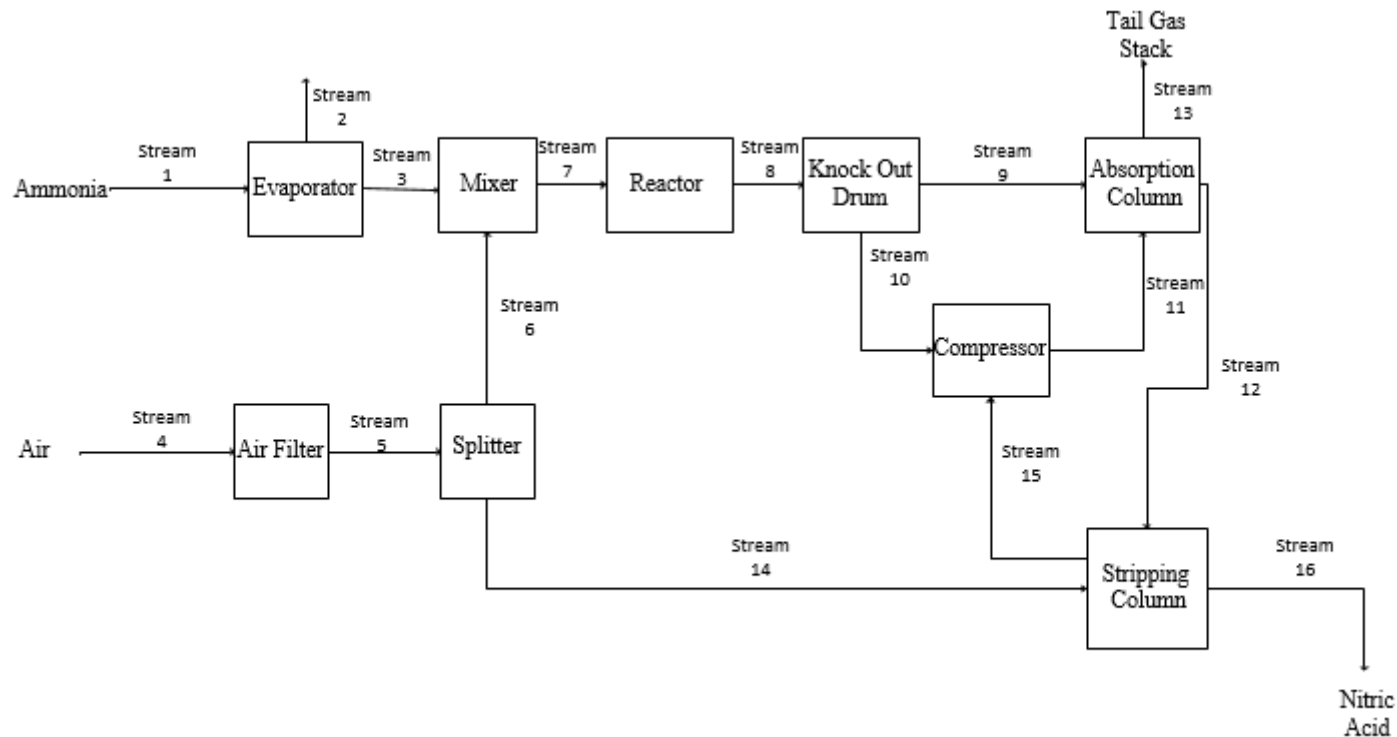
Absorption of
 NO_x to HNO_3



Dual Pressure Process

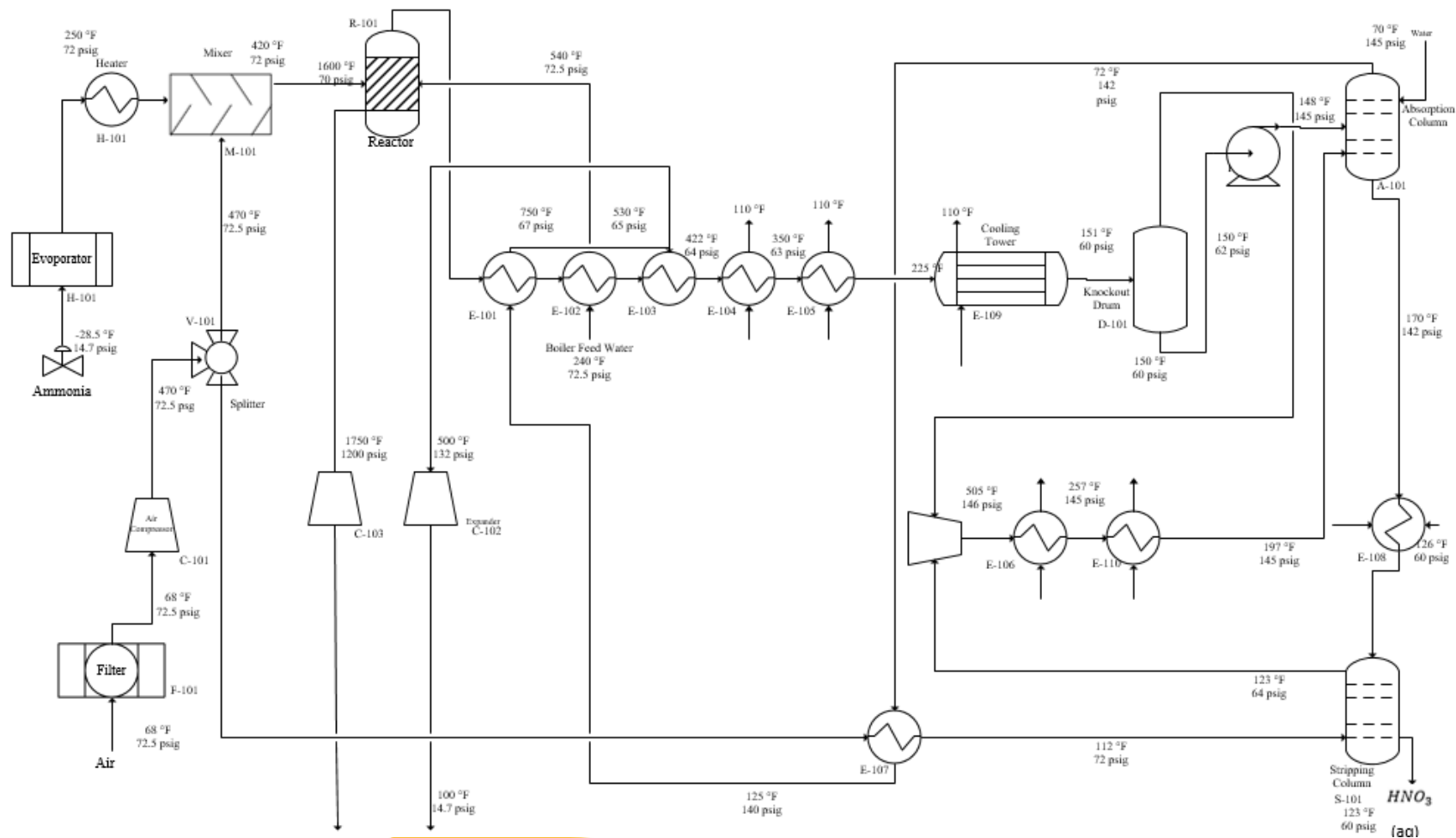
- Can produce up to $1,500 \frac{\text{tons}}{\text{day}}$ with a concentration up to 70%
- Uses two types of pressures:
 - Low to medium pressure for the compressed air in combustion to yield greater NO amounts in reactor
 - High pressure to optimize absorption process

Block Flow Diagram w/ Labeled Streams

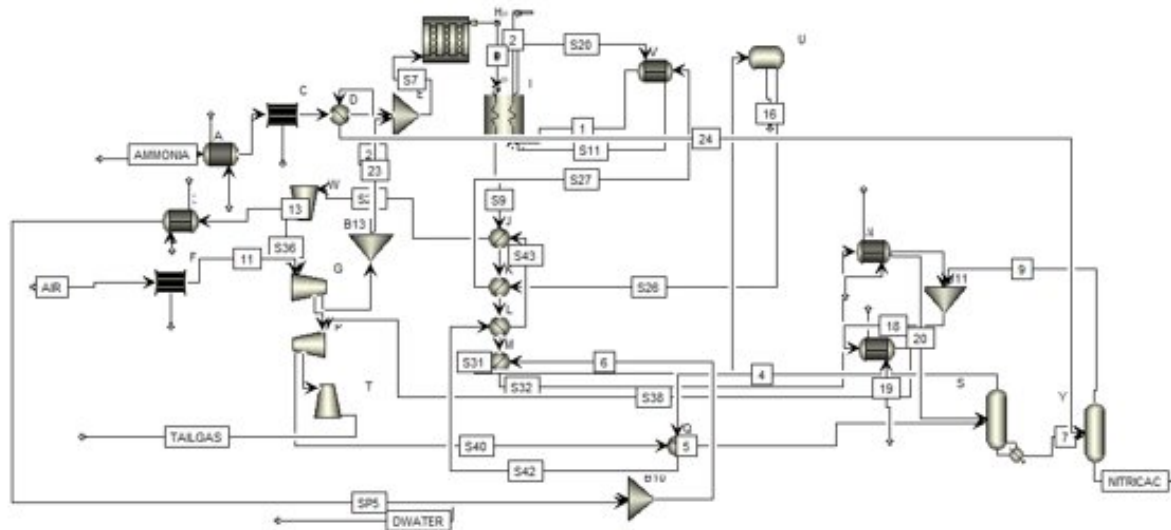


Block Flow Diagram – Dual Pressure Process

Process Flow Diagram



ASPEN Simulation



Aspen Simulation – Dual Pressure Process for Nitric Acid

Materials and Energy Balances

Compound	Stream 1 (lb/hr)	Stream 2 (lb/hr)	Stream 3 (lb/hr)	Stream 4 (lb/hr)	Stream 5 (lb/hr)	Stream 6 (lb/hr)
NH ₃	29762.3	0	29762.3	0	0	0
H ₂ O	1236.41	1093.11	143.30	0	0	0
O ₂	0	0	0	109613.71	109613.71	94269
N ₂	0	0	0	412440.31	412440.31	354635.15
NO	0	0	0	0	0	0
HNO ₃	0	0	0	0	0	0
NO ₂	0	0	0	0	0	0



Materials and Energy Balances

Compound	Stream 7 (lb/hr)	Stream 8 (lb/hr)	Stream 9 (lb/hr)	Stream 10 (lb/hr)	Stream 12 (lb/hr)	Stream 13 (lb/hr)
Ammonia	29762.37	615.09	615.09	0	595.2474	1210.337
Water	143.30	46429.3	46429.3	0	61993.91	55800.99
Oxygen	94269.55	25705.87	0	25705.87	0	41050.03
Nitrogen	354635.17	354635.2	0	354635.2	354635.2	1286212.31
Nitric Oxide	0	0	0	51424.96	18959.73	707384.69
Nitric Acid	0	0	0	0	66138.6	0
Nitrogen Dioxide	0	0	0	0	1481.505	1481.505



Material and Energy Balances

Compound	Stream 14 (lb/hr)	Stream 15 (lb/hr)	Stream 16 (lb/hr)	Stream 17 (lb/hr)
Ammonia	0	0	0	0
Water	0	0	44092.4	9391.69
Oxygen	15344.16	8884.62	0	0
Nitrogen	576941.91	354635.2	0	0
Nitric Oxide	0	1278.68	0	0
Nitric Acid	0	0	66138.6	0
Nitrogen Dioxide	0	16005.59	0	0



Evaporator General Information

- Feed: NH_3
- Molecular Weight of NH_3 : $17.031 \frac{\text{g}}{\text{mol}}$
- Feed amount: $30998.71 \frac{\text{lb}}{\text{hr}}$
- Water amount in the ammonia = $1256.41 \frac{\text{lb}}{\text{hr}}$
- Pure ammonia: $29762.3 \frac{\text{lb}}{\text{hr}}$
- Evaporator Type: Short-Tube Vertical Evaporators, also known as calandria or Robert evaporators

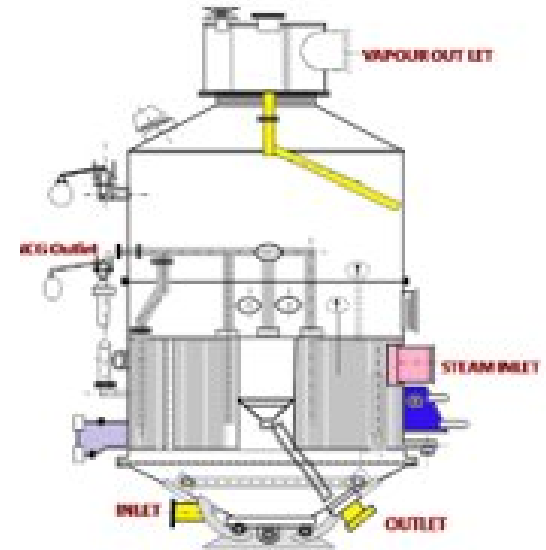


Figure 1 . Calandria type evaporator.

Mechanical Design of the Evaporator

Number of tubes (N)

- *Effective Length of the tube (L) = Tube length – 2(Tube plate thickness)–2(Tube expansion allowance)*
- *Number of tubes = Heating $\frac{\text{Surface}}{\pi \cdot D_m \cdot L}$*
- The thickness of the tube generally take for ammonia heaters and for evaporator 18G and for pans take 16G. (18g = 1.22mm , 16g = 1.625mm, 14g = 1.8mm).



Mechanical Design of the Evaporator

- Dia of the single downtake = Tube plate dia for tubes x % of downtake on tube plate.
- Dia of the central downtake: $\sqrt{[(Area\ of\ singledowntake - total\ area\ of\ peripheral\ downtakes) \times \frac{4}{\pi}]}$
- Final Dia of the tube plate:
 $\sqrt{[(area\ of\ tubeplate\ for\ tubes + downtake\ area) \times \frac{4}{\pi}]}$

Calendria shell thickness :

$$\left(\frac{PD_i}{2FJ - p} \right) + C$$

Tube plate thickness :

$$K = (E_s \times t_s \times (D_o - t_s)) / N_t \times E_t \times t_t \times (D_o - t_t))$$



Mechanical Design of the Evaporator

Vapour outlet pipe dia :

- Vapour volume outlet vapour in ft³/sec

$$\text{heating surface} \times \text{evap. rate} \times \text{sp. volume of outlet} \frac{\text{vapour}}{3600}$$

- Vapour outlet pipe dia in mtrs:

$$\sqrt{\left[\frac{\text{vapour volume}}{0.785 \times \text{velocity of vapour}} \right]}$$

Dia of the condensate line :

Volume of the condensate in ft³/sec:

$$\frac{\text{heating surface} \times \text{evap. rate}}{\text{density of water} \times 3600}$$

- Dia of the each condensate line : $\sqrt{\left(\frac{\text{vol. of condensate}}{0.785 \times \text{velocity of condensate}} \right)}$

Noxious gases connections Dia of the each non condensable gases line :

$$\sqrt{\left(\frac{\text{total area of NCG}}{0.785 \times \text{No. of points}} \right)}$$



Evaporator Specification Sheet

Evaporator				
Identification	Item:	Vertical Vessel		
	Item No.		Date:	04/25/2020
	No. Required	1		
	Cost (\$):			
Function: Evaporation is the removal of solvent (water) as vapor from a solution (Ammonia), slurry or suspension of solid in a liquid.				
Operation: Adiabatic				
	Feed Stream (lb/hr)	Vapor Stream (lb/hr)	Liquid Stream (lb/hr)	
Material Handled: Ammonia				
Oxygen:	0	0	0	
Nitrogen:	0	0	0	
Ammonia:	29762.3	0	29762.3	
Water:	1256.4	1113.1	143.3	
Nitrogen Oxide:	0	0	0	
Nitric Acid:	0	0	0	
Nitrogen Dioxide:	0	0	0	
Total:	31018.7	1113.1	29905.6	
Temperature (°F):		194		
Pressure (psig):				
Design Data:				
Area (ft. ²):				
Height (ft.):				
Diameter (ft.):				
Volume (ft. ³):	2.152			
Material Construction:	Brass			
Vapor Velocity (ft/s):		1.197		1.8



Catalyst Information

- Catalyst Type: Platinum Rhodium
 - Included in gauze at bottom of reactor
 - Mixture improves strength and lowers catalyst loss
 - Rhodium more expensive than platinum
- Platinum – Rhodium 90% - 10%
- Bulk density : 1248 lb/ft³
- Activation of catalyst- 850 Celsius

Reactor

- The rate of ammonia oxidation in terms of a mass-transfer coefficient with the ammonia partial pressure at the catalyst surface assumed to be zero for this rapid reaction

$$(-r_A) = K_{ga}^s a_{wR} P_A$$

- For this rapid reaction assume that partial pressure of ammonia on the catalyst surface is zero. Then the rate of transfer of ammonia becomes

$$(-r_A) dZ = K_{ga}^s a_{wR} y_A P dZ = K_{ga}^s y_A P f_w dn_s$$

- Where n_s is the number of gauzes and f_w is the wire area per gauze cross sectional area for one gauze.

$$(-G/M_f) dy_A = K_{ga}^s y_A P f_w dn_s$$

- or integrating and simplifying by assuming constant number of moles

$$K_{ga}^s P n_s f_w = (G/M_f) \ln(Y_{A1}/Y_{A2}) = (-G/M_f) \ln(1-X_A)$$

- Or ,

$$\ln(1-X_A) = -K_{ga}^s P n_s f_w M_f / G$$

- Where,

$$K_{ga}^s = \frac{0.865 N_{Re}^{-0.648} G}{P N_{Sc}^{2/3} M_m \epsilon_w}$$

- Where M_m is the molecular weight of the mixture.

$$\ln(1 - X_A) = \frac{-0.865 n_s f_w M_f N_{Re}^{-0.648}}{\epsilon_w M_m N_{Sc}^{2/3}} = \frac{-0.865 n_s f_w D^{2/3} \rho_f^{2/3}}{\epsilon_w 0.352 d_w^{0.648} G^{0.648} \mu_f^{0.019}}$$



Reactor

- Where d_w is the diameter of wire. M_F/M_m is approximately unity.

$$\ln(1 - X_A) = - \frac{(0.865) n_s f_w D^{2/3} \rho_f^{2/3}}{\epsilon_w^{0.352} d_w^{0.648} G^{0.648} \mu_f^{0.019}}$$

$$D = 0.227 (T/293)^{3/2} (1/P) \text{ cm}^2/\text{sec}$$

$$M = M_F = (32)(0.21)(1 - Y_A) + (28.01)(0.79)(1 - Y_A) + 17.03 y_{A0} = 28.85 + 11.82 Y_{A0}$$

$$\ln(1 - X_A) = - \frac{5.81761 \cdot 10^{-2} n_s f_w T^{0.222} (28.85 + 11.82 Y_{A0})^{0.62}}{\epsilon_w^{0.352} d_w^{0.648} G^{0.648} \mu_f^{0.019}}$$

- To calculate the rate of Pt losses,

$$R = 1.09 \cdot 10^{10} (T_{O2})^{-1/2} (P_{O2}) P_e \exp(-42500/RT)$$

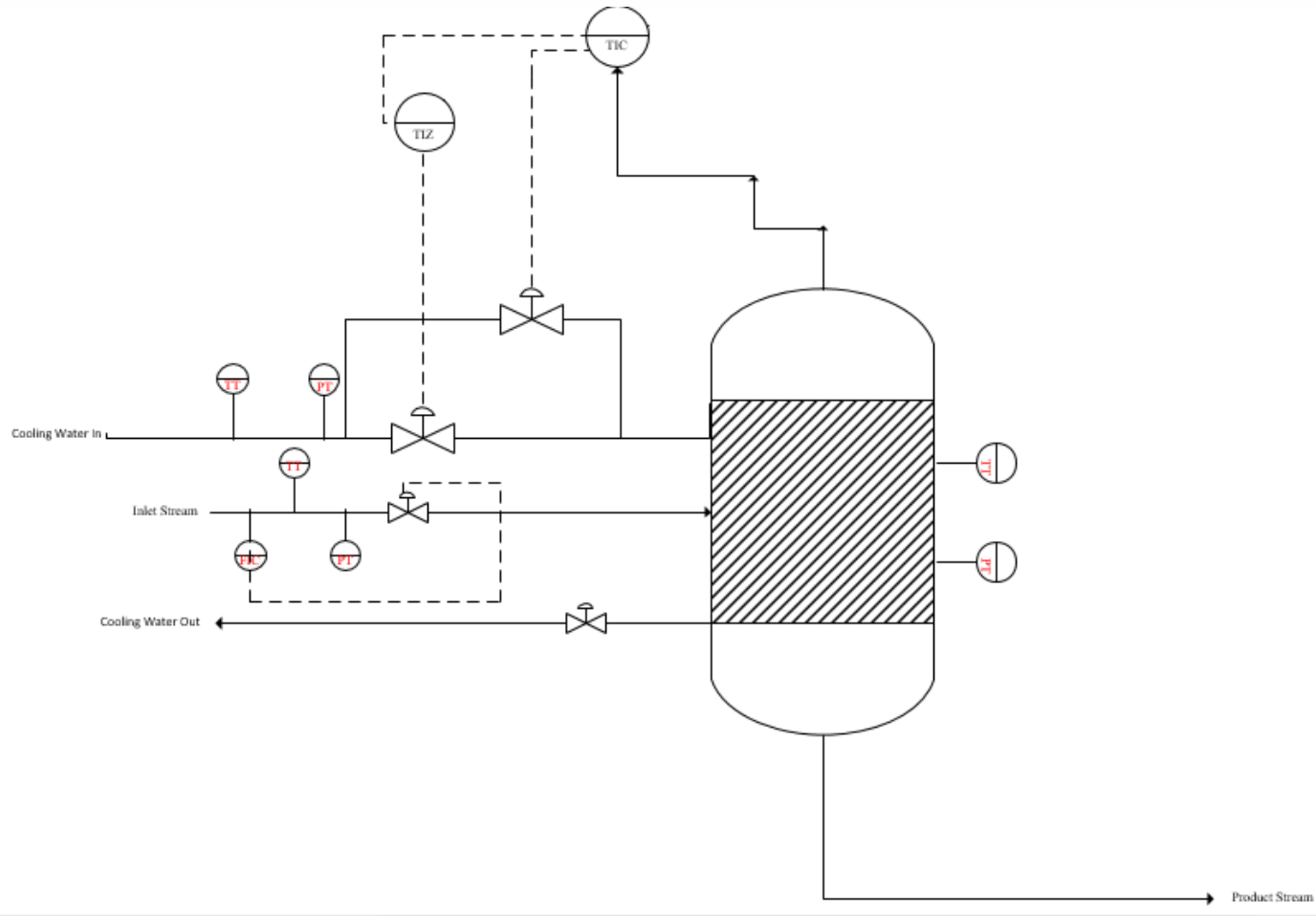


Reactor Specification Sheet

Reactor Specification		
Reactor Temperature	1650	degree Fahrenheit
Reactor Pressure	70	PSIG
Conversion of Ammonia	0.79	
NO Yield	0.41	
Rate	0.6467	(lbmol of NH ₃ /ft ³ of catalyst*hr)
Rate	0.0005	(lbmol of NH ₃ /lb of catalyst*hr)
Catalyst Name		Platinum-Rhodium Gauze Catalyst
Bulk Density	1248.6	lb/ft ³
Volume of Reactor	2707.17	ft ³
Feed Mass Flowrate	478810.4	lb/hr
Oxygen	0.20	
Nitrogen	0.74	
Ammonia	0.06	
Water	0.00	
NO	0.00	
Feed Molar Flowrate	17370.2	lbmol/hr
Product Mass Flowrate	478810.4	lb/hr
Oxygen	0.05	
Nitrogen	0.74	
Ammonia	0.00	
Water	0.10	
NO	0.11	
Product Molar Flowrate	17798.6	lbmol/hr
Product Volumetric Flowrate	77635.0	ft ³ /hr
Diameter	10.45	ft
Height	31.35	ft
Cross sectional Area	85.75	ft ²
Material of Construction	Stainless Steel	
MAWT	2500	Degrees Fahrenheit
MAWP	150	PSIA



P&ID of NH_3 Oxidizing PFR

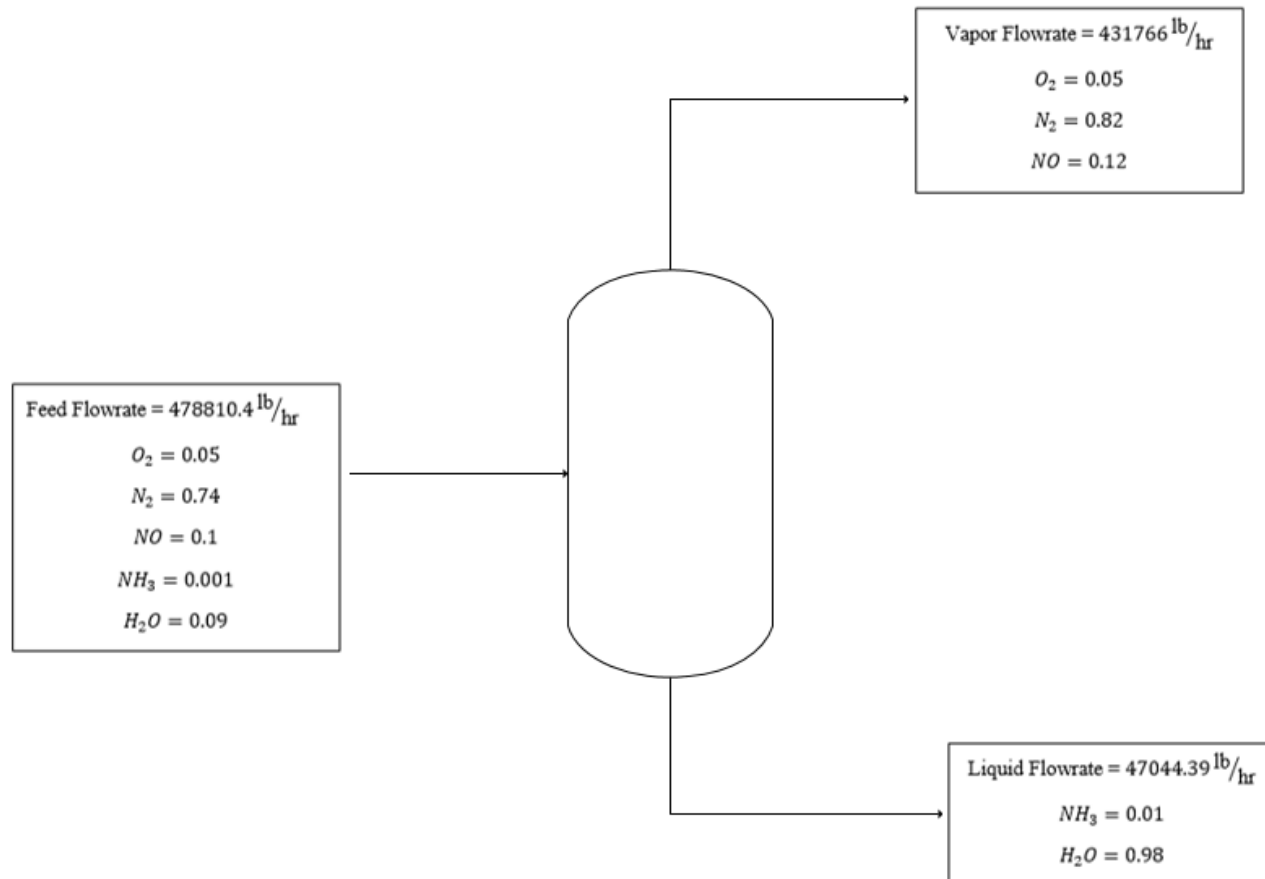


HAZOP Analysis

No.	Item	Function/Purpose	Parameter	Guide Word	Deviation	Consequence	Cause	Hazard
1	2	3	4	5	6	7	8	9
1	Cooling Water	Reactor System	Flow	No	No cooling water flow to reactor	Gives reactor potential to overheat leading to possible explosion	Blockage of cooling water flow pipe, Malfunctioned control valve for cooling water entry. Break in reactor coolant pipe	Overheating of reactor, runaway reaction and potential explosion
2	Cooling Water	Reactor System	Flow	More	Too much cooling water to reactor	Gives reactor potential to overcool and slow down reaction	Malfunctioned control valve for cooling water entry cannot close, Broken valve	Overcooling and decrease reactor temperature
3	Cooling Water	Reactor System	Flow	Less	Not enough cooling water to reactor	Slow down heating of reactor and slow down	Cooling water control valve blockage, Partially open valve	Overheating, increased temperature and runaway reaction
4	Feed Inlet Stream	Reactor System	Flow	More	Too much of the ammonia, air and water mixture is entering into the reactor	Possible overflow of the reactor	Inlet flow rate being above flow rate that can be held by inlet flow, inlet valve malfunction	Overflow of reactor
5	Feed Inlet Stream	Reactor System	Concentration	High	Ammonia, Water or Air concentration is higher than what is needed by the reactor to react	Ammonia is highly flammable at high volumes in		Improper reaction taking place



Knockout Drum (Vapor-Liquid Separator)



Knockout Drum Calculations

Liquid Density

$$MW_L = x_{H_2O} MW_{H_2O} + x_{NH_3} MW_{NH_3} = \left(\frac{.09}{.091}\right) (18 \text{ g/mol}) + \left(\frac{.001}{.091}\right) (17 \text{ g/mol}) = 18 \text{ g/mol}$$

$$V_L = x_{H_2O} \frac{MW_{H_2O}}{\rho_{H_2O}} + x_{NH_3} \frac{MW_{NH_3}}{\rho_{NH_3}} = (.09) \left(\frac{18 \text{ g/mol}}{0.9 \text{ g/cm}^3} \right) + (0.001) \left(\frac{17 \text{ g/mol}}{0.00073 \text{ g/cm}^3} \right) = 25$$

$$\rho_L = \frac{MW_L}{V_L} = \frac{18 \text{ g/mol}}{25} = \mathbf{0.72}$$

Vapor Density

$$\begin{aligned} MW_V &= x_{O_2} MW_{O_2} + x_{N_2} MW_{N_2} + x_{NO} MW_{NO} \\ &= (.06) (32 \text{ g/mol}) + (0.82) (28 \text{ g/mol}) + (0.11) (30 \text{ g/mol}) = 28.18 \text{ g/mol} \end{aligned}$$

$$\rho_V = \frac{PMW_V}{RT} = \frac{(10 \text{ atm})(28.18 \text{ g/mol})}{(82.0575)(333.3 \text{ K})} = \mathbf{0.01}$$

Knockout Drum Calculations

Permissibility

$$u_{\text{perm}} = k_{\text{drum}} \sqrt{\frac{\rho_L - \rho_V}{\rho_V}} = 0.38 \sqrt{\frac{0.72 - 0.01}{0.01}} = \mathbf{1.8 \text{ ft/s}}$$

Cross-Sectional Area

$$A_C = \frac{(V)(MW_V)}{(u_{\text{perm}})(3600)\rho_V} = \frac{(431766)(28.18 \text{ g/mol})(454 \text{ g/lb})}{(3.2 \text{ ft/s})(3600)(0.01)(28316.85 \text{ mL/ft}^3)} = \mathbf{423 \text{ ft}^2}$$

Diameter

$$D = \sqrt{\frac{4A_C}{\pi}} = \sqrt{\frac{4(423)}{\pi}} = \mathbf{23.2 \text{ ft}}$$

Total Height

$$H_{\text{total}} = 3D = (3)(23.2 \text{ ft}) = \mathbf{69 \text{ ft}}$$

Maximum Volume

$$V_{\text{max}} = \frac{\pi D^2 H}{4} = \frac{\pi (23.2)^2 (69)}{4} = \mathbf{29168.5 \text{ ft}^3}$$



Knockout Drum Specification Sheet

Knock Out Drum				
Identification	Item:	Vertical Vessel		
	Item No.		Date:	04/25/2020
	No. Required	1		
	C(\$):			
Function: To separate vapor and liquid mixture of Nitrogen, Ammonia, Water, Nitrogen Monoxide and Nitrogen Dioxide				
Operation: Adiabatic				
	Feed Stream (lb/hr)	Vapor Stream (lb/hr)	Liquid Stream (lb/hr)	
Material Handled: Nitrogen, Ammonia, Water, Nitrogen Monoxide, Nitrogen Dioxide				
Oxygen:	25,705.8	25,705.9	0	
Nitrogen:	354,635.2	354,635.2	0	
Ammonia:	615.09	0	615.1	
Water:	46,429.3	0	46,429.3	
Nitrogen Oxide:	51,424	51,425		
Nitric Acid:	0	0	0	
Nitrogen Dioxide	0	0	0	
Total:	478,810.4	431,766	47,044.4	
Temperature (°F):				
Pressure (psig):				
Design Data:				
Area (ft. ²):				423
Height (ft.):				69
Diameter (ft):				23.2
Volume (ft. ³):				29168.5
Material Construction:	Stainless Steel			
Vapor Velocity (ft/s):				1.8



Stripping Column

- The Kremser equation for theoretical stages:

$$N = \frac{\ln[A + (1-A) \left(\frac{x_2 - \frac{y_1}{m}}{x_1 - \frac{y_1}{m}} \right)]}{\ln\left(\frac{1}{A}\right)}$$

- Where, $1/A = mV/L$, Stripping factor
- Calculation of Efficiency using Drickamer - Bradford Equation
- $E_o = 13.3 - 66.8 \log (\mu)$

Stripping Column

- Since, $N_{\text{theo}} = 5$ stages,

- $E_o = 0.54$ &

$N_{\text{act}} = 9$ stages

- Calculation of vapor velocity

- $$V_{\text{nf}} = K_1 \sqrt{\frac{\rho_l - \rho_v}{\rho_v}}$$



Stripping Column

- $V_{nf} = 4.12 \frac{ft}{s}$
- Actual Vapor Velocity 50-90 % of net vapor velocity
- $V_n = 0.80 \times V_{nf}$
- $V_n = 3.27 \frac{ft}{s}$



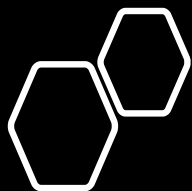
Stripping Column

- Diameter of the stripping column
- Net area for separation process
- $A_n = m' v / V_n$
- $A_n = 7.2 ft^2$
- Assuming down comer occupies 15%
- $A_c = \frac{A_n}{0.85} = 8 ft^2$
- $D_c = 3.7 ft$

$$D_c = \sqrt{\frac{A_c \times 4}{\pi}}$$

Stripping Column

- Height of the Stripping Column
- $H_c = (N_{act} - 1) \times H_s + H$
- $H_c = 21.4\text{ft}$



Stripping Column Specification Sheet

Identification	Product	Aqueous Nitric Acid	
	Item No	S-101	
Operation	Continuous	Operating Temperature & Pressure	125°F, 60 psi
Design Data			
Diameter (ft)	3.7 ft	Tray Spacing (ft)	2 ft
Height (ft)	21.4 ft	Tray Type	Sieve
Theoretical plates	5	Tray Material	Stainless Steel
Actual no of stages	9	Equipment Type	Vertical
Efficiency (%)	54	Plate Pressure	0.16ft
Column Material	Stainless Steel		

Absorption Tower

- Column height: 100.708 ft
- Wall thickness: 0.8125 ft.
- Design pressure: 150 psig.
- Diameter: 12 ft.
- Number of trays: 36
- Wind Load: 25.9 lb/sq.ft @ 0–33 ft.
 - 32.4 lb/sq.ft @ 33–66 ft.
 - 38.9 lb/sq.ft @ 66–99 ft.

Tray	Spacing (ft)
1-2	1
3-4	2
5-20	2
21	3
22-28	2
29-31	3
32-33	4
34-35	5

Absorption Tower Specification Sheet

Absorption Tower				
Identification	Item:	Vertical Vessel		
	Item No.		Date:	04/25/2020
	No. Required	1		
Function: To create Nitric Acid vapor and liquid mixture of Nitrogen, Ammonia, Water, Nitrogen Monoxide and Nitrogen Dioxide				
Operation: Adiabatic				
	Feed Stream 1 (lb/hr)	Feed Stream 2 (lb/hr)	Exit Stream 1 (lb/hr)	Exit Stream 2 (lb/hr)
Material Handled: Nitrogen, Ammonia, Water, Nitrogen Oxide, Nitric Acid, Nitrogen Dioxide				
Oxygen:	0	0	0	0
Nitrogen:	0	354635.2	0	354636.2
Ammonia:	595.25	0	595.25	0
Water:	61993.91	0	61993.91	0
Nitrogen Oxide:	0	3218.745	0	18959.73
Nitric Acid:	0	0	66138.6	0
Nitrogen Dioxide	0	73920.91	0	1481.505
Total:	62589.16	431774.8	128727.76	375077.435
Temperature (°F):	148	197	170	70
Pressure (psig):	145	145	142	145
Wall Thickness (ft):	0.8125			
Height (ft.)	100.7			
Diameter (ft):	12			
Number of Stages	36			
Material Construction:	Stainless Steel			
Tray Type	Sieve			



Storage Tank Specification Sheet

Equipment Type	Nitric Acid storage tank
Shape	Cylindrical
Nature	Insulated
Material of Construction	Stainless Steel
Capacity	50000000kg/hr
Volume(m3)	23.8
Diameter(m)	4.6
Height(m)	13.9

Equipment Type	Ammonia Storage tank
Shape	Cylindrical
Nature	Insulated

Material of Construction	Stainless Steel
Capacity	13565kg/hr
Volume(m3)	66.8
Diameter(m)	6.5
Height (m)	19.6



Chemical Safety

- Ammonia
 - Rescue Personnel
 - Self-contained breathing apparatus
 - Stop the flow of gas
 - Large Concentrations
 - Evacuation of the area
 - Water or fog spray to lower concentrations
 - Low Concentrations
 - Eye irritations (temporary blindness)
 - Skin burn
 - Inhalation causes coughing, lung irritation, laryngitis, bronchitis



Chemical Safety

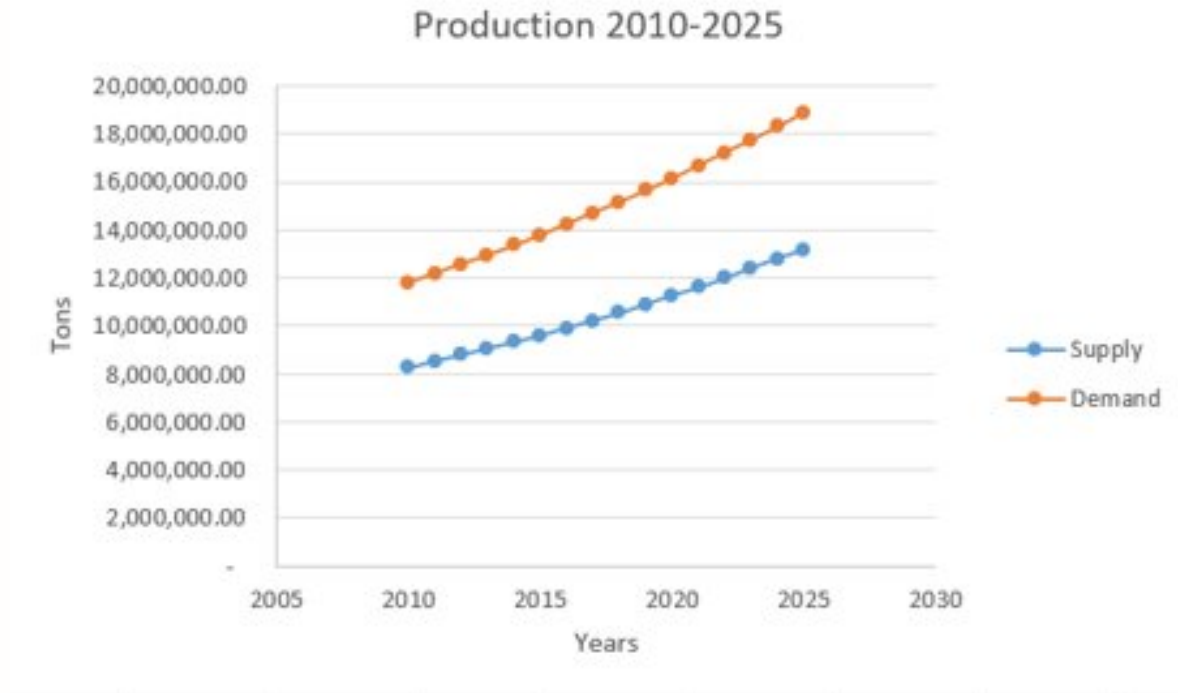
- Nitric Acid
 - Large Concentrations
 - Water spray or resistant foam; not straight streams
 - Eliminate all sources
 - Safety Signs
 - Location where's pipes are in proximity
 - Safety Gear
 - Wear or be near to positive self-contained breathing apparatus
 - SafeAir chemical detection badges
 - Reacts explosively with all metallic powders, hydrogen sulfide, ethanol,

Safety Analysis

- Platinum Rhodium Catalysts replaced periodically – degrades over time
- Air filters must be replaced and disposed of via waste management contractor
- Tail gas is in regulation with EPA before being released to atmosphere

Species	Limit
NO_x	100–3500 ppm
O_2	1–4 % by volume
H_2O	0.3–2% by volume

Supply and Demand



Supply and Demand Curves for Nitric Acid Production



PRAIRIE VIEW
A&M UNIVERSITY

Raw Material and Product Cost — El Dorado Nitrogen, LLC

- Raw Material
 - $\text{NH}_3 = \$0.37/\text{kg}$
 - NH_3 per year = \$108 M/yr
- Product
 - $\text{HNO}_3 = \$0.31/\text{kg}$
 - HNO_3 per year = \$240M/yr



Capital Cost

Project Identifier: Illustration 101	Fluid processing plant	User: copy from values at left or	Calculated values, million \$
Direct Costs			
Purchased equipment, E'			40.800
Delivery, fraction of E'	0.10	0.10	4.080
Subtotal: delivered equipment			44.880
Purchased equipment installation	0.47	0.47	21.094
Instrumentation&Controls(installe	0.36	0.36	16.157
Piping (installed)	0.68	0.68	30.518
Electrical systems (installed)	0.11	0.11	4.937
Buildings (including services)	0.18	0.18	8.078
Yard improvements	0.10	0.10	4.488
Service facilities (installed)	0.70	0.70	31.416
Total direct costs	2.60	2.60	161.568
Indirect Costs			
Engineering and supervision	0.33	0.33	14.810
Construction expenses	0.41	0.41	18.401
Legal expenses	0.04	0.04	1.795
Contractor's fee	0.22	0.22	9.874
Contingency	0.44	0.44	19.747
Total indirect costs	1.44	1.44	64.627

Return on Investment , *ave* %/yr: -17.0

Payback period, y: -9.4



PRAIRIE VIEW
A&M UNIVERSITY

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Thank you to...

- El Dorado Nitrogen, LLC
 - Michael Griffin
 - James Cartwright
- Technical Advisors
 - Dr. L. Martin
 - Dr. E. Dada
- Roy G. Perry College of Engineering - Chemical Engineering Department
 - Chemical Engineering Class of 2020



PRAIRIE VIEW
A&M UNIVERSITY

Questions?

Thank you!

Cost of Major Units

- Evaporator - \$78,000.00
- Reactor - \$88,800.00
- Knockout Drum - \$88,700.00
- Absorption Column - \$1,920,000.00
- Stripping Column - \$1,430,000.00

**SENIOR DESIGN AND PROFESSIONALISM I
FALL 2021**

Title of Assignment: HOMEWORK 1 and 2

TOPICS COVERED IN HOMEWORK 1 and 2

Test 1 covered the following topics:

1. Problem statement
2. Problem definition
3. Drafting memoranda (content and audience)
4. HOMEWORK 2 is a revision of HOMEWORK 1

SENIOR DESIGN AND PROFESSIONALISM I FALL 2019

HOMEWORK #1 (AND #2) QUESTION

Please draft and submit a problem statement and design basis comprising the elements we discussed in class at the beginning of the semester for your group's project (see your group's sharepoint folder for the full description of your project requirements). Use the sample problem statement and sample design basis documents for guidance purposes.

In completing this assignment, please be mindful and follow the parameters and guidelines for your final project to tailor your problem statement and design basis appropriately.

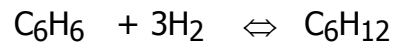
SAMPLE SOLUTION ON NEXT PAGES

September 12, 2021

TO: Prof. L.L. Martin
FROM: YOUR NAMES
RE: Simulation Case Study for the Design of a Cyclohexane Plant

In response to increased demands for polymer-grade cyclohexane, a local petrochemical chemical company is contemplating the addition of a cyclohexane plant. This company has asked our team to come up with preliminary designs for this addition. The sales department has conservatively estimated that they can sell 30×10^6 kg of poly-grade cyclohexane per year.

Cyclohexane will be made from benzene and hydrogen, via the solid-catalyzed gas-phase reaction:



Benzene is an increasingly banned, carcinogenic product formed during the catalytic reforming of naphtha, while cyclohexane is a useful intermediate in the production of nylon. Process development engineers at the company assures us that, with the new RI204 catalyst, the reaction is extremely fast; we can expect near-equilibrium conversions of benzene to cyclohexane, provided that the minimum reaction temperature is 425 K.

Please have your team do preliminary energy and material balances for a cyclohexane plant, including the sizing of all heat exchangers. For the time being, the sizing of the reactors is not critical. However, to ensure favorable equilibrium conversions and to preserve the integrity of the catalyst, the reactor temperatures should not exceed 500 K. Additionally, the molar $\text{H}_2/\text{C}_6\text{H}_{12}$ ratio in the reactor(s) should be nowhere less than 5/1. We have been informed more than once that energy costs must be minimized, so please have your team make every effort to make this an energy-efficient process.

A design basis and some basic data are attached. We will submit a simulation and final report that summarizes our analysis by December 3, 2021.

DESIGN BASIS

Plant Capacity

Design capacity: 30,000,000 kg/yr
Design operating time: 8320 hr/yr

Raw Materials

Hydrogen (gas, 99.95+% pure), at 80°F and 25 psig
Benzene (liquid, 99.95+% pure), at 80°F and 25 psig

Product Cyclohexane Specification

Liquid, 99.9% pure, at 105°F max and 25 psig

Utilities Available at Battery Limits

Steam: High pressure, saturated, at 300 psig
Medium pressure, saturated, at 150 psig
Low pressure, saturated, at 50 psig
Condensate return at 2 psig, min.
Cooling water: Available at 55 psig and 85°F, ave.
Return at 25 psig, min., and 115°F, max.

Pressure Drops for Process Streams

Heat Exchangers: 2 psi for gases (or condensation)
5 psi for liquids (or boiling)
Reactors: 10 psi maximum total

Ambient Conditions

Maximum temperature: 95°F
Minimum temperature: -10°F
Relative humidity: 25-95%
Maximum windspeed: 30 mph

ABOVE AVERAGE

September 14, 2021

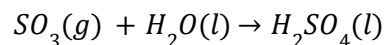
To: Prof. L.L. Martin

From: Tyecia Franklin, Taylor Linton, Wasil Mahmood and Franck Nangomoko

RE: Preliminary design of a Sulfuric acid Plant

With the growing demand for highly concentrated pure grade sulfuric acid, a fertilizer company is looking into the construction of a new sulfuric acid plant. This company has asked our team to begin preliminary designs for this addition. The sales division has estimated that they will be able to sell 2.5 million tons of sulfuric acid per year.

Sulfuric Acid will be produced from sulfur trioxide and water, as shown in the following reaction.



Sulfur trioxide is formed in a plant converter from the oxidation of sulfur dioxide with the use of a catalyst. With the combination of sulfur trioxide, water and a catalyst it leads to the generation of sulfuric acid, which acts as a building block in the formation of phosphoric acid. Process development engineers have assured us that with the use of a catalyst, it greatly decreases the reaction process time. We can expect to maintain near equilibrium conversions, with a minimum reaction temperature of 130°F.

Our team will be carrying out preliminary energy and material balances for a sulfuric acid plant along with the sizing of all reactors and heat exchangers. However, in order to ensure that the final product is in the form of a liquid, the water-treated sulfur trioxide must also be reacted with concentrated sulfuric acid. Therefore, sulfuric acid will not only be our desired product but will also act as a raw material. We are aware that the energy cost must be minimized and will make a strong effort to create an energy efficient process.

Our design basis along with other basic information is attached. We will be submitting a simulation and final report of our analysis by November 30th 2021.

Very good!!

Design Basis

Plant Capacity

Design Capacity : 2.5 million tons/year

Design Operating Time : 7200 hr/ year

Raw Materials

Oxygen (gas, 21%) at STP

Sulfur (liquid, 98.5% pure) at STP

Water (liquid 1.5%) at 77°F and 25 psig

Sulfur Dioxide (gas, 99.95+% pure)

Sulfuric acid (liquid, 98.5% pure)

Product Sulfuric Acid Specification

Liquid, 98.9% pure 250°F max and 30 psig

Utilities Available at Battery Limits

Steam:

High Pressure, saturated, at 350 psig

Medium Pressure, saturated at 150 psig

Low Pressure, saturated, at 50 psig

Cooling Water:

Available at 60 psig and 88°F

Return at 35 psig, min., and 125°F, max.

Pressure Drops for Process Streams

Heat Exchangers: 3 psi for gases (or condensation)
7 psi for liquids (or boiling)

Reactor: 15 psi maximum total

Ambient Conditions

Maximum Temperature: 116°F

Minimum Temperature: 130°F

Relative Humidity: 40-90%

Maximum Wind Speed: 20 mph

good?

To: Dr. L.L. Martin

From: Anh Nguyen
Bryson Marshall
Dayna Butler
Kennedi Henderson

RE: Design of a Phosphoric Acid Plant

In response to increased demands for merchant-grade phosphoric acid, a local fertilizer company is contemplating the addition of a phosphoric acid plant. This company has asked our team to come up with preliminary designs for this addition. The sales department has conservatively estimated that they can sell 200,000 tons of phosphoric acid per year.

Phosphoric Acid will be made from sulfuric acid and naturally occurring phosphate rock,



As the phosphate rock is continuously fed into the reactor with sulfuric acid, the reaction combines calcium, and forms gypsum (calcium sulfate). Filtration is used to separate gypsum from the reaction. Process development engineers at the company assure us that, with 93 percent sulfuric acid, this will produce the strongest product possible and decrease evaporation cost. We can expect near-equilibrium conversions of sulfuric acid to phosphoric acid, provided that the reaction temperature is kept at 340 - 350K.

Our team will do preliminary energy and material balances for a phosphoric acid plant, including the sizing of all heat exchangers and reactors. However, to ensure the gypsum is completely washed away, approximately 0.7 acres of cooling and settling pond area will be needed for every ton of daily P_2O_5 capacity. Additionally, excess H_2SO_4 is fed through several reactors until the desired conversion of phosphoric acid is reached. We have been informed more than once that energy costs must be minimized, so we will make every effort to make this an energy-efficient process.

A design basis and some basic data are attached. We will submit a simulation and final report that summarizes our analysis by November 15th, 2021.

very good

Design Basis

Capacity

Design capacity: 200,000 tons/yr
Design operating time: 8400 hr/yr

Raw materials

Phosphate rock (solid), grounded 0.15 – 2 mm (5.9×10^{-3} – 78.7×10^{-3} in)
Sulfuric acid (liquid, 93%)

Product Specification

Liquid, 75% H_3PO_4 (54% available P_2O_5)

Process

Wet process: Reaction, Filtration, Concentration

Utilities Available at Battery Limits

Reactor: stirring speed 200 rpm, pressure 15 psig
Warehouse: maximum 10% moisture for phosphate rock
Electricity: 110V
Cooling air: Available at 77°F, average
Return at 115°F, average
Wash water: Available at 85°F, 15 psig average
Emission monitor
Fuels: Liquid natural gas

Ambient Conditions

Location: Brandon, Florida
Max Temperature: 90.6°F
Min Temperature: 50.1°F
Humidity: 74%
Rainfall: 51.3 in
Windspeed: 10 mph

Very good.

AVERAGE

September 14, 2021

TO: Prof. L.L. Martin

FROM: Jarred Essissima, Doron Montgomery, Frederick Williams, Ike Anaghara

RE: Simulation Case Study for the Design of a Acetonitrile Plant

no question

Acetonitrile's continued growth worldwide has produced an opportunity to design an Acetonitrile production plant. In response to increasing acetonitrile consumption at a rate of 5-6% over a five year span, There is an increased demand of acetonitrile for use in the pharmaceutical industry as a solvent for use in pharmaceutical drugs. We were asked by one of three major producers of acetonitrile to Construct a plant to meet the increasing demand.

The process of acetonitrile formation from acetic acid and ammonia is equilibrium two-stages reaction:



Preliminary Energy, and Material balances needed for an acetonitrile plant will be completed promptly. Although at this time sizing of reactors is not critical; to ensure favorable equilibrium conversions and preserve purity of product, reaction temperatures should not exceed 400°C. Energy costs and cost efficiency are also highly suggested to be minimized.

Included you will find a design basis for the case study of our acetonitrile plant. A final simulation and report will be submitted on/before December 7, 2021.

How much?

Design Basis

Plant Capacity

Design capacity:
Design operating time:

10,000,000 to 50,000,000 lb per yr
2920 hr/yr

ok

lbs? °C?

do not mix
units.

Raw Materials

Acetic acid (liquid, 99.9+% pure), at 25°C
Ammonia (gas, 99.9+% pure), at 25°C
Water (liquid 99.9+% pure), at 25°C
 $\gamma\text{-Al}_2\text{O}_3$

Product Acetonitrile Specification

Liquid, 99.9% pure, 100°C at max and 0.20 MPa

do not
mix
units!

Ideal Pressure for Process Streams

Ammonia Catalyst: 0.217-3.045 partial pressure psi

Reactors: 14.696 psi (Fixed Packed Bed Reactor)

Ambient Conditions

Maximum temperature: 81
Minimum temperature: 60
Relative humidity: 56 - 89%
Maximum wind speed: 9.4 mph

⇒

what temperature
scale?

why?

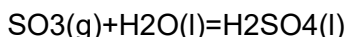
To: Prof. L.L. Martin

From: Tyecia Franklin, Taylor Linton, Wasil Mahmood and Franck Nangomoko

RE: Preliminary design of a Sulfuric acid Plant

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Sulfuric Acid will be produced from sulfur trioxide and water, as shown in the following reaction.



Sulfur trioxide is formed in a catalytic converter from the oxidation of sulfur dioxide with the use of a catalyst. With the combination of sulfur trioxide, water and a catalyst it leads to the generation of sulfuric acid, which acts as a building block in the formation of phosphoric acid. Process development engineers have assured us that with the use of a catalyst, it greatly decreases the reaction process time. We can expect to maintain near equilibrium conversions, with a minimum reaction temperature of 1800°F.

Our team will be carrying out preliminary energy and material balances for a sulfuric acid plant along with the sizing of all reactors and heat exchangers. However, in order to ensure that the final product is in the form of a liquid, the water-treated sulfur trioxide must also be reacted with concentrated sulfuric acid. Therefore, sulfuric acid will not only be our desired product but will also act as a raw material. We are aware that the energy cost must be minimized and will make a strong effort to create an energy efficient process.

Our design basis along with other basic information is attached. We will be submitting a simulation and final report of our analysis by November 30th 2021.

Design Basis

Plant Capacity

Design Capacity : 200 thousand tons/year

Design Operating Time : 8400 hr/ year

Raw Materials

Oxygen (gas, 21%) at STP

Sulfur (liquid, 98.5% pure) at STP

Water (liquid 1.5%) at 77°F and 14.7 psig

Sulfur Dioxide (gas, 99.95+% pure)

Sulfuric acid (liquid, 98.5% pure)

Product Sulfuric Acid Specification

Liquid, 98.9% pure 100°F max and 30 psig

impurity limits?

Utilities Available at Battery Limits

Steam:

High Pressure, saturated, at 350 psig

Medium Pressure, saturated at 150 psig

Low Pressure, saturated, at 14.7 psig

Cooling Water:

Available at 60 psig and 88°F

Return at 35 psig, min., and 125°F, max.

Pressure Drops for Process Streams

Heat Exchangers: 3 psi for gases (or condensation)
7 psi for liquids (or boiling)

Reactor: 15 psi maximum total

Ambient Conditions

Maximum Temperature: 110°F

Minimum Temperature: 15°F

Relative Humidity: 74%

Maximum Wind Speed: 30 mph

BELOW AVERAGE

Date??

TO: Professor Lealon. L. Martin

FROM: Ibrahim Arogundade, Ebonie Henderson, Jacquelyn Fuller, Tyree Madison

RE: Simulated Model for a plant design of L-Methionine

Agreement
or
metric?

L-methionine has been used in various industrial applications such as production of feed and food additives. L-methionine is one of the essential amino acids in all animal species. Most mammals depend on outside sources to replenish themselves with L-methionine as mammals are unable to synthesize it naturally. This has created a huge demand in several industries. In response to this demand our company devises a design of a plant that produces 50,000 tons of L-methionine per year.

L- Methionine is industrially produced from the acetylation of DL-methionine which is manufactured using the following raw materials hydrogen cyanide, acrolein, methyl mercaptan, and ammonium carbonate (All About Feed, 2020). Along with cysteine, these two compounds are the only Sulphur-containing proteinogenic and essential amino acids. Methionine is an intermediate in the biosynthesis of cysteine, carnitine, taurine, lecithin, phosphatidylcholine, and other phospholipids. Figure 1.1 depicts the process of which L-methionine is derived from

red?

??

no figure
needed for
problem statement

statement

what about
production
conditions?

product purity?
Tons? price?

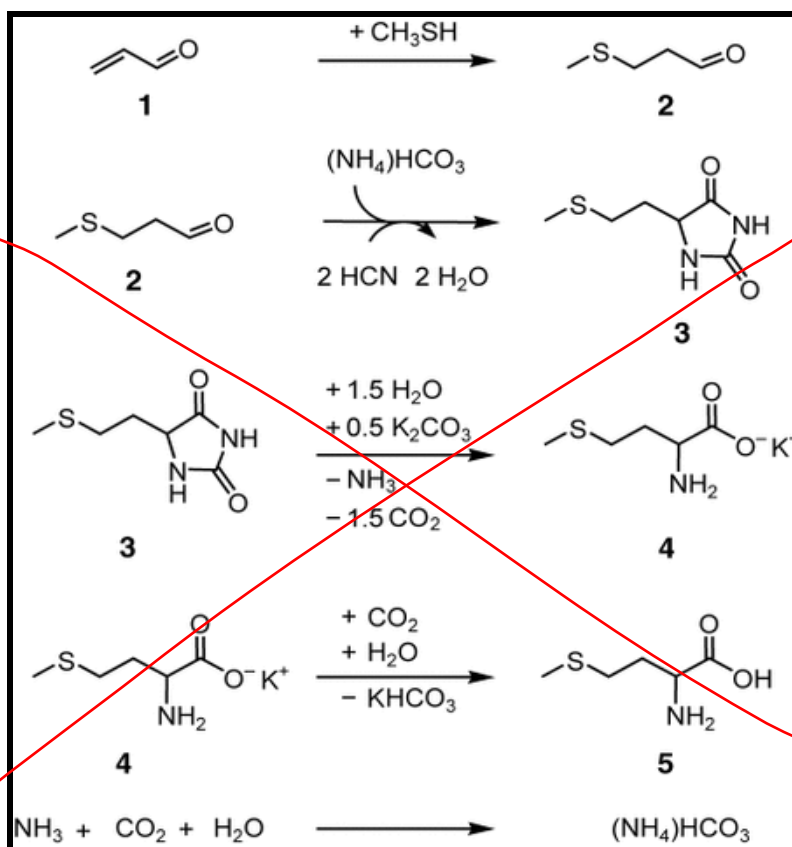


Figure 1.1 Industrial methods for the production of optically active intermediates

The team will complete preliminary energy and material balances for the manufacturing of L-Methionine; for the time being, sizing of the reactors is not critical. Furthermore, environmental factors are always important as well as staying within the guidelines of environmental protection agencies so the team will do so by preserving the amino acid by operating at moderate pressures and temperatures to reduce emission rates. Our team has been informed that operating costs must be minimized. Our team will make an effort to create an efficient process. A design basis and basic data are attached. Our team will submit a simulation and final report that summarizes our analysis by December 18, 2021.

DESIGN BASIS

Plant capacity

Design capacity: 50,000 tons/yr

Raw Materials

Acrolein (solid, pure 99.9% at 20 degrees Celsius)
Methyl mercaptan (solid, pure 99.5% at 20 degrees Celsius)
Hydrogen Cyanide (solid, pure 99.9% at 20 degrees Celsius)
Ammonia Carbonate (solid, pure 99.5% at 20 degrees Celsius)

should be in
AES

Product L-methionine Specification

Dry, 99.9% pure, at 38 degrees C max

Utilities Available

Steam:

Medium Pressure, saturated at 800 kpa
Low Pressure, saturated at 101.0 kpa

Cooling Water:

Available at 20 degrees
Return at 80 degrees Celsius max

Why??

Ambient Temperatures

Maximum Temperature: 80 degrees Celsius

Minimum Temperature: 20 degrees Celsius

80°C ambient
temperature??
This is too
hot!!

Appendix

1. The complex process of manufacturing methionine. All About Feed. (2020, December 18). Retrieved September 15, 2021, from <https://www.allaboutfeed.net/animal-feed/feed-processing/the-complex-process-of-manufacturing-methionine/>.
2. Breuer, M., Ditrich, K., Habicher, T., Hauer, B., Keßeler, M., Stürmer, R., & Zelinski, T. (2004, February 2). Industrial methods for the production of optically active intermediates. Wiley Online Library. Retrieved September 15, 2021, from <https://onlinelibrary.wiley.com/doi/full/10.1002/anie.200300599>.

TO: Prof. L.L. Martin

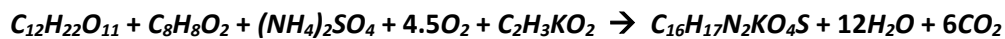
FROM: Tiarra Rodrigues, Katelynn Inman, Chiebuka Ejimadu, Caleb Myers

RE: Simulation Case Study for the Design of a Penicillin Production Plant

According to the Centers for Disease Control and Prevention (CDC), 101,567 cases of syphilis were reported in the U.S. in 2017, yielding a rate of 31.4 cases per 100,000 population as compared to previous years. The inception of the pandemic of 2020 is a prime case as well, that is projected to fuel the demand for penicillin antibiotics forecasted for 2026. The demand for medicinal penicillin in the U.S. is approximately 83 million pounds per year based on percentage of dependence on China's production.

In response to this high demand for penicillin, our team will produce a preliminary design of a penicillin plant to produce 20% of the U.S. demand. The sales department has conservatively estimated that they can sell 17 million pounds of penicillin per year to various wholesalers and pharmaceutical companies in the U.S.

Penicillin G Potassium will be synthesized from *Penicillium chrysogenum* and media containing lactose, ammonium sulfate as a nitrogen source, and an acidic precursor (phenylacetic acid) via aerobic fermentation:



It is important to note that phenylacetic acid ($C_8H_8O_2$) serves as a precursor and is fed to the reaction in lesser amounts.

Penicillin is a fungal antibiotic that is derived from the species *Penicillium chrysogenum*; it is used to treat many varieties of bacterial infections. The main two forms of first-generation penicillin – penicillin G and penicillin V – differ in that penicillin V is a derivative of penicillin G and is taken orally, unlike penicillin G, which is intravenous. Potassium acetate is introduced within the extraction phase to contribute potassium ions to the broth and further synthesize Penicillin G Potassium, which is the powder medicine used to treat various bacterial infections.

Within the design parameters we have given the annual production, cost parameters, time horizon, thermodynamic properties, and performance models of the units. Please have your team determine the optimal process design, including equipment sizes, structural alternatives and operating conditions that simultaneously maximizes the economic performance and minimize the environmental impact according to LCA principles.

A design basis is also attached to this problem statement. Our team will submit a simulation and a final report by the conclusion of this course.

What does this mean?

DESIGN BASIS

Plant Capacity

- Design Capacity: 17 million lb./yr.
- Design Operating time: 330 days/yr. (7920 hr./yr.)

low

Raw Materials

- Must provide:
 - An abundant growth of mycelium (a vegetation produced that is later recycled)
 - Maximum penicillin accumulation
 - Simply extraction and purification of the antibiotic
- Penicillin Chrysogenum (high yielding strain)
 - Necessary for antibiotic product
- Medium Materials
 - Nitrogen source - Ammonium Sulfate
 - Mineral sources
 - Oxygen
 - Carbon Source- Lactose
 - Precursor - Phenylacetic acid
- Extraction Process Materials
 - Potassium Source - Potassium Acetate
 - Acid source - Sulfuric acid
 - Solvent source - Butyl acetate
 - Activated Carbon

*no! provide
raw materials
and
conditions
of
availability*

Product Penicillin Specification

- Solid, Penicillin G K (99.5% pure)
 - Fine crystallization

ok

Utilities Available

- Heat Sterilization = 250°F, 30 psi (2.04 atm)
- Fermentation = 68°F-86°F, 15 psi (1.02 atm), pH = 6.5
- Cooling water = 77°F
- Cooler = 36°F
- Heater = 77°F

Pressure Drops for Process Streams

- Heat Sterilization = 30 psi (2.04 atm)
- Fermenter = 15 psi (1.02 atm)

Temperature Conditions

- Maximum Process Temperature = 250°F
- Minimum Process Temperature = 36°F
- Culture & Medium Ambient Temperatures = 77°F

No material balance due to laboratory-scale values. We have not completed the scale-up process based on the articles we utilized.

**SENIOR DESIGN AND PROFESSIONALISM I
FALL 2021**

Title of Assignment: HOMEWORK 3

TOPICS COVERED IN HOMEWORK 3

- 1. Literature review**
- 2. Process selection**
- 3. Production route analysis**
- 4. Process description**

**SENIOR DESIGN AND PROFESSIONALISM I
FALL 2019**

HOMEWORK #3 QUESTION

**CHEG 4472 Senior Design & Professionalism I (Fall 2019):
Assignment 3**

September 12, 2019

Due: September 26, 2019

You will be graded based on your ability to define and plan the project. Clarity of presentation is essential if you are to avoid losing points. Use the below cover page.

- (a) Create a list of major tasks and their respective duration to be accomplished to enable you achieve the goals and objectives for your project**
- (b) Organize the tasks into phases/module**
- (c) Identify sub-tasks and their respective duration**
- (d) Link major tasks and/or sub-tasks when required**
- (e) Identify milestones and deadlines to track an important event**
- (f) Prepare a Gantt Chart print out using Microsoft Project or Excel**

**DEPARTMENT OF CHEMICAL ENGINEERING
SENIOR DESIGN & PROFESSIONALISM I CHEG 4472
COURSE ASSESSMENT GRADING & OUTCOME
ASSESSMENT SHEET FOR FALL 2019 SEMESTER**

ABET Outcome 2: An ability to apply engineering design to produce solutions that meet specified needs with consideration of public health, safety, and welfare, as well as global, cultural, social, environmental, and economic factor.

Assignments that test competency in this area will include problems testing students' understanding of the design process, identification of a need, problem definition, project planning, project management, information gathering, idea generation and creativity, feasibility studies and evaluation of ideas to select the most feasible and suitable concept, appropriate of the process, performing design calculations and evaluating the design solution.

Name: _____

Title of Assignment: _____ Due Date _____

Competency Area	Max for this Assignment	Student's Score
ABET Outcome 2: An ability to design a system, a component, or process to meet desired needs within realistic constraints		
2.1. Ability to Plan the Project Students ability to (i) Define the design strategy and methodology, (ii) Identify and break down work into tasks and subtasks and identify the personnel and deliverables for each. .		
2.2. Ability to Plan the Project Students ability to (iii) Develop a Gantt chart and critical path analysis for managing the project (iv) Establish major milestones for tracking progress and define performance metrics to measure success		
TOTAL	100	

MAJOR TASKS

1. Project Conception and Definition
2. Flow sheet development
3. Reporting

PHASES

1. Phase 1 – Project conception and definition
2. Phase 2 – Flow sheet development
3. Phase 3 – Reporting

SUB-TASKS

- A. Project conception and definition
 - a. Client identification and recognition of need
 - i. Market analysis and trends: Define market- volume, quality, uses and cost of product
 - b. Process screening of alternatives
 - i. Process chemistry: Reactants, reactions (reaction stoichiometry) and products; catalysts, incomplete reactions and decomposition
 - ii. Screening processes using gross profit analysis
 - iii. Reaction kinetics and rate equations
 - iv. Handling, storage and safety: Physical and chemical properties; EPA, OSHA regulations and waste disposal
 - c. Defining process conditions and capacities
 - i. Plant capacity where product demand or raw material supply defines the feed rate
 - ii. Defining temperatures, pressures and other process variables; process description
- B. Flow Sheet Development
 - a. Process description
 - b. Preliminary Process Flow Diagram
 - i. Equipment symbols
 - ii. Process stream flow lines
 - iii. Equipment numbers and names
 - iv. Utility designations
 - v. Temperature and pressure designations on process lines
 - c. Materials and energy balances
 - i. Basis of calculations
 - ii. Material and Energy balances around each process unit: use of degree of freedom analysis, assumptions and use of heuristics

- d. Finalized Process Flow Diagram
 - i. Equipment symbols
 - ii. Process stream flow lines
 - iii. Equipment numbers and names
 - iv. Utility designations
 - v. Temperature and pressure designations on process lines
 - vi. Selected volumetric and molar flow rates
 - vii. Material balance table showing flow summary of process
- e. Computer (ASPEN/HYSYS) simulation of process
 - i. Fluid package selection
 - ii. Assumptions for modeling process units

C. Reporting

- a. Homework Assignments
- b. Midterm Report and Presentation
- c. Final End of Semester Presentation
- d. Final End of Semester Report

ABOVE AVERAGE

CHEG 4247: SENIOR DESIGN & PROFESSIONALISM I

FALL 2021

ASSIGNMENT STATEMENT/QUESTIONS

Senior Design & Professionalism I (Fall 2021): Home Work 3
Due October 26, 2021

You will be graded based on your ability to engage in life-long learning. Start each question on a new page. Clarity of presentation is essential if you are to avoid losing points.

Present a comprehensive literature review/survey of your project, citing all sources. Include (a) an introduction, (b) review of literature on production of your product including process/production routes, physical and chemical properties, handling and storage, uses and product specification, (c) process selection (using process sorting), (d) process description, stating the main steps involved in the production, and providing details of the steps involved.

Note: Make sure to use effective and well-placed subheadings, so that the sections and subheadings follow the logical sequence of the report outline.

Limiting your sources to only the internet or merely copying what you find in the literature without a brief discussion highlighting the relevance or otherwise of the information will be considered inadequate.

DEPARTMENT OF CHEMICAL ENGINEERING

SENIOR DESIGN & PROFESSIONALISM I CHEG 4247

COURSE ASSESSMENT GRADING SCHEME & OUTCOME

ABET Outcome 7: An ability to acquire and apply new knowledge as needed, using appropriate learning strategies

Assignments that test competency in this area will include problems that test a student's ability to identify, retrieve, and organize information needed for a particular new task even if the task is outside of their area of expertise.

Name: Taylor Linton, Tyecia Franklin, Wasil Mahmood, Franck Nangomoko

Title of Assignment: Homework #3 Due Date: October 26, 2021

Competency Area		
7. Ability to engage in in life-long learning	Max for this Assignment	Your Score
<i>Effectively use library and online resources for research and are abreast with current developments relating to the project</i>		
(i) Identify the types of information needed for a complete understanding of all aspects of the project (Based on task described in the project planning).	25	20
(ii) Gather information on relevant fundamentals, theory / concept (demonstrate technical competence) and relate them to the design.	50	47
(iii) Provide the sources in a list of references properly cited in the literature review section and relevant sections of the report.	25	25
TOTAL	100	92

OK. But
could be organized
better

start with the
earliest chemical
production of
sulfuric
acid

A) introduction

The origin of sulfuric acid is unknown; however, it is estimated that the first appearance of the acid can date back to the 10th century. Moving to the 15th century, the burning of sulfur with saltpeter became the first documented process for creating the compound. The implementation of the lead chamber process (first sulfuric acid mass production process) by John Roebuck in 1746 opened usability pathways for sulfuric acid by other processes. The lead chamber process, however, was made obsolete early 85 years later by the process currently utilized by modern Sulfuric Acid production systems (Austin, 1984).

In 1831 Peregrine Phillips introduced the contact process. While being known as the modern-day industry standard, the contact process was not a commercial success for nearly 40 years post-introduction. Many aspects such as lack of demand, slow technological development, and confusion related to catalytic gas reactions were all determinants for the lack of commercial success. The process first gained momentum through a boom in the dye industry, for which sulfuric acid became a necessary compound in the production of organic coloring matter.

The process itself utilized the feeding of sulfur dioxide and air over a catalyst to form sulfur trioxide, followed by its absorption in sulfuric acid (98-99%). The contact process would be later refined in modern usage; however, the foundational reaction would remain the same (Austin, 1984).

(b) Review of literature on production of your product including process/production routes, physical and chemical properties, handling and storage, uses and product specification

Production routes

As explained previously, the production of sulfuric acid is conducted through the contact process in modern production setups. A refined version of the contact process (double absorption) was utilized within our production system. The process is derivative of the foundational contact process, as it utilizes two absorption towers instead of a single a tower, to yield a higher conversion of sulfur dioxide (produced through sulfur burning) to sulfur trioxide. Vanadium pentoxide was determined to be the catalyst utilized to facilitate the double absorption process (Austin, 1984).

Physical and chemical properties

As the name suggests, sulfuric acid is a strong dibasic acid which exists as both an oxidizing and dehydrating compound. Sulfuric acid is a clear colorless, oily liquid which has a tendency of turning yellowish-amber upon aging. Physical properties and special considerations that must be taken in the processing and storage of sulfuric acid can be found below (OSHA, n.d).

Property	Value
Formula	H ₂ SO ₄
Molecular Weight	98.08 g/mol
Melting Point	51 F
Boiling Point	554 F
Relative Density (Water = 1)	1.84 (93% H ₂ SO ₄)
Odor	Odorless when cold; acrid odor upon heating
Appearance	Clear, colorless, oily liquid
Heat Capacity	1.34 kJ/(kg K)

Handling

Sulfuric acid is an extremely corrosive chemical. Special consideration must be taken into account with storage, transport, and general safety associated with sulfuric acid plant operation.

What?

The most common system utilized for the transport of sulfuric acid is through trucking, hence adequate PPE (personal protective equipment) is essential for the safe operation and handling of sulfuric acid for both plant and transportation personnel. Further information on PPE and general safety guidelines is given below.

Due to the physical nature of sulfuric acid, an emphasis must be placed on the wellbeing of all personnel working with the compound. The NFPA hazard rating diagram for sulfuric acid is shown below.



The diagram shown outlines four key safety aspects that individuals must be weary of when working with sulfuric acid. The red diamond establishes a value of 0 for compound flammability (will not burn under normal fire conditions). The yellow diamond assigns a value of 2 for instability, as the compound undergoes violent chemical changes at elevated temperature and pressures. The white diamond displays a W, which indicates a violent reaction with water. The last and possibly most important section, the blue diamond assigns a value of 3 indicating that the compound can cause serious or permanent injury. (cameochemicals, n.d; Teck, 2015)

To mitigate the dangers involved with sulfuric acid interactions the table below shows 4 separate classes of PPE, depending on an individual's expected exposure. (Veolia, n.d)

Need to connect chemical safety to your process

Class D: for low risk of exposure	• Safety glasses with side shields • Steel-toe safety shoes with PVC, neoprene or composite soles • Pants and sleeved shirt, or coveralls, made of acid-resistant polyester, acrylic or wool • Hard hat
Class C: for moderate risk of exposure	• Coverall splash goggles (a face shield can be added over the goggles if desired, but is not a replacement for goggles) • Acid-resistant gauntlet gloves • Optional, acid-resistant jacket • Optional, face shield

Class B: for high risk of exposure	• Head Protection: splash hood and hard hat (limit duration of tasks to avoid oxygen deficiency in hood) • Eye Protection: chemical splash goggles • Respiratory: not required for non-fuming sulfuric acid • Hand Protection: acid-resistant gauntlet length gloves with sleeves over gloves • Body Protection: acid suit, 1 piece or 2 piece (fabric must pass ASTM testing for $\geq 93\%$ sulfuric acid) • Foot Protection: acid-resistant boots with pant legs over boots
Class A: or maximum risk of exposure, used during an emergency leak/spill situation	• hard hat • Eye Protection: full face mask • Respiratory: NIOSH approved respiratory protection • Body Protection: acid-resistant, fully-encapsulated suit (Fabric must pass a 45 min breakthrough ASTM F739 chemical permeation test for $\geq 93\%$ Sulfuric Acid) • Foot Protection: acid-resistant boots with pant legs over boots

Storage

As mentioned previously, sulfuric acid is an aggressive oxidizer. This physical property makes it difficult to process and store sulfuric acid, as corrosion becomes a major concern for any material which is utilized in the production and storage tanks for the acid. Another major cause for concern is the relative density of sulfuric acid (Relative Density (Water = 1): 1.84 (93% H_2SO_4)). Any material which is utilized must retain structural integrity (especially in the bottom third portion of the tank where static load is highest), as sulfuric acid is nearly twice the density of water. A handful of industry standard storage systems are listed in the table below.

Steel Tanks	• Ideal for 98% sulfuric acid • May require additional lining if utilized for other concentrations
FRP (Fiberglass Reinforced Plastic) Tanks	• Can be purchased with a variety of linings • Structural layer consisting of chopped fiber glass and resin
Polyethylene or Plastic Tanks	• Consist of linear or high-density cross-linked polyethylene • Specialized in chemical containment

Secondary containment measures are recommended to mitigate the risks and hazards associated with chemical spills and leaks (PolyProcessing, n.d).

(c) Process selection (using process sorting)

The production of sulfuric acid can be carried out in several different ways. In order to determine the most efficient and cost-effective process, necessary research was conducted.

Research shows that there are three different sets of raw materials that can be used to achieve the desired product of sulfuric acid.

The first set includes the use of elemental sulfur. In this process the elemental sulfur is burned in the presence of oxygen to form sulfur dioxide. This is the most common way of producing sulfur dioxide because it is the easiest to carry out and its main raw material is relatively inexpensive and easy to obtain. The second method for producing sulfur dioxide is the

metallurgical method. It involves the use of metal ores and smelter gas burning. The use of these raw materials accounts for 20% of world production. However, it requires use of large and expensive equipment. The third way of achieving sulfur dioxide to eventually produce sulfuric acid is by way of acid regeneration. This method involves the use of spent sulfuric acid and accounts for only 10% of world production, due to its high transportation cost and production of transportation emissions.

There are different process methods of creating sulfur acid. This includes the contact method and the lead chamber method. However, the lead chamber method is almost obsolete due to its costly equipment and low concentration yield. The contact process is carried out by passing sulfur dioxide and oxygen over the catalyst vanadium pentoxide. This process is more cost effective and produces higher concentration. Within this process there are 2 types of absorption, double and single. The single absorption method yields a lower sulfuric acid concentration and involves the use of only one absorption tower. Double absorption is the most used method due to its greater conversion of SO_2 to SO_3 and greater concentration yield.

Process Sorting for Sulfuric acid production, scored 1-3 with 3 being the highest

	Sulfur Burning	Metallurgical	Acid Regeneration
Cost Effectiveness	3	1	2
Operation/ Safety	3	2	1
Usage of process	3	2	1
	9	5	4

Based on our research we have concluded that our process will involve the burning of elemental sulfur to obtain sulfur dioxide. It will be carried out using the double contact absorption process and will contain the catalyst vanadium pentoxide.

(d) process description, stating the main steps involved in the production, and providing details of the steps involved.

There are four main reactions that place within our process to produce sulfuric acid. These reactions are as listed below:

- 1) $\text{S(l)} + \text{O}_{2\text{(g)}} = \text{SO}_{2\text{(g)}}$
 - 2) $\text{SO}_{2\text{(g)}} + \frac{1}{2} \text{O}_2 = \text{SO}_{3\text{(g)}}$
 - 3) $\text{SO}_{3\text{(g)}} + \text{H}_2\text{SO}_{4\text{(l)}} = \text{H}_2\text{S}_2\text{O}_7\text{(l)}$
 - 4) $\text{H}_2\text{S}_2\text{O}_7\text{(l)} + \text{H}_2\text{O(l)} = 2\text{H}_2\text{SO}_{4\text{(l)}}$
- 

A stream of air with a composition of 21% O₂ and 79% N₂ blows into an air separator at 122,427 lb/hr. After separating the air, the nitrogen is purged out and stored in for nitrogen consumers and the oxygen is compressed to a sulfur burning furnace. The sulfur burner includes a feed of molten sulfur being pumped at 294°F and 35 psi with a flowrate of 17,140 lb/hr and the oxygen being compressed inside. Once the sulfur is oxidized, SO₂ leaves the furnace and is cooled at 770°F it will lead into the 4-pass catalytic converter.

The 4-pass converter has a 99.7% conversion rate of sulfur trioxide. The first and second stage of the converter has a 92.4% conversion rate, therefore once SO₃ and SO₂ leaves the reactor at 908°F and 29.4 psi it is slightly cooled down to 302°F so gases will be able lead into the first absorbing tower. In the third and fourth stage of the converter the gases are cooled down even more. The gases will then be 810°F and cooled to 302°F, so it now has a 7.3% conversion and leads to the second absorbing tower.

Using the absorption process of SO_2 and SO_3 assists with producing the intermediate component oleum. After the absorption process in the first absorber, oleum will pump into the first dilution tank at 203°F and 14.7 psi and SO_2 is recycled directly back into the reactor at the same temperature and pressure. When the absorption is complete in the second absorber, oleum is pumped to the second dilution tank and SO_2 is recycled back to the stream that leaves the sulfur burner and enters the reactor.

Inside of the dilution tanks oleum and water will react to make sulfuric acid. The first dilution tank pumps sulfuric acid at 97,294 lb/hr, 89°F , and 14.7 psi for storage into the acid storage tank and the concentrated sulfuric acid splits from the stream and recycled to the first absorbing tower at 48,647 lb/hr. Last, from the second dilution tank, sulfuric acid is pumped at 7,685 lb/hr, 89°F , and 14.7 psi for storage in and having concentrated sulfuric acid split from the stream to be recycled to Stream 9 at 3,842 lb/hr to lead back into the reactor. This process will lead us to producing 52,491 pounds of sulfuric acid every hour.

good.
But how will
you use this information
to make your design?

References

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AVERAGE

CHEG 4247: SENIOR DESIGN & PROFESSIONALISM I

FALL 2021

|ASSIGNMENT STATEMENT/QUESTIONS

**Senior Design & Professionalism I (Fall 2021): Home Work 3
Due October 26, 2021**

You will be graded based on your ability to engage in life-long learning. Start each question on a new page. Clarity of presentation is essential if you are to avoid losing points.

Present a comprehensive literature review/survey of your project, citing all sources. Include (a) an introduction, (b) review of literature on production of your product including process/production routes, physical and chemical properties, handling and storage, uses and product specification, (c) process selection (using process sorting), (d) process description, stating the main steps involved in the production, and providing details of the steps involved.

Note: Make sure to use effective and well-placed subheadings, so that the sections and subheadings follow the logical sequence of the report outline.

Limiting your sources to only the internet or merely copying what you find in the literature without a brief discussion highlighting the relevance or otherwise of the information will be considered inadequate.

DEPARTMENT OF CHEMICAL ENGINEERING
SENIOR DESIGN & PROFESSIONALISM I CHEG 4247
COURSE ASSESSMENT GRADING SCHEME & OUTCOME

ABET Outcome 7: An ability to acquire and apply new knowledge as needed, using appropriate learning strategies

Assignments that test competency in this area will include problems that test a student's ability to identify, retrieve, and organize information needed for a particular new task even if the task is outside of their area of expertise.

Name: Caleb Myers, Chiebuka Ejimadu, Katelynn Inman, Tiarra Rodrigues

Title of Assignment: _____ Due Date: October 26, 2021

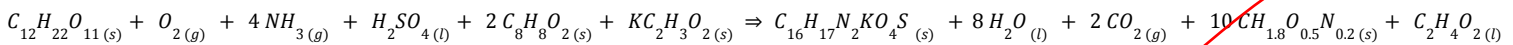
Competency Area		
7. Ability to engage in in life-long learning	Max for this Assignment	Your Score
<i>Effectively use library and online resources for research and are abreast with current developments relating to the project</i>		
(i) Identify the types of information needed for a complete understanding of all aspects of the project (Based on task described in the project planning).	25	20
(ii) Gather information on relevant fundamentals, theory / concept (demonstrate technical competence) and relate them to the design.	50	45
(iii) Provide the sources in a list of references properly cited in the literature review section and relevant sections of the report.	25	15
TOTAL	100	80

(a) An Introduction

Problem Statement (Tiarra)

According to the Centers for Disease Control and Prevention (CDC), 101,567 cases of syphilis were reported in the U.S. in 2017, yielding a rate of 31.4 cases per 100,000 population as compared to previous years. The inception of the pandemic of 2020 is a prime case as well, that is projected to fuel the demand for penicillin antibiotics forecasted for 2026. The demand for medicinal penicillin in the U.S. is approximately 34.3 million kg per year based on the percentage of dependence on China's production. In response to this high demand for Penicillin G, our team will produce a preliminary design of a Penicillin plant to produce 20% of the U.S. demand. The sales department has conservatively estimated that they can sell 6.86 million kg of penicillin per year to various wholesalers and pharmaceutical companies in the United States.

Penicillin G potassium will be synthesized from *Penicillium Chrysogenum* and media containing lactose, ammonium sulfate as a nitrogen source, and an acidic precursor (phenylacetic acid) via aerobic fermentation:



Penicillin is a fungal antibiotic that is derived from the species *Penicillium chrysogenum*; it is used to treat many varieties of bacterial infections. The main two forms of first-generation penicillin – penicillin G and penicillin V – differ in that penicillin V is a derivative of penicillin G and is taken orally, unlike penicillin G, which is intravenous. Potassium acetate is introduced within the extraction phase to contribute potassium ions to the broth and further synthesize Penicillin G Potassium, which is the powder medicine used to treat various bacterial infections. Within the design parameters we have given the annual production, cost parameters, time horizon, thermodynamic properties, and performance models of the units. Our team will present a design proposition that includes equipment sizes and structural alternatives. The facility will present stable operating conditions that simultaneously maximizes the economic performance and minimize the environmental impact.

Client Identification and Recognition of Need (Caleb)

The widespread growth of bacteria with resistance to standard antibiotics has been a topic of concern over the past few decades. Figure 1a shows the growth in the percentage of infectious bacteria that possess this resistance since 2000. Based on the trend, although the data only extends to 2014, it reveals a 2% increase in the concentration of resistant bacteria about every 6-7 years; based on this assumption, it is safe to expect over 12% of infectious bacteria to be resistant to standard antibiotics by 2022. This phenomenon has undoubtedly increased the

Content is low
but it is poorly
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demand for higher-level penicillins that are able to eradicate these evolved bacteria. Figure 1b shows the expected growth in the demand for amoxicillin over the course of the next 6 years. Amoxicillin is a penicillin antibiotic that specifically treats stomach ulcers. It is assumed that the market for other high-level penicillins will see similar increases within the decade. The primary goal of the plant is to supply its pharmaceutical clients an adequate amount of penicillin G potassium to synthesize enough high-level penicillins that can reverse this trend.

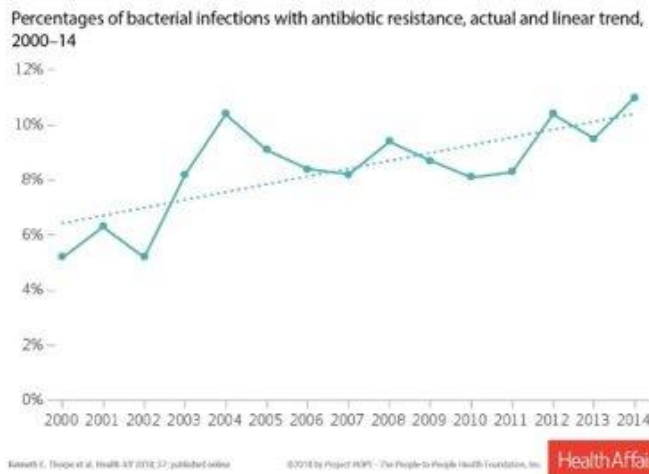


Figure 1a. Growth of bacterial infections with resistance to antibiotics from 2000-2014

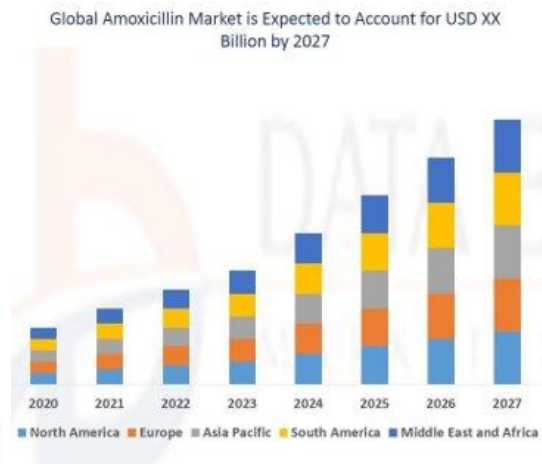


Figure 1b. Expected Growth of the Amoxicillin Market by 2027

The plant's clientele mainly consists of pharmaceutical companies, specifically Pfizer, Baxter, King Pharmaceuticals, and Sandoz. After being dried and grinded, the final penicillin G potassium recovered is in the form of crystal powder which allows for easier and more efficient handling and distribution. The powder is sent to a solid hopper via conveyor belt, and is dispensed into bulk bags that will be transported to clients by road. Once shipped to pharmaceutical buyers, the penicillin G potassium may be diluted with solution to form intravenous benzylpenicillin, or, in most cases, used to synthesize higher-level penicillins that are specialized to treat specific bacterial infections.

Project Goals and Objectives (Tiarra)

1. Determining an optimal process design simultaneously maximizes the economic performance and minimizes the environmental impact.
2. We will be selling biomass which is one of the byproducts from the process. It is created within our production and is great for outsourcing agriculturally. This will be explained further in the report.
3. Our process will also produce a purity of 99.5% Penicillin G Potassium.

Contemporary issues and impact of project on society (Tiarra)

1. Contemporary issues relevant to project

where is [1] - [7]?

The Center for Disease Control and Prevention, more commonly known as CDC, is an American government-based organization that helps stabilize the infrastructure of public health and aid in stopping the spread of diseases. From their statements, antimicrobial resistance is the leading issue concerning antibiotics [8]. The resistance occurs when bacteria evolve and develop counterattacks to withstand the drugs designed for them. These evolved bacteria continue to grow and spread and are very difficult to maintain. In more severe cases, they are impossible to kill. In the United States every year, there are 2.8 million people who become infected with antimicrobial resistant bacteria and they most likely will have to be admitted into hospitals and receive stronger doses of toxic medications [8]. Even still more than 35,000 individuals will die each year from the 2.8 million people infected [8]. Even during the COVID-19 pandemic, the CDC monitors what possible effects antimicrobial resistance could have on the nation. Below is a chart provided by the CDC of antibiotics and their resistant bacteria that evolved over time.

Table 1. List of Antibiotics and their Identified Resistant Bacteria since the Creation of each Antibiotic [8]

Antibiotic Approved or Released	Year Released	Resistant Germ Identified	Year Identified
Penicillin	1941	Penicillin-resistant <i>Staphylococcus aureus</i>	1942
		Penicillin-resistant <i>Streptococcus pneumoniae</i>	1967
		Penicillinase-producing <i>Neisseria gonorrhoeae</i>	1976

Vancomycin	1958	Plasmid-mediated vancomycin-resistant <i>Enterococcus faecium</i> Vancomycin-resistant <i>Staphylococcus aureus</i>	1988 2002
Methicillin	1960	Methicillin-resistant <i>Staphylococcus aureus</i>	1960
Extended-spectrum cephalosporins	1980 (Cefotaxime)	Extended-spectrum beta-lactamase- producing <i>Escherichia coli</i>	1983
Azithromycin	1980	Azithromycin-resistant <i>Neisseria gonorrhoeae</i>	2011
Imipenem	1985	<i>Klebsiella pneumoniae</i> carbapenemase (KPC)-producing <i>Klebsiella pneumoniae</i>	1996
Ciprofloxacin	1987	Ciprofloxacin-resistant <i>Neisseria gonorrhoeae</i>	2007
Fluconazole	1990 (FDA approved)	Fluconazole-resistant <i>Candida</i>	1988
Caspofungin	2001	Caspofungin-resistant <i>Candida</i>	2004
Daptomycin	2003	Daptomycin-resistant methicillin-resistant <i>Staphylococcus aureus</i>	2004

Ceftazidime-avibactam	2015	Ceftazidime-avibactam-resistant KPC-producing <i>Klebsiella pneumoniae</i>	2015
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[9] and [10]

2. Potential impact of project on society

Since our company's goal is to decrease the United States dependency of Penicillin G from China, our impact will come from how much product is created. The United States in theory should buy from our company to save money on import cost and support local businesses. The most damaging greenhouse gas, carbon dioxide, is released into the atmosphere from the burning of fossil fuels. Factory emissions contribute greatly to the release of carbon dioxide into the atmosphere. Industry and electrical generating factories contribute slightly more than 50 percent of greenhouse gases [11]. To combat this epidemic, our company will be implementing a carbon capture system (CCS) in place. There are three steps to this process:

1. **Capture:** the CO₂ is separated from other gases produced in industrial processes, such as those at coal and natural-gas-fired power generation plants or steel or cement factories [11].
2. **Transport:** the CO₂ is then compressed and transported via pipelines, road transport or ships to a site for storage [11].
3. **Storage:** finally, the CO₂ is injected into rock formations deep underground for permanent storage [11].

The mycelium biomass from our process is captured and sold as a byproduct for animal feed. Due to our location, Magnolia, TX, this will play a major role in our economic breakdown. There is a lot of agriculture related businesses that we will sell to. To support a large production scale, the design team must take into account the effect of the production process on the environment while utilizing inexpensive substrates and achieving high production yields. The development of a plant will provide a moderate amount of jobs for engineers, contractors and operators alike be they local or outsourced from different locations.

(b) Review of Literature on Production of Penicillin G Potassium

Penicillin G was first synthesized as..... (Tiarra)

Before the creation of antibiotics, there were no effective treatments for infections like pneumonia, and gonorrhea. Someone could contract a serious disease from a simple cut/scratch. In 1928, Professor Alexander Fleming accidentally discovered the first strain of *penicillium notatum* within his staphylococcus petri dishes. This penicillium was capable of killing a wide range of harmful bacteria. Now that scientists were able to separate the strain and cultivate it, they wanted to increase their yield to a large-scale production to be used during WWII. Penicillin was named the “wonder drug” that saved millions of lives. By 1949, the US successfully industrialized penicillin production to be distributed to pharmacies throughout the nation. After the rise of resistant bacteria, in 1961, scientists sought out alternatives to the original antibiotics. The idea of synthetic drugs formulated from the original properties was executed and this was only the beginning. Modern day penicillin is derived from a newer fungal bacteria strand *penicillium chrysogenum*. Today, penicillin is still used to treat various bacterial infections like syphilis, strep throat, meningitis and so on. Higher level penicillins are used to combat the evolved bacteria.

refs?

Production Route (Katelynn)

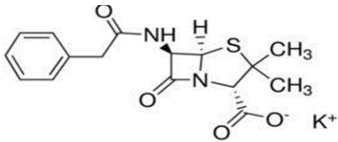
The production of Penicillin G is done through fermentation. All penicillin G is derived from the fermentation of a microorganism, *Penicillium chrysogenum*, with an addition of a precursor, phenylacetic acid. The fermentation process starts with a cell culture, a pure strain of *Penicillium chrysogenum*. In a lab the cells are added to a petri dish to increase their size, from there they are put in a flask with more medium to multiply. Once the cells have reached the max growth phase in the flask, they are transferred to the inoculum. From the inoculum into the fermenter where penicillin is produced. Then the penicillin G is sent to the extraction phase.

include
look
figura

Physical and Chemical Properties (Tiarra)

Table 2. List of Chemical and Physical Properties of the Product Penicillin G Potassium [5]

Chemical Properties	Physical Properties

Chemical Formula	$C_{16}H_{17}KN_2O_4S$	Color	White
Drug Class	Penicillin	Odor	Odorless
pH	6.5	Phase	Solid powder
Stability	Stable	Molecular Weight	372.5 kg/kmol
Solubility	Soluble in Water	Density	1.36 kg/L
Structure		Melting Point	214-217 °C
Flammability	This material is combustible, but will not ignite readily	Particle Size	10 microns
Reactivity	High accumulation results in combustion (dust explosion)	Flash Point	335 C

Handling, Storage and Safety (Tiarra)

1. Handling

- When handling, use appropriate personal protective equipment (ppe listed in safety). Individuals with direct exposure to the product should avoid inhalation and contact with skin, eye, and clothing. This is to ensure that there is no contamination transferred from

the individual to the product. Individuals should wash their hands before and after leaving the facility post PPE removal.

- When handling the product, it would be optimal to minimize dust generation and accumulation by regularly maintaining the facility, equipment, and storage of any exposed areas.

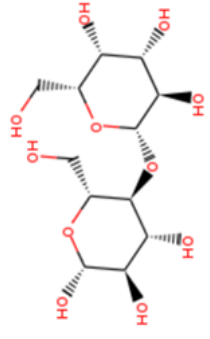
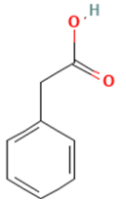
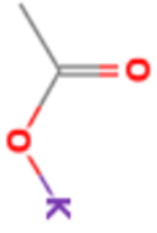
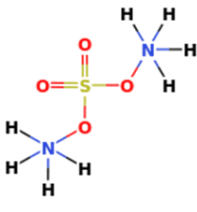
Accidental spills

- **Health and Safety Precautions:** Personnel involved in clean-up should wear appropriate personal protective equipment (listed in Safety) to limit their exposure.
- **Measures To Take for Cleaning / Collecting:** Contain the source of spill if it is safe to do so. Collect spilled material by a method that controls dust generation such as a damp cloth or a filtered vacuum. These ways are great for thoroughly cleaning spills of dry solids.
- **Additional Consideration for Large Spills:** Non-essential personnel should be evacuated from affected areas. Report emergency situations immediately. Clean up operations should only be undertaken by trained personnel.

2. Storage

Table 3 : Raw Process Materials

	Lactose	Phenylacetic Acid	Sulfuric Acid	Potassium Acetate	Ammonium Sulfate
Molecular Weight	342.3 kg/kmol	136.15 kg/kmol	98.079 kg/kmol	98.142 kg/kmol	132.14 kg/kmol
Chemical Formula	$C_{12}H_{22}O_{11}$	$C_8H_8O_2$	H_2SO_4	$C_2H_3KO_2$	$(NH_4)_2SO_4$

Chemical Structure					
Boiling Point	668.9 °C	265 °C	337 °C	117.1 °C	330 °C
Freezing Point	202.8 °C	76.5 °C	10 °C	292 °C	235 °C
Flash Point	357.8 °C	132 °C	-	> 250 °C	-
Critical Temperature	-	-	654 °C	-	250 °C
Density	1.76 kg/L	1.081 kg/L	1.83 kg/L	1.57 kg/L	1.77 kg/L

- Lactose
 - This material should be stored in a cool and ventilated place to replicate dry conditions. This material should avoid any heat source and oxidizing agents. Similar to Penicillin G Potassium, this is a white crystalline powder that if accumulated can become combustible.[4] This will be stored with materials that have similar storage requirements. This material will be transported in bulk and it is classified as not dangerous.[4]
- Phenylacetic Acid
 - This material will be stored in an airtight container with a ventilated and cooled room. This material should be kept away from incompatible substances like strong bases.[10] This will be stored with materials that have similar storage

requirements.[10] This material will be transported in bulk and it is classified as not dangerous.

- Sulfuric Acid
 - This material is a level 8 transport hazard and will be handled as such. Sulfuric acid is typically transported within an high-density polyethylene (HDPE) tank car. When arriving at the facility, this material will be placed in a cool dry room.
- Potassium Acetate
 - This material will be stored in an airtight container with a ventilated and cooled room.[12] This material should be kept away from incompatible substances. This will be stored with materials that have similar storage requirements. This material will be transported in bulk and it is classified as not dangerous.
- Ammonium Sulfate
 - This material should be stored in a cool and ventilated place to replicate dry conditions. This material should avoid any heat source and oxidizing agents. This will be stored with materials that have similar storage requirements. This material will be transported in bulk and it is classified as not dangerous.

3. *Safety*

Personal Protective Equipment:

- **Hands:** Wear suitable protective gloves according to EN 374. It is recommended to test the chemical resistance of the gloves with the supplier. The gloves should be made of nitrile rubber (NBR) and have a 0.11 mm layer thickness. There should be a minimum level 6 permeation of breakthrough.
- **Eyes:** Wear safety glasses or goggles if eye contact is possible.
- **Skin:** Wear protective clothing when working with large quantities.
- **Respiratory protection:** If airborne exposures are within or exceed the Occupational Exposure Band (OEB) range, wear an appropriate respirator with a protection factor sufficient to control exposures to the bottom of the OEB range. Respiratory protective gear is necessary when dust formation is visible. At this point the individual should wear a respirator with a particulate filter (P2) meeting EN 143 standards. The filters should be able to combat 94% of airborne particles.

First Aid Measures:

- **Eye Contact:** If contact is made, the individual must immediately flush their eyes with water for at least 15 minutes. If the irritation occurs or persists, they will need to receive medical attention.[7]
- **Skin Contact:** Any articles of contaminated clothing must be removed. Flush area where the product came in contact with with large amounts of water and use soap (wash clothing).[7]

- **Ingestion:** One should never give anything by mouth to an unconscious person. Rinse out the individual's mouth with water. Lastly, do not induce vomiting unless directed by medical personnel.[7]
- **Inhalation:** The individual should remove themselves from the contaminated environment and move to fresh air and rest. Also they should seek medical attention immediately.[7]

Reactivity: Initially, the state of the product at delivery is not explosive, however, when there is a large accumulation of fine particles this will lead to a dangerous dust explosion.[9] A dust explosion is defined as a combustion of suspended particles in the air within an enclosed area. These dangerous situations can happen where there is a powdered combustible material in high concentrations within the air and another oxidizing gas (i.e., pure oxygen).[9]

Measures for Environmental Protections: Place waste in an appropriately labeled, sealed container for disposal to avoid environmental release. The product should be kept from drains, ground and surface water as well. We are choosing to implement appropriate technical and procedural waste water and waste disposal measures to prevent occupational exposure or environmental releases. Potential points of process emissions of this material to the atmosphere should be controlled with dust collectors, HEPA filtration systems, or other equivalent controllers.

What are process implications?

Uses (Tiarra & Caleb)

The two main uses of Penicillin G Potassium are to treat various bacterial infections like pneumonia, strep throat, and syphilis, and to serve as a precursor to high-level penicillins that may be resistant to natural antibiotics. Because antimicrobial resistance has become one of the greatest global health threats in recent years, new synthetic strains of antibiotics are created to eradicate the bacteria entirely rather than simply inhibiting growth.

Penicillin G in its natural state, is a white powder. The powder can be dissolved in water and injected into a muscle or vein, but the solution may also be administered directly into the lining of the chest cavity, into the fluid surrounding the spinal cord, or into a joint. Conventional antibiotics are derived from natural sources, typically from certain fungi or soil bacteria, and therefore rely on timely fermentation processes that require large-scale bacterial cultures and several subsequent purification stages. They are not designed to avoid resistance. In contrast, synthetic antibiotics are exclusively synthesized in labs to be potent enough to mitigate the threat posed by these evolved bacteria. Unlike their precursor, penicillin G, many synthetic penicillins, such as amoxicillin, may be administered orally.

Product Specification (Tiarra & Katelynn)

Table 4: Product Specification

Purity	99.5% Penicillin G Potassium
Product Recovery	78%

Our product Penicillin G Potassium is a white crystalline powder which is odorless and moderately hygroscopic.[6] Penicillin G potassium is very soluble in water. The pH of the reconstituted product is between 6.0–8.5.[6] The particle size of the will be around 10 microns which is not visible to the naked eye. We chose this size because we wanted a fine particle that is able to be produced consistently and easily stores away. Our product purity is specified as 99.5% Penicillin G Potassium.

(c) Process Selection

Market Analysis and Trends (BUKA)

Natural Penicillin like Penicillin G or V, are major active ingredients for higher-level synthetic penicillin that combat more aggressive bacterial infections/diseases. The global market of penicillin is a very dynamic space, but the demand is forecasted to increase in the coming years due to the increase of drug-resistant bacterial infections. For this project, Penicillin G is our focus. Due to limited market data because most were restricted since it's mostly under China's control, we made a few educational assumptions based on literature study and various historical data that we found. The world production of penicillin was about 105,000 metric tons/year, which is equivalently 95.3 million kg/yr. Based on literature study, China is the main manufacturer of Penicillin G. They produce nearly all of the Penicillin G globally so we assumed a basis of 90 %. Also, the United States is a major importer of Penicillin G from China and they receive about 40-45% of the production [2]. As a desired plant capacity, we assumed 20 % of US demand to fulfill the lack of Penicillin G manufacturing in the United States and to relinquish some percentage of dependence from China in terms of major ingredients to make higher-level penicillin. The calculation to find the desired plant capacity is shown below:

World Production – 105,000 Tons/yr (95.3 million kg/yr)

Nearly all of Penicillin G Production is in China (Assumed 90%)

US demand from China (40% Import)

Desired Plant Capacity (Assumed 20% of US Demand)

To find Plant Capacity ...

$(95.3 \text{ million kg/yr} * 0.9 * 0.4 * 0.2) = 6.86 \text{ million kg/yr}$

fermenting

good!

Medium routes to producing products (Katelynn)

- 1. Penicillin G industrial process and lab/patent routes have been reported to be used for producing Penicillin*

The production process to produce penicillin G has two parts, fermentation and extraction. The Fermentation process starts with a cell culture, a pure strain of penicillium chrysogenum. The cell culture is freeze dried and transferred with viable spores of the microorganism. In a lab the microorganism is introduced to a medium that will provide nutrients for it to grow. Once the

cells have reached maximum growth it will be transferred to the inoculum tank to start the production of penicillin G. Once the cells have reached peak production of penicillin G it will be transferred to a fermenter. In the fermenter it will continue to produce penicillin G at its peak production rate, allowing the cells to produce the highest yield possible of Penicillin G. The medium was chosen due to it producing the highest yield of Penicillin G compared to others. A carbon source is needed in the medium most being some type of sugar. A simple sugar is best to use as it is easily absorbed by microorganisms allowing a higher number of primary metabolites to be produced. In figure 3 it shows the relation of 5 mediums, one being potato dextrose broth and the other various carbon sources contain, glucose, lactose, maltose, and sucrose; to the concentration of penicillin G those mediums produce. From figure 3 it shows that the potato dextrose medium broth and lactose medium broth produced the highest concentration of penicillin G.

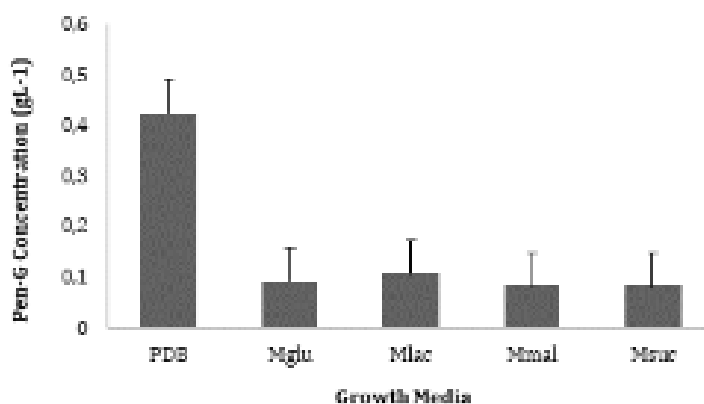


Figure 3. Penicillin G production from *Penicillium chrysogenum* in Various Mediums

In the industry of penicillin G production, a precursor is needed. The precursor allows a higher change of microbes to produce a specific penicillin depending on the precursor. The precursor, phenylacetic acid, acts as a hydrophobic side chain of benzylpenicillin allowing *P. chrysogenum* to specifically produce Penicillin G. The mediums with an addition of a precursor, phenyl acetic acid, give a significantly different result. The penicillin G produced with varied carbon sources have a much lower concentration than the mediums with an addition of PAA. With proper doses the PAA allows optimum Pen G production. The mediums that produced the highest concentration of Pen G without PAA were potato dextrose broth and lactose medium broth. Figure 4 shows the comparison of the 2 mediums with various concentrations of phenylacetic acid and the concentration amount of pen g that they produced. From the graph the Lactose Medium F produced the highest concentration of penicillin G with a PAA concentration of 0.6g/L to be used to derive a relationship in order to find the scaled up concentration for our industrial-size plant.

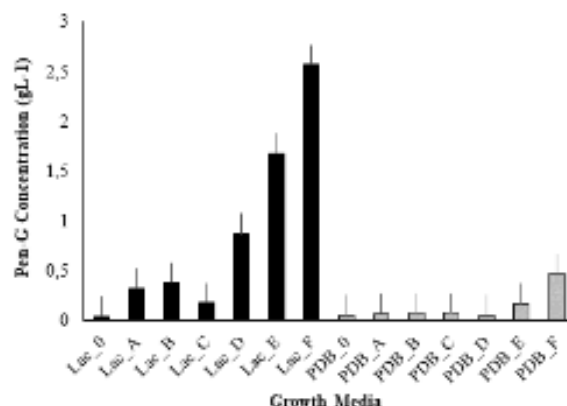


Figure 4. Penicillin Production from *Penicillium chrysogenum* with Various Concentrations of Phenylacetic Acid

2. Medium route 1

The medium is the nutrition factor that governs growth and production of penicillin G by *P. chrysogenum*. The penicillin G medium is first introduced as lab-scale of the process. The medium broth is a standard medium with a lactose carbon source and phenyl-acetic acid precursor. The medium is composed of the following components shown in figure 5. In figure 5 the carbon source chosen is lactose and the composition of the precursor, phenyl-acetic acid, is 0.6g/L. The *penicillium chrysogenum* is inoculated in the medium at room temperature for 48 hours. The medium is then incubated for 10 days with agitation at room temperature. Phenyl acetic acid is added 3 days after the bio production of fungi takes place. Once inoculation is complete the medium produces a 2.46 g/L yield of penicillin G (Sari 2020).

No.	Production medium	Weight (g)
1	KH_2PO_4	0.4
2	$(\text{NH}_4)_2\text{SO}_4$	0.45
3	$\text{MgSO}_4 \cdot 7\text{H}_2\text{O}$	0.05
4	$\text{Na}_2\text{SO}_4 \cdot 7\text{H}_2\text{O}$	0.15
5	$\text{ZnSO}_4 \cdot 7\text{H}_2\text{O}$	0.2
6	Yeast Extract	0.5
7	Phenylacetic Acid (PAA)	0-0.6
8	Carbon Source Variation (Lac, Glu, Suc, Mal) and PDB	1.5

Notes: Lac= Lactose, Glu= Glucose, Suc= Sucrose, Mal= Maltose and PDB as standard medium. PAA concentration variation (0, A, B, C, D, E, F). 0= 0 gL⁻¹; A= 0.1 gL⁻¹; B= 0.2 gL⁻¹; C= 0.3 gL⁻¹; D= 0.4 gL⁻¹; E= 0.5 gL⁻¹; F= 0.6 gL⁻¹

Figure 5. Penicillin G Production Medium Composition with Various Carbon Sources

The information from this article was utilized to derive a relationship to create an industry scaled process. The composition of the components in the medium were scaled up to find the mass fractions needed to produce penicillin G in a process plant.

3. *Medium route 2*

Another medium that was reflected upon was a potato dextrose broth medium. This broth is created by the fermentation of potato skins in distilled water. This medium was economically cheaper than the lactose medium selected. The reason this medium was eliminated from the process was due to it producing a smaller yield of penicillin g compared to the lactose medium once the precursor, phenyl-acetic acid, was added. As well the potato dextrose broth medium contains complex sugars that would need to be hydrolyzed by enzymes into simple sugars (Sari 2020). In order for the fungus to hydrolyze these sugars it would have to produce the enzymes to break down the complex sugar into a simple sugar making the fungus work harder.

Process Economy of Overall Reaction (Katelynn)

Overall Reaction Path:

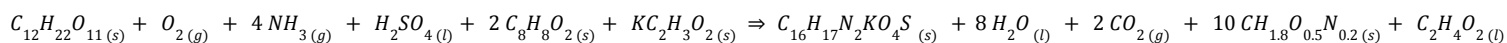


Table 5. Overall Reaction Component Cost

Components	kg-mole	Molecular Weight (g/mol)	kg	kg/kg of Penicillin G Potassium	\$/kg
Lactose	1	342.3	0.342	0.917	
Oxygen	1	16	0.016	.043	
Ammonia	4	17.031	3200 kg/h of ammonium sulfate		
Sulfuric Acid	1	98.079	0.098	0.263	
Potassium Acetate	2	98.15	0.098	0.263	
Penicillin G Potassium	1	372.5	0.373	1	

Martin Team 2

Water	8	18.01528	0.018	0.048	
Carbon Dioxide	2	44.01	0.044	0.118	
Biomass	10				
Acetic Acid	1	60.052	0.060	0.161	

Theoretical Profit = [Cost of Products] - [Cost of Reactants]

$[\$(1) + \$(1) + \$(4) + \$(1) + \$(2) + \$(1)] - [\$(1) + \$(8) + \$(2) + \$(10)] =$

The theoretical profit indicator is about... showing that our process is profitable.

(d) Process Description

Very good

In the creation of penicillin, there are two main reactions that occur within the process. Reaction (1) is the fermentation process occurring with the presence of a carbon source, nitrogen source, oxygen and other components to produce Penicillin G. Reaction (2) is the crystallization reaction that occurs with the addition of potassium acetate to form Penicillin G Potassium crystals from Penicillin G. Each reaction has a letter that corresponds to each component. It has been shown below:

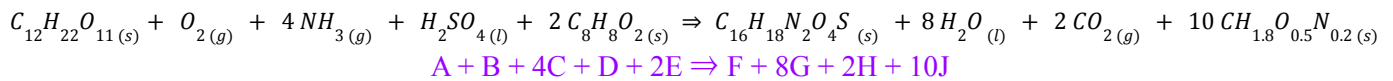
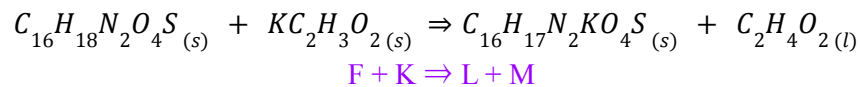
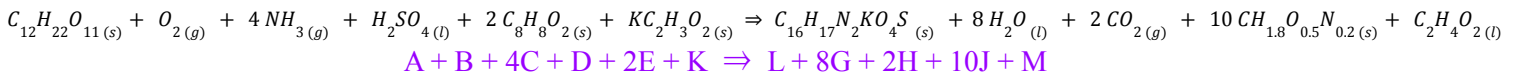
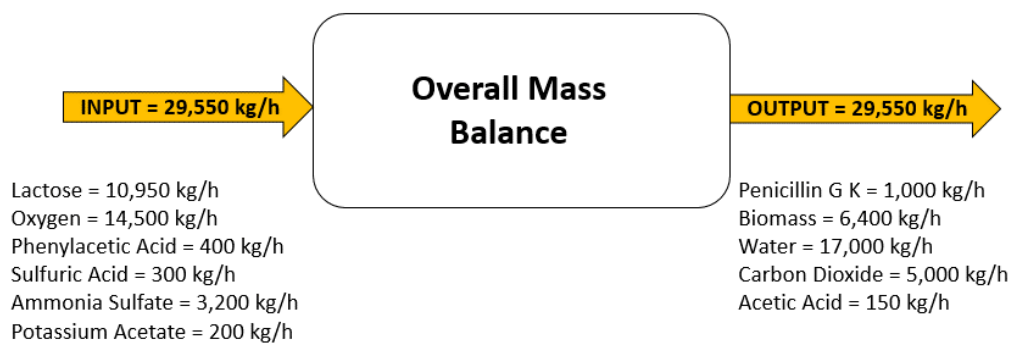
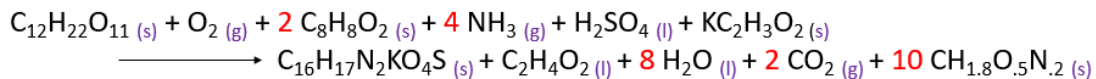
Reaction Mechanisms (BUKA)**Reaction 1: Fermentation****Reaction 2: Crystallization of Penicillin G Potassium****Overall Reaction:****Overall Mass Balance (Buka)**

Figure 6. Overall Mass Balance across the Entire Process

Raw Material Preparation (Caleb)

Raw Materials

- ***P. chrysogenum* cells**
 - Obtained in a freeze-dried state from a laboratory. Cell culture will ultimately be grown to a concentration of 66 g/L before entering the bioreactor.
- **Lactose**
 - Pure lactose solids in powder form. Exists as a solid at room temperature. Being the carbon source for biomass, lactose has a much higher concentration in the medium than the other minerals.
- **Phenylacetic acid**
 - Highly concentrated powder (54.8 g/L). Exists as a solid at room temperature. Is necessary for the growth of penicillin G, but fed at a considerably low concentration to avoid inhibiting fungal growth.
- **Sulfuric acid**
 - Highly concentrated sulfuric acid. Exists as a liquid at room temperature. Centrifugally pumped to tank V-202 to substantially decrease the pH of the agitated mixture.
- **Potassium acetate**
 - Used in powder form. Exists as a hygroscopic solid at room temperature. Potassium ion is necessary to deprotonate penicillin G within the crystallizer.
- **Ammonium Sulfate**
 - Powder that is very soluble in water. Exists as a solid at room temperature. Because it serves as the nitrogen source for biomass, ammonium sulfate is the second-most concentrated species within the design medium, behind lactose.
- **Butyl acetate**
 - Serves as the solvent for the penicillin extraction process. Exists as a colorless liquid at room temperature. Supplied in large amounts for liquid-liquid extraction and in many instances of crystal washing.
- **Air**
 - Approximately 78% N₂ and 22% O₂. Enters with a massive flow rate to satisfy the needs of the aerobic fermentation.

Utilities

- **Cooling water**
 - Used to maintain a steady fermentation temperature within the jacketed bioreactor. Also used as a heat transfer medium to reduce the temperature of penicillin G broth from the bioreactor before passing through the rotary vacuum filter.
- **Chilled water**

- Used to reduce the temperature of the penicillin G broth from the first rotary vacuum filter before entering the mixing tank. Also used in the jacketed heat sterilizers to reduce the streams back to their inlet temperatures after sterilization.
- **Steam**
 - Used to sterilize inlet air and medium impurities before they enter the bioreactor. Also used to slightly increase the temperature of the air and medium to the fermentation temperature after sterilization.

Reaction and Fermenter Operation (BUKA & Caleb)

Prior to the bioreaction, in which *P. chrysogenum* cells will undergo fermentation within bioreactors to produce penicillin G, the raw materials must first be properly prepared. The inlets of the bioreactor include the inoculum and the fermentation medium, which will be fed to the reactor separately from each other.

The growth and multiplication of *P. chrysogenum* cells occurs in four phases: the lag phase, growth phase, stationary phase, and decline phase. In the lag phase, the cells become acclimated to the medium they have been introduced to and undergo the necessary metabolic processes for eventual cell multiplication. After this, they enter the growth phase and the concentration of cells in the inoculum increases exponentially. At a certain point, the cells will have absorbed most of the nutrients in the medium and the concentration will converge to a certain range (stationary phase) before eventually decreasing again due to the absence of adequate carbon and nitrogen sources within the broth. This fungal cell growth from the growth to stationary phase occurs in logarithmic fashion.

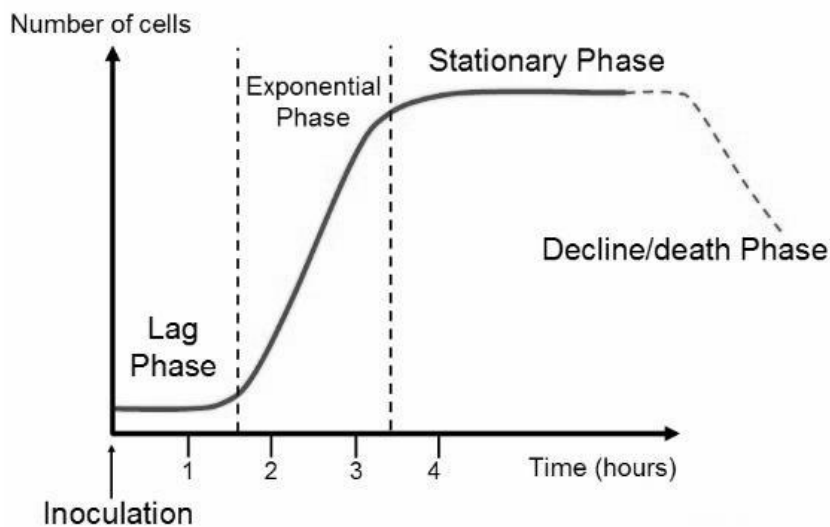
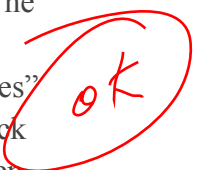


Figure 7. Phased Fungal Cell Growth Curve

In order to thoroughly explain the processes preceding fermentation, both the inoculum and fermentation medium will be discussed independently.

Inoculum

The inoculum, which is a conglomerate of both fungal cell biomass and fermentation medium minerals, must undergo preparation prior to being ready for admission into the bioreactor. The goal of the preceding process is to increase the concentration of cells in broth to a value sufficient enough for a resulting yield of penicillin G by introducing the cells to “food sources” (primarily sources of carbon and nitrogen) that will promote rapid cell growth. Initially, stock cultures of freeze-dried *P. chrysogenum* cells are obtained via laboratory. These cells are then extracted from their stock container and brought to an agar plate, which will serve as the site for the cells’ initial introduction to the fermentation medium. Before the cells can multiply, they must first enter the *lag phase*, in which they may become accustomed to their new environment before being able to multiply. A small amount of medium must be added to the agar plate containing these fungal cells in order to initiate this process. During the lag phase, cells synthesize enzymes necessary for growth; although the cell concentration does not yet increase, the cells do increase in size. 

Following the conclusion of the lag phase is the *growth phase*, in which the cells use nutrients from the fermentation medium to increase in concentration. The new cells, having increased in size after exiting the lag phase, are transferred from the agar plate to a flask and reintroduced to fermentation medium. By this time, the cells have adapted to these conditions and the concentration of cells begins to increase. This process will have to be repeated various times to increase the cell concentration to a level sufficient enough for the full-scale bioreactor. For this specific design, a cell concentration of 66 g/L and temperature of 30 degrees Celsius within the agitated inoculum tank (V-103) are desired before releasing it into the bioreactor. Once this concentration is reached, the contents are pumped to the fermenter (V-104) to eventually coexist with a high concentration of fermentation medium.

The overall material balance across the fermenter is shown below. Because this fungal fermentation is an aerobic process, an inlet stream of air is required to provide an adequate supply of O₂ for the biochemical reaction. The extracted air first enters a compressor (C-101) in order to increase its pressure to 2.04 atm, and is then passed across a heat sterilizer (E-103) to destroy lingering microorganisms. Afterwards, the air reaches a heater (E-104) and its temperature raised from ambient conditions to 30 degrees Celsius before entering the fermenter from the bottom. Another stream to consider is that of the exhaust gas leaving from the top of the fermenter, which is composed of O₂ and N₂ (from inlet air) and CO₂ (fermentation byproduct).

Unit Balance: Fermenter

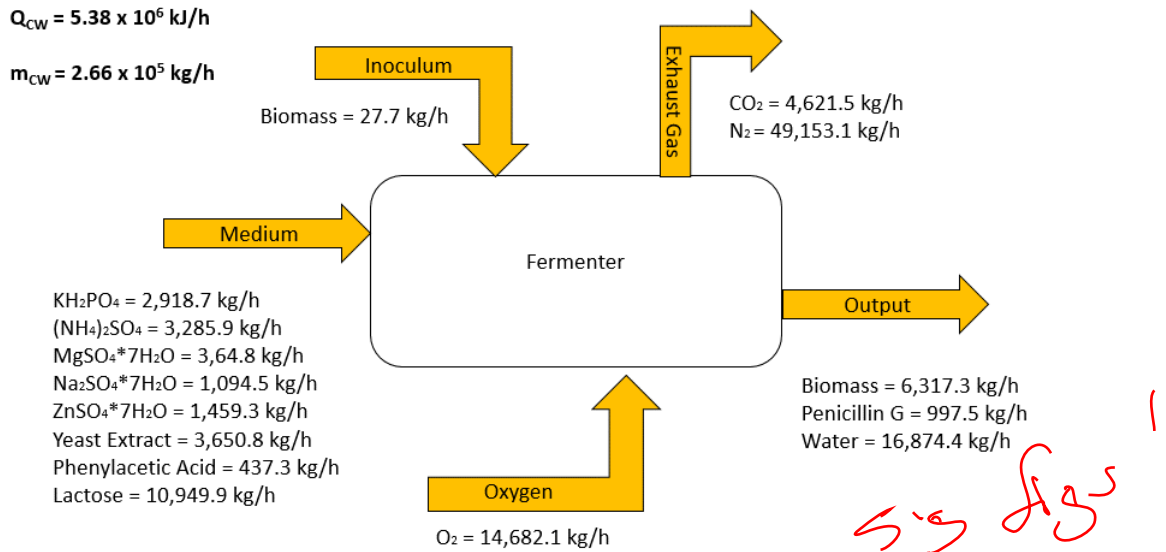


Figure 8. Material Balance across Fermenter

Medium

Because the growth of fungal cells primarily requires an abundance of a carbon source (lactose), it is initially stored separately from the rest of the minerals and phenylacetic acid in the medium, which are stored together.

Lactose will be in solid form stored in a hopper (TK-101) before being transported to an agitated medium tank (V-102) via conveyor belt. The rest of the medium components, before entering the agitated mineral tank (V-101), must be stored in their respective tanks or hoppers; liquid constituents will be pumped through pipes to V-101, while solid constituents, like lactose, must also be stored in solid hoppers and transported via conveyor. The mineral solution will then be pumped into the agitated medium tank. The design will feature multiple batch medium tanks in parallel to compensate for time required for solids to dissolve into the broth. After exiting the medium tank, the complete medium will be pumped to a heat sterilizer (E-101) to eliminate any impurities from the solution and then heated (E-102) to 30 degrees Celsius prior to entering the fed-batch fermenter (V-104). At the same time, the biomass will be entering in the fermenter from the inoculum tank (V-103). The fermentation process will be conducted at 30 degrees Celsius and 1.02 atm. The fermentation time will be 120 hours, which includes the growth phase, production phase, cleaning and so on. The design includes multiple fermenters in parallel to maintain a continuous process, as certain fermenters will undergo cleaning at different times. The fermenter's output stream includes the intermediate product penicillin G, high amounts of water and lots of biomass. The full fermentation phase of the *P. chrysogenum* is shown below:

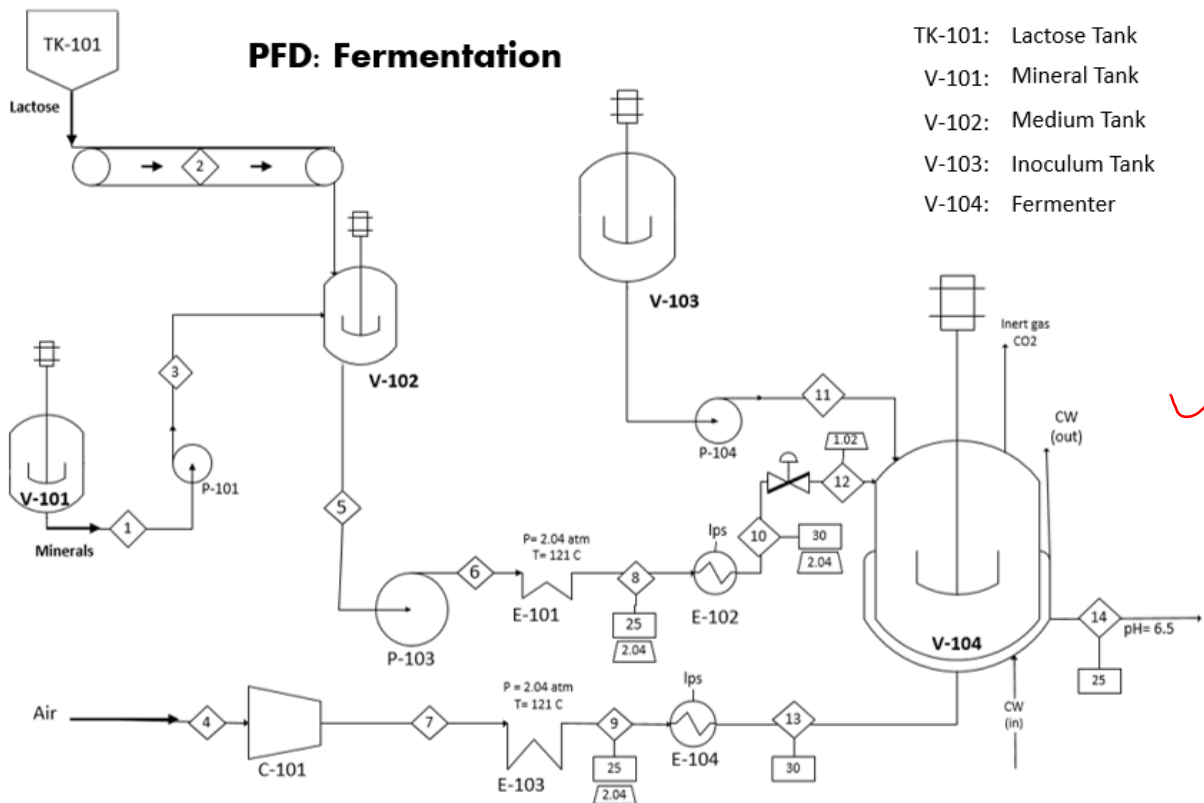


Figure 9. Process Flow Diagram of the Fermentation of *P. chrysogenum* to Produce Penicillin G

Separation Units (BUKA)

The extraction process begins after the fermentation process. The main purpose is to stabilize and isolate our final product at a high purity to be sold to our various clients. This process involves various units and equipment that performs different separations of solids from liquid like rotary vacuum filters, and liquid-liquid extraction like solvent extractor, that can transfer mass based on solubility of desired component from one liquid to liquid. As a result of fermentation, a mixture of biomass, water and Penicillin G goes through a rotary vacuum filter (V-201) to remove the biomass, which will be sold for agricultural purposes and animal feed. It will be cooled with a cooler (E-202) to 2 degrees celsius to prevent the product intermediate to degrade. Next, the mixing tank (V-202) is introduced to add sulfuric acid and butyl acetate (solvent) together, which results in penicillin G being soluble in solvent to be extracted in the solvent extractor (V-201). The carbon adsorption tower (T-201) removes the color and odor for a pure, colorless hue for the broth. Next step is to introduce it in the crystallizer to form crystals of Penicillin G Potassium with the presence of potassium acetate. It will go through the first crystal filter (V-205), re-washed in a crystal washing tank (V-206) and filtered again in another crystal filter (V-207). Finally, it is sent to a vacuum dryer (E-203) to dry off the product crystals before

being sent to a grinder (V-208). It is stored in a hopper (TK-206) and then packaged in bulk bags. The image below shows the process of the Penicillin G broth going through each separation unit until it is ready for product storage:

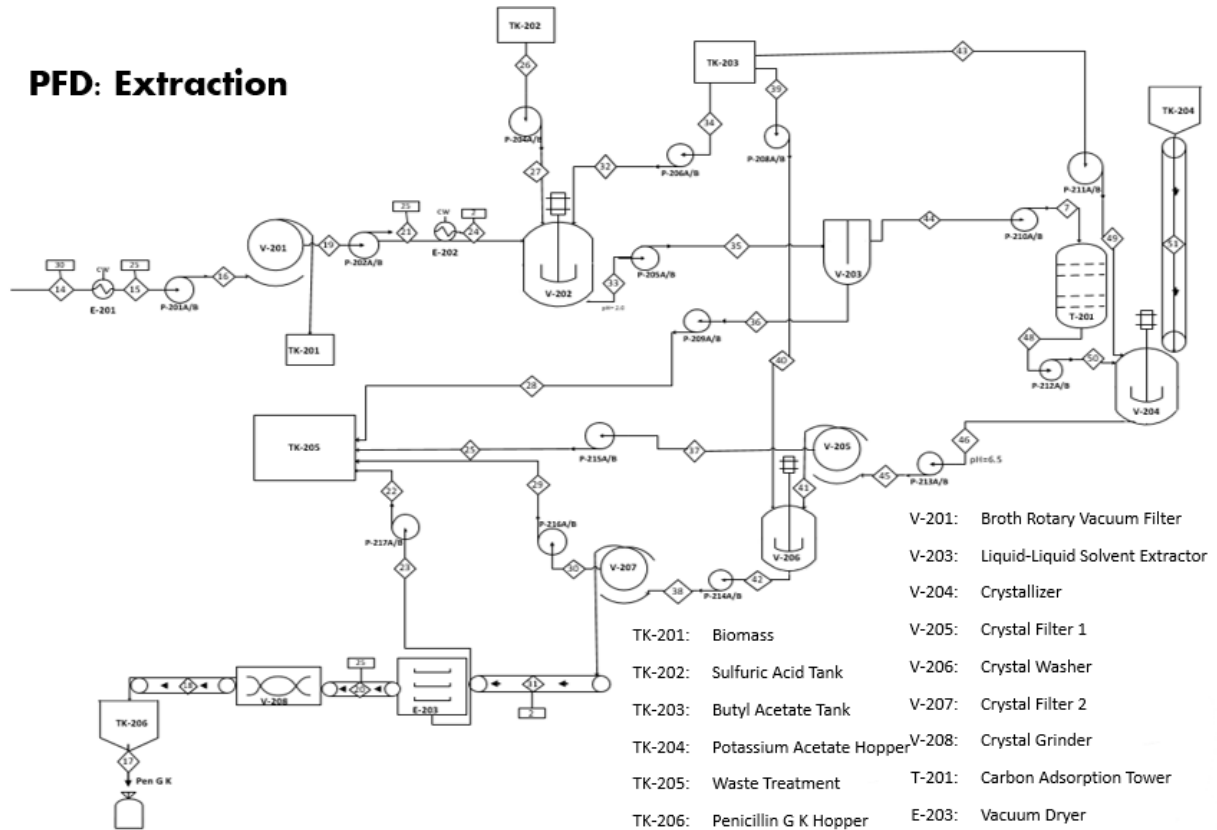


Figure 10. Process Flow Diagram of the Extraction of Penicillin G Potassium

Product Storage (Tiarra & Buka)

The product will be stored in super sacks (bulk bags) post-process and placed in a dry refrigerated room awaiting transportation to our clients. Our product, Penicillin G Potassium, has a 7-day maximum life expectancy at room temperature before it degrades. However, the product will be stored in a refrigerated room at 4 °C. This condition helps extend the shelf life of the product for up to 3 months.

Basis of Calculations and Major Assumptions (Buka & Caleb)

Based on the previously discussed global market analysis conducted by the team of engineers, a production capacity of 6.86 million kg/yr was determined to be feasible to satisfy 20% of the U.S. demand for penicillin. Our plant will have about 90% uptime, based on the fact that it will

operate for 330 days (7,920 hours) out of the year; the other 35 days will be used as a buffer for unscheduled downtime. The plant efficiency was also determined to be 78%, which was obtained from literature analysis for general penicillin processes. Lastly, a feasible specific production rate of 0.15g penicillin G/Lhr was obtained from literature and used to determine the necessary working volume.

The team's basis calculations were obtained for a period of 1 year for simplification purposes. A molar mass ratio of 1.11 was derived from the division of penicillin G potassium's molar mass by that of penicillin G. Dividing the plant capacity by this ratio revealed that 6.18 million kg penicillin G is required as a fermenter output. Because the plant is 78% efficient, it became apparent that more than 6.18 million kg penicillin G is required in order to satisfy the resulting losses of penicillin G potassium. Dividing the plant capacity by 0.78 yields a temporary capacity of 8.80 million kg penicillin G potassium that was solely used to calculate the required production rate of penicillin G. Dividing this plant capacity by the molar mass ratio (1.11) once more yielded a production rate of 7.90 million kg penicillin G, which is the required capacity of the fermenter. Next, dividing this penicillin G by the plant's operating time of 7,920 hours resulted in a required flow rate of 1 million g penicillin G/hr from the fermenter. Finally, the team manipulated the specific production rate of penicillin G (0.15g/Lhr) to obtain a mass flow rate on the basis of 1 L working volume (0.15g penicillin G/hr/1L). A proportional relationship between this production rate and the required flow rate of penicillin G out of the fermenter (1 million g/hr) was used to solve for the required working volume of the full-scale process, which was determined to be about 6.65 million liters.

The extraction process recovers 78% of the desired product output. The extraction process includes various equipment like rotary vacuum filters for both removal of biomass and crystal filtration, mixing tanks, solvent extractor, carbon adsorption tower, crystallizer, and vacuum drying. Based on literature, the product recovery percentage for each major unit was obtained. The first major unit, solid-liquid separator called rotary vacuum filter, recovers 93% of the penicillin G while the rest leaves with the majority of biomass. Following, the solvent extractor recovers 80% - 90% of penicillin G based on current process research so we assumed 86% for our process. The rotary vacuum filters for both of the crystal filters were assumed to have a product recovery of 99%. For the rest of the units being used for the extraction process, we assumed the output was 100%. Our basis with the crystallizer was assumed that all of the penicillin G is converted to penicillin G potassium when introduced to potassium acetate.

Based on these calculations for the required production rate of penicillin G and total working volume, the team worked backwards to find required feed conditions for the fermenter and eventually find material balances across each unit using their product recoveries as well.

Material Balance of each Unit (Buka)

After exiting the fermenter, the resulting mixture of Penicillin G, water and biomass will be heading towards the extraction process. There are several units used to transform the product intermediate of Penicillin G to our desired product of Penicillin G Potassium to be stored and sold to our clients. The units are shown below:

Rotary Vacuum Filter (RVF)

A rotary vacuum filter is used to separate solids from liquids. In this case, we are trying to remove biomass in order to concentrate the Penicillin G in the broth solution. We assumed that the large amount of biomass removed will be 93%, but also small amounts of Penicillin G (7%) and water (8%) are lost at this stage as well.

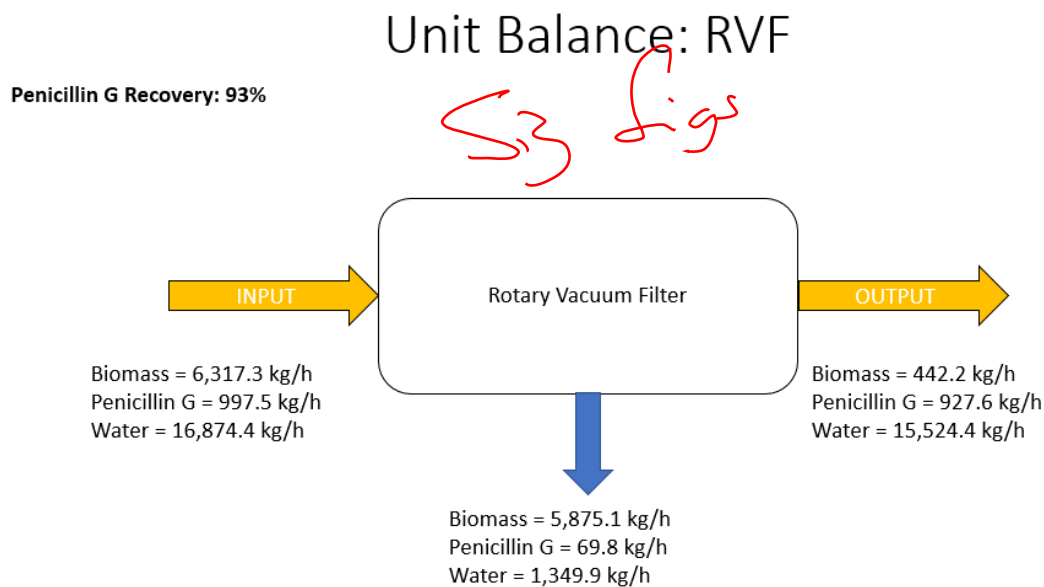


Figure 11. Material Balance across Broth Rotary Vacuum Filter

Mixing Tank

The purpose of this mixing tank is to agitate the combination of Penicillin G broth with the newly added components of sulfuric acid and butyl acetate, which is the solvent. Sulfuric acid was added based on the relationship between itself and Penicillin G produced on Reaction (1). Based on literature review, butyl acetate is added at 0.25 g butyl acetate/ g broth. Adding sulfuric acid is for adjusting the pH level down to 2, which is when Penicillin G exists as an undissociated acid making it soluble in organic solvents like butyl acetate.

Unit Balance: Mixing Tank

Penicillin G Recovery: 100%

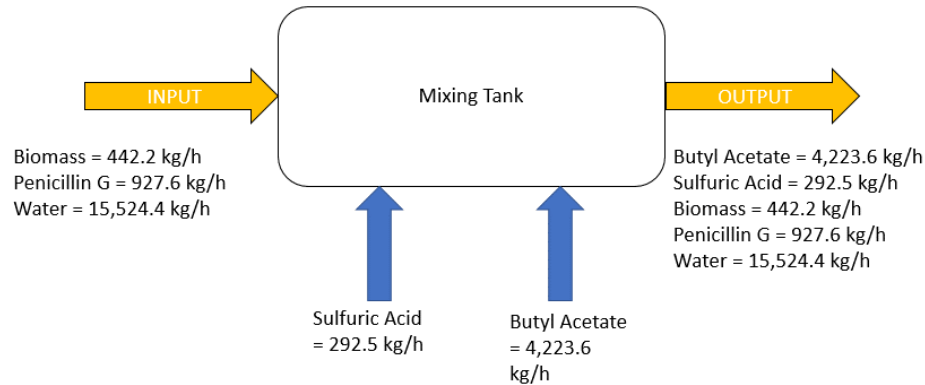


Figure 12. Mass Balance across Mixing Tank

Solvent Extractor

The purpose behind the solvent extractor is to conduct a liquid-liquid extraction which transfers some constituents of one liquid into the other one. In this process, the constituent will be Penicillin G being moved from the broth to the solvent, which will be extracted while the rest is sent to a waste treatment to recover the lost butyl acetate of 10% for reuse. Penicillin G recovery in this unit will be 86% based on literature parameters. However, we made assumptions that 95% of water is lost and all of the sulfuric acid is lost as well because it's very soluble in water. Also, we assumed that 96% of biomass that was left after the rotary vacuum filter is removed at this step.

Unit Balance: Solvent Extractor

Penicillin G Recovery: 86%

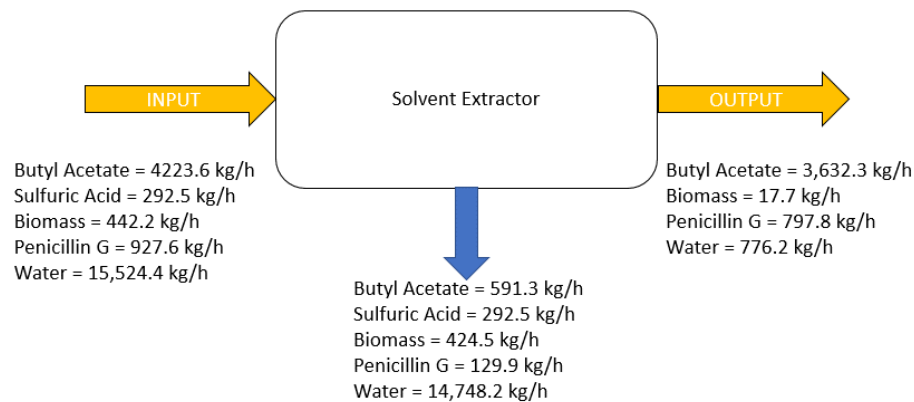


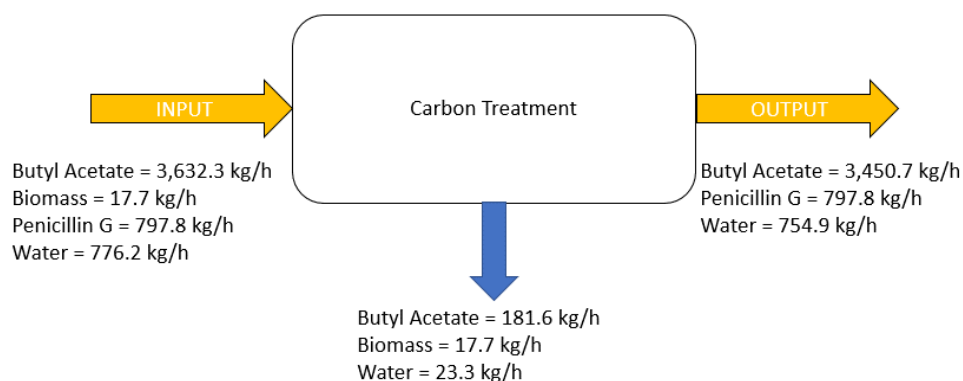
Figure 13. Mass Balance across Solvent Extractor

Carbon Treatment

Carbon treatment is done in an adsorption tower with carbon trays with carbon particle sizes between 10-20 microns. This step focuses on removing the color and odor of the solution coming from the solvent extractor. It also removes impurities like the remaining biomass. Solution particles and impurities stick or adhere to the surface of the carbon molecules on the trays, which can be replaced when the trays are overused. We assumed that there was a 5% loss on butyl acetate and 3% of remaining water. No Penicillin G was lost at this stage.

Unit Balance: Carbon Treatment

Penicillin G Recovery: 100%

**Figure 14.** Material Balance across Carbon Adsorption Tower

Crystallizer

This stage is for creating the crystals. Penicillin G broth is sent into the crystallizer with the addition of butyl acetate and potassium acetate. As Penicillin G is in contact with potassium acetate, Reaction 2 comes into effect making penicillin G a negative ion which also makes it insoluble in butyl acetate. This process is by the deprotonation of penicillin G molecule by the strong base of potassium acetate, which removes the hydrogen atom from penicillin G, and then protonated with the potassium atom to form Penicillin G Potassium crystals. Then, the free-floating hydrogen atoms will bond with the negatively-charged remainder of potassium acetate to form acetic acid.

Unit Balance: Crystallizer

Penicillin G K Recovery: 100%

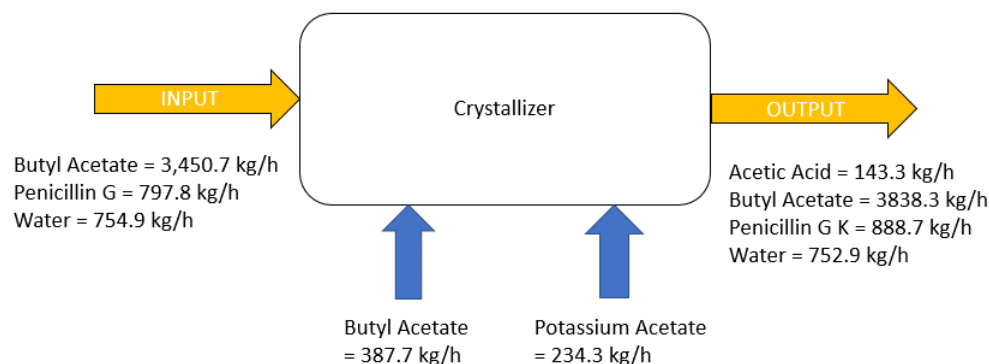


Figure 15. Material Balance across Crystallizer

Crystal Filter 1

Following the crystallizer, the crystal filter is another rotary vacuum filter that separates solids from liquid solution. In this case, we are separating the Penicillin G Potassium crystals from the solvent solution. The solvent solution will be heading off to a waste treatment to re-extract the butyl acetate for re-use in the process. We assumed that 88% of butyl acetate is removed with 95% of water content and all of the acetic acid is gone because it's soluble and fully miscible in water. We assumed that we will experience a 99% recovery of Penicillin G Potassium.

Unit Balance: Crystal Filter 1

Penicillin G K Recovery: 99%

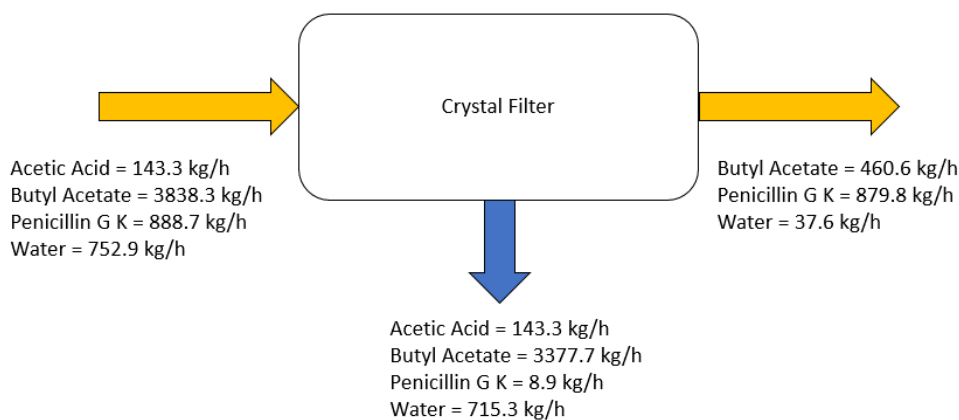


Figure 16. Material Balance across Crystal Rotary Vacuum Filter 1

Crystal Washing

At this stage, the crystals need to be rewashed with more solvent while still using the 0.25 g butyl acetate/ g broth ratio.

Unit Balance: Crystal Washing

Penicillin G K Recovery: 100%

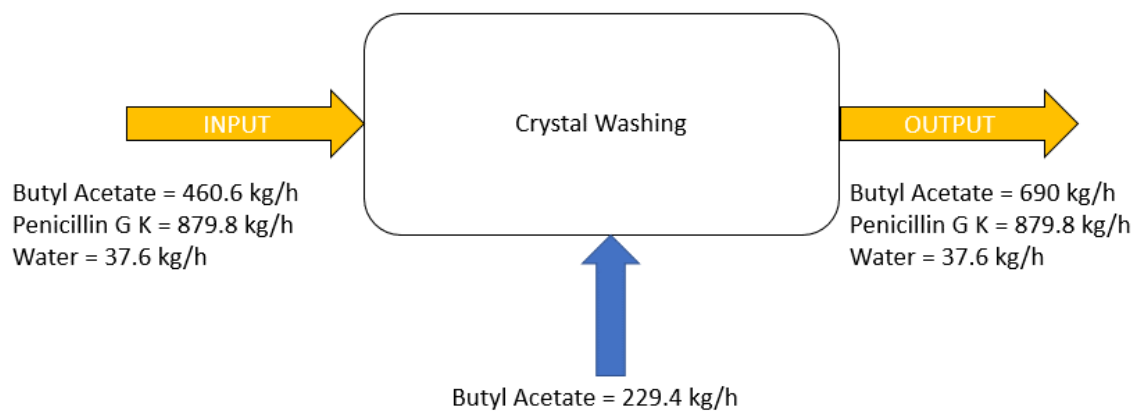


Figure 17. Material Balance across Crystal Washer

Crystal Filter 2

The crystals are re-filtered with the same assumed parameters from the first crystal filter since both equipment are the same.

Unit Balance: Crystal Filter 2

Penicillin G K Recovery: 99%

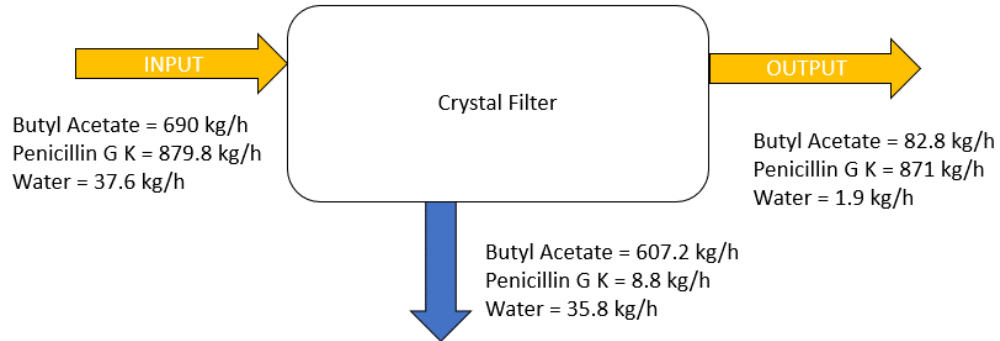


Figure 18. Material Balance across Crystal Rotary Vacuum Filter 2

Vacuum Drying

Finally, the crystals are dried at an ambient temperature with a pressure slightly below atmospheric. Butyl acetate is assumed to be retained at 5% of its content and water is retained at 4 % of its content. At the end, the product is at a purity of 99.5% before being transported to the grinder to be converted to a fine powder.

Unit Balance: Vacuum Drying

Penicillin G K Recovery: 100%

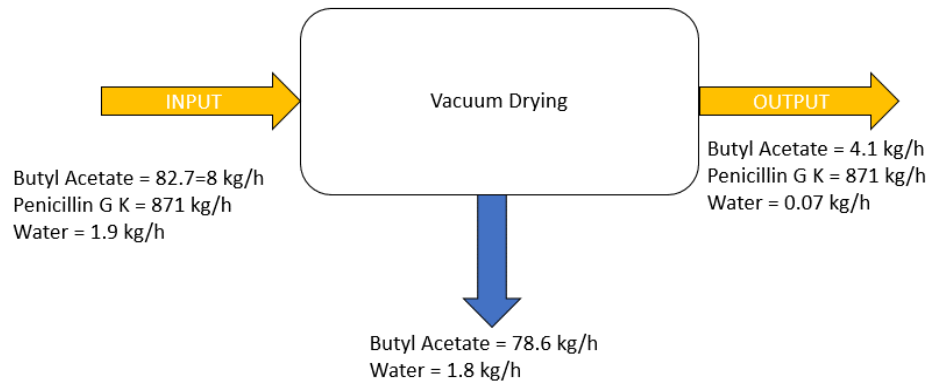


Figure 19. Material Balance across Vacuum Dryer

Degree of Freedom Analysis (Caleb)

According to Gibbs's Phase Rule, the number of degrees of freedom can be calculated using the following relationship:

$$F = C - P + 2$$

Where F = # degrees of freedom; C = # of components; P = # of phases

The following table shows the number of degrees of freedom corresponding to each process unit in the team's design:

Table 8. Degrees of Freedom for all Major Process Units

good!

Process Unit	C [# of components]	P [# of phases]	F [C - P + 2]
V-104	10	2	10
V-201	3	2	3
V-202	5	2	5
V-203	5	2	5
T-201	4	2	4
V-204	4	2	4
V-205	4	2	4
V-206	3	2	3
V-207	3	2	3
E-203	3	3	2

Energy Balance (Caleb)

Figure 16 shows the specifications for all heat exchangers used in the team's design. Each exchanger requires a utility/requires utilities that serve as mediums for heat transfer. The heat duties of the exchangers and the flow rate of the inlet utilities for each exchanger are shown below:

Energy Balance: Utility Equipment Table

Exchanger	Inlet Temp [°C]	Outlet Temp [°C]	Pressure [atm]	Utility	Heat flow [kJ/h]	Utility flow rate [kg/h]
E-101 (jacketed)	25	25	2.04	Steam	-1.33 x 10 ⁷	74,324.9
				Chilled water	1.33 x 10 ⁷	33,112.3
E-102	25	30	-	Steam	-6.02 x 10 ⁵	64,592.3
E-103 (jacketed)	25	25	2.04	Steam	-1.2 x 10 ⁷	67,060.1
				Chilled water	1.2 x 10 ⁷	29,875.7
E-104	25	30	-	Steam	-6.23 x 10 ⁵	66,845.5
E-201	30	25	-	Cooling water	9.44 x 10 ⁵	45,124.3
E-202	25	2	-	Chilled water	3.03 x 10 ⁶	31,486.4

Figure 20. Utility Equipment Table

According to the table, steam utilities all have negative heat flow values, while those of cooling and chilled water are all positive. This is a reasonable occurrence due to the fact that both steam and liquid water serve opposite purposes as utilities for the heat exchangers. Because the steam is supplying the process stream with the heat it needs to see a temperature increase, heat is being transferred from the steam to the process stream. For this reason, heat flow values for steam should be negative because the steam is losing heat while serving as the heat flow medium; conversely, the purpose of cooling/chilled water is to remove heat from the process streams, thus decreasing their temperatures. Moreover, heat flow values for cooled and chilled water should be positive because heat is being transferred from the process streams to the water.

After calculating the heat duties of each heat exchanger unit, utility flow rates were determined by the equation

$$\dot{Q} = \dot{m}c_p\Delta T$$

use proper notation

Solving for $\dot{m}$,

$$\dot{m} = \dot{Q}/c_p\Delta T$$

It is important to note that mass, $\dot{m}$, in this situation represents a mass flow rate, not simply a mass. This is true because the calculated heat duty, $\dot{Q}$, is in units of [kJ/hr] or [kW]. c_p represents the specific heat capacity of the water utility (liquid water or steam, depending on the exchanger) and ΔT is the temperature difference between the utility and the inlet stream. The

All variables should be included in a nomenclature section

mass flow rates of the utilities in the heat exchangers appear considerably high, but this is because a large flow of water is needed to facilitate the transfer of so much heat.

In-depth calculations concerning the derived heat flow and utility flow rate values can be found within the appendix of this report.

Aspen Simulation (Buka)

After all process parameters and designing the Process Flow Diagram, the Aspen Simulation was created. Due to the fact that some equipment wasn't available in Aspen, we simulated our process using closely related equipment that was applicable which resulted in our process converging and having practical values close to our hand calculations. Also, our process was a bioprocess which requires a bio-simulator with the correct raw material component and accurate fluid package as well. Aspen Model is visible below:

Aspen Simulation

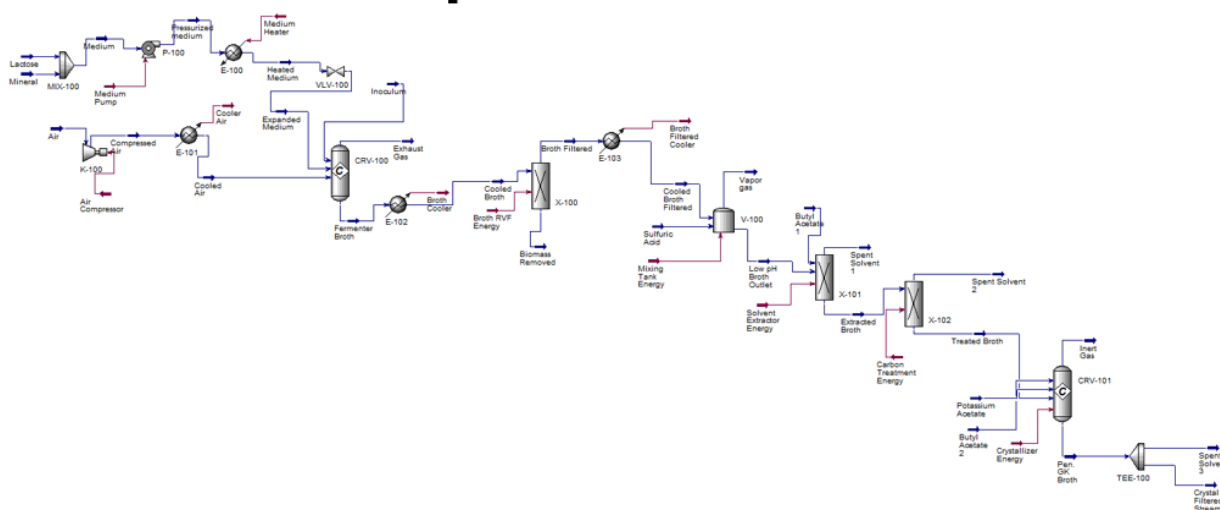


Figure 21. Aspen Simulation

Conclusion and Recommendations (Buka & Caleb)

All in all, the design project satisfied all objectives and revealed itself to be feasible. According to the growth profit indicator, the total cost of necessary raw materials (excluding transportation costs) is less than the total value of products manufactured for sale (penicillin G potassium and biomass), indicating that this plant is profitable and thus worth constructing. Although this analysis does not take into account transportation and utility costs, it is useful in determining the validity of a premature design plan. Regardless, the proximity of the plant to its raw material

suppliers on either side of the country significantly reduces the effect of transportation costs on overall profit.

One recommendation the Team has to ultimately increase profit in the long run is to utilize multiple liquid-liquid extractors in series, rather than one extractor for the whole process. As mentioned earlier in the report, the plant has an overall efficiency of 78%, meaning that the remaining 22% represents the extra amount of penicillin G potassium that could be produced in the event of a theoretically seamless process. By attempting to minimize these potential losses and make the process more efficient, less raw materials will be required and more penicillin G potassium can be manufactured with minimal extra effort. The liquid-liquid extractor in the design has an efficiency of 86%, meaning that 86% of incoming penicillin G is admitted onward to the next unit in the process. By placing multiple liquid-liquid extractors in series, the design will permit for the process stream to be more penicillin G-rich. Adding multiple extractors will lead to a 92% - 96% efficient extraction process, which is around an 8% higher efficiency. While adding multiple extraction units does initially cost, that cost will pale in comparison to the total operating cost because it will maximize the amount of penicillin G potassium that can be made from the same amount of raw materials.

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BELOW AVERAGE

No references
or citations!

I. Introduction

Acetonitrile is a chemical compound with the formula CH_3CN . It is a clear, colorless liquid with a sweet and ethereal odor. It is the simplest organic nitrile and was first prepared by French Chemist Jean-Baptiste Dumas in 1847. Acetonitrile is one of the most frequently used eluents used in reverse phase chromatography and is a critical solvent in pharmaceutical applications for the production of vaccines and antibiotics. In this comprehensive literature review, we will be going over a review of literature on production routes, uses, and handling, as well as process selection and description for our design of production of acetonitrile.

II. Production Literature Review

Many reaction routes for the production of acetonitrile have been studied. Below are the main production routes found in our research.

II.A.1 Production of Acetonitrile from the Sohio Process

A very common way to produce Acetonitrile is via the Sohio process. This process involves the catalytic oxidation of propylene in the presence of ammonia and air. However, we determined this production route was not a route we wanted to take. The primary dealbreaker is because Acetonitrile would be produced as a by-product. Since this would limit our production then it was determined to avoid this process.

II.A.2 Reacting acetic acid with ammonia

II.A.3 Ammoxidation of ethanol

Another way to produce acetonitrile is the ammoxidation of ethanol. The main reaction in this process begins with the reactants entering in a fluidized bed reactor. The process has a low yield without the presence of a catalyst, but with aid from a catalyst the process can achieve high conversions of ethanol. The ideal catalyst to use for this process is vanadium oxide.

II.B. Handling and storage

Acetonitrile is commonly delivered to customers in: ISO tank container, bulk truck, rail car, drum, and ship. Storage capacity should be carefully considered for optimum handling and transport of material. Acetonitrile storage and handling are subject to regulatory policies, and requirements from regulations either local or national must be considered to operate under law. Acetonitrile should be stored in a cool, dry and well ventilated area. The storage area should be out of direct sunlight. The container should be sealed to prevent exposure to air. Temperatures should never exceed 86 degrees Fahrenheit. For quantities larger than a liter, storage should be in a metal container. Acetonitrile should be kept away from oxidants, acids, anhydrides and alkali metals. To prevent accidental explosions or health hazards, several measurements should be taken. Acetonitrile should be handled alongside a colleague. It should be handled under a fume hood if direct contact is required. Fume hoods help minimise exposure. It is important to avoid skin, eyes, inhalation and ingestion. Furthermore, it should be kept away from

Key findings
Sohio process
by-product
dealbreaker
avoid this process

steam, flames, direct heat and combustible substances. Protective clothing such as a long sleeved lab coat or gown, rubber gloves, safety goggles and a face mask are required.

II.C Physical and Chemical Properties

Acetonitrile is a clear colorless liquid with a sweet ethereal odor. Although it is a hazardous chemical, its chemical properties are well understood and is a stable chemical under conditions of normal use. Physical properties include its boiling point at 81.60°C and a flash point at 6°C which makes it a highly flammable fluid. The chemical reactions of acetonitrile are essentially engaged on the nitrile, or -CN, group. Acetonitrile can be utilized to prepare amines, amides, amidines, carboxylic acids and esters, aldehydes, ketones, imines, and many other mixtures. In any case, the essential modern utility of acetonitrile is as a solvent. As a magnificent polar aprotic solvent, with a high dipole movement and dielectric constant. Acetonitrile is preferably appropriate for chemical analysis, extractive purification and organic and biochemical reactions.

II.D Uses

Acetonitrile is utilized to make drugs, perfumes, rubber products, pesticides, acrylic nail removers and batteries. It is also used to remove unsaturated fats from animal and vegetable oils.

III. Process selection

In our process selection we considered three process routes. Our first process is acetonitrile via the sohi process. It is the most common production route as the sohi process in the main widely used production route but due to it making a product of acrylonitrile, it wasn't highly favored in our design in order to produce mass amounts of acetonitrile. Our second consideration is acetonitrile from acetic acid and ammoxidation. This is the least common production route with not much historical literature to build a grass root plant design around. Its purity level is at 98.5% for this process route. Our process was acetonitrile via pressure swing distillation. In this case there was a good selection of literature to study and create a design around. At its highest purity (99%), it is our most favorable specification. Our issues with design were waste treatment issues and excess by-products in process flow.

IV. Process description

Mixing of Ethanol:

The liquid ethanol flows at an ambient temperature of 77°F. The alcohol is then mixed with ammonia. The mixture then passes through a heat exchanger to increase its temperature to 788°F. Air also flows through a heat exchanger to be heated to 788°F in a separate stream.

Ammoxidation reaction:

The heat ethanol and ammonia are fed into the fluidized bed reactor. The heated air is fed into the reactor separately. The reactor operates at a temperature of 788°F and 29psi to provide a conversion of 100 mol% ethanol. The reactor produces vent gas, acetonitrile, water, and co-products.

Separation/purification:

The first gas separator separates carbon dioxide and ammonia from the product mixture. The product mixture consisting of acetonitrile, water and hydrogen cyanide goes through swing distillation for further purification. In the first distillation column hydrogen cyanide with any remaining carbon dioxide and ammonia is extracted. Acetonitrile and water is extracted in the second distillation column. Due to the similar boiling points of acetonitrile and water the second distillation operates at 145psi and involve more trays to achieve the desired 99.9% acetonitrile product.

- poorly written
missing key information

**SENIOR DESIGN AND PROFESSIONALISM I
FALL 2021**

HOMEWORK 4

TOPICS COVERED IN HOMEWORK 4

1. Ethics

CHEG 4472-P02: SENIOR DESIGN & PROFESSIONALISM I

FALL 2019

ASSIGNMENT STATEMENT/QUESTIONS

Senior Design & Professionalism I (Fall 2019): Home Work 4 Due: November 7, 2019

You will be graded based on your understanding of professional and ethical responsibilities as they relate to your project. Clarity of presentation is essential if you are to avoid losing points.

- 1. Write a 2-page synopsis comparing the National Council of Examiners for Engineering and Surveying (NCEES) code of professional conduct with the American Institute of Chemical Engineers (AIChE) and National Society of Professional Engineers (NSPE) code of ethics.**
- 2. Using the NSPE Code of Ethics, analyze the following case study. For the case study, justify your opinions by quoting relevant sections of the NSPE Code of Ethics that supports the opinion you make and why the opposite opinion may not be right.**

Case Study

Fact pattern:

Engineer A is a principal in a medium-sized engineering firm with expertise in mechanical and electrical engineering. Engineer A's firm is retained on a speculative basis by Engineer B, a local civil engineer, to assist City X in applying for a federal grant for certain wastewater treatment equipment upgrades for the city's wastewater treatment facility. The application is successful, City X obtains the grant, and Engineer B is retained to design the waste water equipment upgrades. In recognition of Engineer A's work in securing the grant, Engineer C, the chief city engineer, verbally promises to select Engineer A's firm on a future engineering project for City X.

Question: Was it ethical for Engineer C to offer to select Engineer A's firm on a future engineering project for City X?

CHEMICAL ENGINEERING DEPARTMENT
SENIOR DESIGN & PROFESSIONALISM I CHEG 4472
GRADING SCHEME AND OUTCOME ASSESSMENT SHEET FOR FALL 2019

ABET OUTCOME 4: An ability to recognize ethical and professional responsibilities in engineering situations and make informed judgments, which must consider the impact of engineering solutions in global, economic, environmental, and societal contexts

Assignments that test competency in this area will include problems that test the student knowledge in the Professional Code of Ethics, ability to apply relevant aspects of the professional code of ethics when considering alternative decisions or solutions, ability to ethically evaluate the short and long term impact of engineering solutions on community and environment.

Name: _____

Title of Assignment: _____

Competency Area	Max for this Assignment	Your Score
4.1 An understanding of professional and ethical responsibility <i>This assignment tests the student knowledge in the Professional Code of Ethics, and ability to apply relevant aspects of the professional code of ethics when considering alternative decisions or solutions.</i>	100	
TOTAL	100	

ABOVE AVERAGE

CHEG 4247-P01: SENIOR DESIGN & PROFESSIONALISM I FALL 2021

ASSIGNMENT STATEMENT/QUESTIONS

Senior Design & Professionalism I (Fall 2021): Home Work 4 Due: November 16, 2021

You will be graded based on your understanding of professional and ethical responsibilities as they relate to your project. Clarity of presentation is essential if you are to avoid losing points.

- 1. Write a 2-page synopsis comparing the National Council of Examiners for Engineering and Surveying (NCEES) code of professional conduct with the American Institute of Chemical Engineers (AIChE) and National Society of Professional Engineers (NSPE) code of ethics.**
- 2. Using the NSPE Code of Ethics, analyze the following case study. For the case study, justify your opinions by quoting relevant sections of the NSPE Code of Ethics that supports the opinion you make and why the opposite opinion may not be right.**

Case Study

Facts:

Engineer A is a principal in a medium-sized engineering firm with expertise in mechanical and electrical engineering. Engineer A's firm is retained on a speculative basis by Engineer B, a local civil engineer, to assist City X in applying for a federal grant for certain wastewater treatment equipment upgrades for the city's wastewater treatment facility. The application is successful, City X obtains the grant, and Engineer B is retained to design the waste water equipment upgrades. In recognition of Engineer A's work in securing the grant, Engineer C, the chief city engineer, verbally promises to select Engineer A's firm on a future engineering project for City X.

Question:

Was it ethical for Engineer C to offer to select Engineer A's firm on a future engineering project for City X?

1. Codes of Conduct Synopsis

The National Council of Examiners for Engineering and Surveying, or NCEES, has a code of professional conduct Which was revised in September 2021. The preamble states that these rules protect the health, safety, and wellbeing of the public in engineering professions. These rules shall be followed by every licensee and firm that is able to perform engineering or surveying services. This section contained three sections the first being Licensee's Obligation to the Public, next Licensee's Obligation to Employer and Clients, and last Licensee's Obligation to Other Licensee's.

The AIChE, the American Institute of Chemical Engineers, adopted a code of ethics that contained eleven rules its members must follow to achieve their goals. This code of conduct was approved by the board in November 2015. Their intro states that All members of the shall uphold integrity, honor, and dignity of the engineering profession. It then goes on the explain how the rules should be upheld by actions such as using their knowledge and skill for the enhancement of human welfare.

The NSPE, National Society of Professional Engineers, stated that their code of ethics. The Ethical review background states their standards were first drafted at the end of the nineteenth century. The current code of ethics was adopted in 1964 and has been revised to fit today's standards. It then goes on to the introduction, or preamble of the current code of ethics. This addresses member of the engineering profession. It states that engineering had a direct vital impact on the quality of life for all people, then states the standards an engineer shall act accordingly. This set of codes, like the NCEES, separated its code into three sections. The three sections were Fundamental Canons, which were some of the originals created in 1964, Rules of practice, and professional obligations.

The NCEES, AIChE, and the NSPE all start with the same rule, that being an engineer's responsibility for the protection of the public safety, health, and welfare when performing. Other regulations are written in these codes that they all share are:

- It is an engineer's responsibility to inform and advise their employer if they believe that their duties could possibly endanger the health, welfare, or safety of the public in the present or future.
- Only perform services that they are authorized to do. To give colleagues and coworkers credit for the engineering work they have done and recognize their interests, capabilities, and contributions.
- Always act in a professional matter for every employer, client, or contractor.
- Accept responsibility for professional activities, and seek and heed reviews of their work and offer objective criticism to others.

Along with those stated above, the codes of conduct for each of these organizations are similar in essence. They express ethical values that engineers should uphold. The professional codes of conduct not only help protect the public and the reputation of the profession but also help engineers avoid legal consequences. Following the codes lays the foundation for a minimal consequence in many situations that an engineer may face and allow him/her/them to obtain and build a positive reputation in the profession.

How are the codes different?

2. Ethics Case Study

It was not ethical for engineer C to offer to select Engineer A's firm on a future project for City X according to the NSPE Code of Ethics. Engineer A has expertise in mechanical and electrical engineering. According to NSPE Code of Ethics section 2, rule 2, part a, "Engineers shall undertake assignments only when qualified by education or experience in the specific technical fields involved." Engineer A is not qualified by education or experience to choose necessary treatment equipment. A better source would be An engineer with expertise in chemical engineering.

Reason 2 that the case study is not ethical is Engineer C verbally promised to select Engineer A's firm on a future engineering project for City X. According to NSPE Code of Ethics section 2, rule 5, part b, "Engineers shall not offer, give, solicit, or receive, either directly or indirectly, any contribution to influence the award of a contract by public authority, or which may be reasonably construed by the public as having the effect or intent of influencing the awarding of a contract. They shall not offer any gift or other valuable consideration to secure work. They shall not pay a commission, percentage, or brokerage fee to secure work, except to a bona fide employee or bona fide established commercial or marketing agencies retained by them." The correct way to choose an engineer for a project would be going through a bidding process. Each engineering firm would give estimates and plans for how they will carry out the project and the firm that best serves the project should be chosen.

Reason 3 that the case study is not ethical is because Engineer A's firm is retained on a speculative basis by Engineer B. Engineer B was chosen with no proof of work or reputability.

CHEMICAL ENGINEERING DEPARTMENT
SENIOR DESIGN & PROFESSIONALISM I CHEG 4247
GRADING SCHEME AND OUTCOME ASSESSMENT SHEET FOR FALL
2021

ABET OUTCOME 4: An ability to recognize ethical and professional responsibilities in engineering situations and make informed judgments, which must consider the impact of engineering solutions in global, economic, environmental, and societal contexts

Assignments that test competency in this area will include problems that test the student knowledge in the Professional Code of Ethics, ability to apply relevant aspects of the professional code of ethics when considering alternative decisions or solutions, ability to ethically evaluate the short and long term impact of engineering solutions on community and environment.

Name: _Shumpert Kirksey, Meredith Meyer, Cherish Vaughn, Garred Essissima

Title of Assignment: _Homework #4: Ethics and Professionalism

Due Date: November 16, 2021

Competency Area	Max for this Assignment	Your Score
4.1 An understanding of professional and ethical responsibility <i>This assignment tests the student knowledge in the Professional Code of Ethics, and ability to apply relevant aspects of the professional code of ethics when considering alternative decisions or solutions.</i>	100	
TOTAL	100	93

AVERAGE

CHEG 4247-P01: SENIOR DESIGN & PROFESSIONALISM I

FALL 2021

ASSIGNMENT STATEMENT/QUESTIONS

Senior Design & Professionalism I (Fall 2021): Home Work 4 Due: November 16, 2021

You will be graded based on your understanding of professional and ethical responsibilities as they relate to your project. Clarity of presentation is essential if you are to avoid losing points.

1. Write a 2-page synopsis comparing the National Council of Examiners for Engineering and Surveying (NCEES) code of professional conduct with the American Institute of Chemical Engineers (AIChE) and National Society of Professional Engineers (NSPE) code of ethics.
2. Using the NSPE Code of Ethics, analyze the following case study. For the case study, justify your opinions by quoting relevant sections of the NSPE Code of Ethics that supports the opinion you make and why the opposite opinion may not be right.

Case Study

Facts:

Engineer A is a principal in a medium-sized engineering firm with expertise in mechanical and electrical engineering. Engineer A's firm is retained on a speculative basis by Engineer B, a local civil engineer, to assist City X in applying for a federal grant for certain wastewater treatment equipment upgrades for the city's wastewater treatment facility. The application is successful, City X obtains the grant, and Engineer B is retained to design the waste water equipment upgrades. In recognition of Engineer A's work in securing the grant, Engineer C, the chief city engineer, verbally promises to select Engineer A's firm on a future engineering project for City X.

Question:

Was it ethical for Engineer C to offer to select Engineer A's firm on a future engineering project for City X?

CHEMICAL ENGINEERING DEPARTMENT
SENIOR DESIGN & PROFESSIONALISM I CHEG 4247
GRADING SCHEME AND OUTCOME ASSESSMENT SHEET FOR FALL 2021

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Name: __Tyecia Franklin, Taylor Linton, Wasil Mahmood, Franck Nangomoko_____

Title of Assignment: _____

Due Date: November 16, 2021

Competency Area	Max for this Assignment	Your Score
4.1 An understanding of professional and ethical responsibility <i>This assignment tests the student knowledge in the Professional Code of Ethics, and ability to apply relevant aspects of the professional code of ethics when considering alternative decisions or solutions.</i>	100	
TOTAL	100	85

The AIChE code of ethics seems to be targeting the important aspects of developing your character as a chemical engineer. In the beginning of this document, the organization starts with stating that they "...shall uphold and advance the integrity, honor and dignity of the engineering profession..." which proves that they do not just want the ethics to be performed as if someone is just going with the flow. AIChE's code of ethics is based on personal development and safety of oneself and others. Although this code of conduct provides numerous ethics to follow as a chemical engineer, yet it does not thoroughly explain each point. Not being specific can lead to miscommunication between the employers and employees within the work environment.

Unlike the previous code of ethics for engineers, the National Society of Professional Engineers (NSPE) has written out the details about each ethic that should be performed. This code of ethics breaks down each section by the fundamental canons, rule of practices, and professional obligations. Beneath each ethical statement are at least two additional statements that are similar to the rule of practice or professional obligations. For example, the statement "2. Engineers shall perform services only in the areas of their competence" is a common ethics that organizations imply. In the NSPE code of ethics it provides additional ethical behaviors that pertain to the subject such as, "a. Engineers shall undertake assignments only when qualified by education or experience in the specific technical fields involved." Along with statement a, are two other ethical behaviors that carry on the behaviors of the second rule of practice.

The NCEES code stands for the National Council of Examiners for Engineering and Surveying. The purpose of the code is to convey the rules of professional conduct. These specific rules apply to all that hold a certificate of licensure to perform engineering services.

These rules are put in place to protect life, health, and property. It is imperative for licensees to adhere to the regulations and meet the standards of moral and ethical conduct. The NCEES is comprised of three sections, those sections are as follows: Licensee's obligation to society, Licensee's obligation to employer and clients and the Licensee's obligation to other licensees. Section one describes licensees' performance standards as it pertains to their community and all of society. They are obligated to hold themselves accountable for producing quality work that includes safety considerations. Section two involves the licensees quality of work that they provide to clients and employers. Section three describes licensees obligation to complete their own work honestly and provide other credit when it is necessary.

Overall, the code of conduct for AIChE, NSPE, and NCEES are all upholding their members to a high standard. Each of the above codes is unique to the specific group of people that it addresses. As stated the AIChE code of ethics specifically targets chemical engineers. The NSPE code of ethics targets all engineers. While the NCEES code of ethics can apply to anyone that holds a certificate of licensure to perform acts of engineering.

Very good!

Case Study

After taking an honest review of the case study, we concluded that it was unethical for Engineer C to select engineer A's firm on a future engineering project for city X. So, according to NSPE section (II.5.b), "engineers shall not offer, give, solicit, or receive, either directly or indirectly, any contribution to influence the award of a contract by public authority, or which may be reasonably construed by the public as having the effect or intent of influencing the awarding of a contract..." based on this, we can say that it will be unfair to other companies that are not only qualify but also supersede the requirements to receive the contract being offer to Engineer A's firm.

other actions?

BELOW AVERAGE

CHEG 4247-P01: SENIOR DESIGN & PROFESSIONALISM I

FALL 2021

ASSIGNMENT STATEMENT/QUESTIONS

Senior Design & Professionalism I (Fall 2021): Home Work 4 Due: November 16, 2021

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Case Study

Facts:

Engineer A is a principal in a medium-sized engineering firm with expertise in mechanical and electrical engineering. Engineer A's firm is retained on a speculative basis by Engineer B, a local civil engineer, to assist City X in applying for a federal grant for certain wastewater treatment equipment upgrades for the city's wastewater treatment facility. The application is successful, City X obtains the grant, and Engineer B is retained to design the waste water equipment upgrades. In recognition of Engineer A's work in securing the grant, Engineer C, the chief city engineer, verbally promises to select Engineer A's firm on a future engineering project for City X.

Question:

Was it ethical for Engineer C to offer to select Engineer A's firm on a future engineering project for City X?

CHEMICAL ENGINEERING DEPARTMENT
SENIOR DESIGN & PROFESSIONALISM I CHEG 4247
GRADING SCHEME AND OUTCOME ASSESSMENT SHEET FOR FALL 2021

ABET OUTCOME 4: An ability to recognize ethical and professional responsibilities in engineering situations and make informed judgments, which must consider the impact of engineering solutions in global, economic, environmental, and societal contexts

Assignments that test competency in this area will include problems that test the student knowledge in the Professional Code of Ethics, ability to apply relevant aspects of the professional code of ethics when considering alternative decisions or solutions, ability to ethically evaluate the short and long term impact of engineering solutions on community and environment.

Name: _____

Title of Assignment: _____

Due Date: November 16, 2021

Competency Area	Max for this Assignment	Your Score
4.1 An understanding of professional and ethical responsibility <i>This assignment tests the student knowledge in the Professional Code of Ethics, and ability to apply relevant aspects of the professional code of ethics when considering alternative decisions or solutions.</i>	100	
TOTAL	100	70

Established in 1934, the National Society of Professional Engineers (NSPE) has always put the interests of professionally licensed engineers first with a central goal of protecting engineers from unlicensed entities and creating a safe inclusive environment for all engineers. Their code of ethics reflects these same ideals to ensure not only those engineers are conducting honest business, but they're also ensuring the safety of the public. Deception is frowned upon within the organization, which is very reasonable, when conducting a business, being as transparent as possible with your consumers is the most ethical you can do, lying or leaving important details out that people should know only creates ignorance to the truth of the matter and could put others at risk. If you're working with another company but you choose to leave important information about certain measurements of chemicals you're working with, you're creating a viral situation that could hurt someone if they don't handle the substances properly due to the information you gave them. The inclusive side of the code of ethics outlaws the criticism or down talking of another engineer to further yourself throughout a company. This is just common courtesy, because if you must rely on making someone who's supposed to be your colleague look bad in order to make yourself look good to boost your stock with a company or to get a job, you're obviously not doing your job right to begin with and deserve you be in the position you're already.

Not sure I understood this

Not the NCEES provides proper examination to grant engineers their license to be able to conduct work legally and properly in that field. Conflicts of interests are outlawed meaning giving someone an engineering license because you know them or just because their family is an extreme violation of ethics and it's grounds for termination and depending on if a accident were to occur based off of that type licensing, jail time. Conflicts of interest are also not allowed in

NSPE and AIChE which is common sense given that the goals of the three are to be honest with how engineers are supposed to operate. For AIChE the main focus of the code of ethics for chemical engineers is to ensure the absolute safety of the public. Given what chemical engineers work with, they work in a field that not only puts them a risk, but general citizens at risk everyday which is why their jobs must be executed to perfection. Chemical leaks or explosions can affect the breathing and water conditions for hundreds of citizens if it isn't contained, a reason why chemical engineers receive high praise for what they do.

After reading the Case Study, engineer C was not acting in an ethical manner for verbally agreeing to select engineer A's firm for a future project. The agreement is only on the basis of an IOU for engineer A securing the grant for engineer B's company which goes down as a conflict of interest. Something like that would require an interviewing process to review the list of candidates that's suitable for the project, so the best output of production can be optimized. Quality over quantity is always valued at with anything, especially in terms of work conducted by engineers, if we had our buddies working important projects for us instead of a highly trained and renowned professional, the result would probably be terrible.

Where are your citations?

Also, there are at least 3 sections for unethical behavior

**SENIOR DESIGN AND PROFESSIONALISM I
FALL 2021**

FINAL PROJECT REPORT

- 1. Apply a systematic design process, incorporate engineering codes, standards, and realistic constraints that include economic; environmental; sustainability; manufacturability; ethical; health and safety; social; and political considerations in solving the design problem.**
- 2. Work in groups**

GROUP 4 DESIGN PROJECT

Project: Plant design for production of ethylene oxide

Problem Statement Summary

Design a grass-roots plant for production of ethylene oxide.

Option Sorting:

You will have to defend any decisions you make throughout the design, noting that the best defense is economic justification. You should begin your design effort with a comparative evaluation of published feasible reaction routes to ethylene oxide.

Your comparison between the various process technologies should be a screening but not a rigorous process optimization or design for each published process option or route. Feasible flow sheets for each process option are available in the literature. Some important considerations for these process options include:

- ✓ Availability and cost of raw materials
- ✓ Reaction selectivity: A process with low selectivity will require additional purification and storage units for byproducts, or some means of recycling them. The market values of the byproducts are also very important; some streams may have no salable value and require disposal
- ✓ Reaction yield: A process with low yield will have large recycle streams, requiring larger and higher operating costs for the reaction and crude separation sections
- ✓ Thermodynamic barriers to separating key components: Separating components that form azeotropes and distillation pinches at moderate conditions may require more complicated processes or operation at more extreme conditions
- ✓ Safety and operability

PROCESS DESIGN:

Once you have considered the process options, proceed and select, with justification, your best option for the detailed process design.

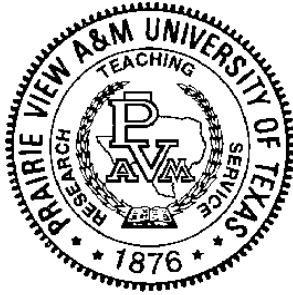
Scope of design work and deliverables

- Set up a HYSYS model of the process and prepare the material and heat balances, using an appropriate thermodynamic fluid property package
- Prepare a complete simulation report of the process
- Assume 80% polytropic efficiency for compressors and the 75% HYSYS default adiabatic efficiency for the pumps
- Assume 5 psi pressure drop for coolers, and for shell and tube heat exchangers such as the water cooler, use 5 psi for both the shell and tube sides
- Prepare material and energy balances of the preferred complete process
- Prepare a complete simulation report of the preferred process
- Provide a process description and prepare a Process Flow Diagram (PFD) for the plant showing the major items of equipment, and indicating the materials of construction and the operating temperatures and pressures
- Prepare a chemical engineering design of any (i) reactor(s), (ii) absorption column(s) and (iii) product distillation units
- Prepare a mechanical engineering design of the reactor(s) with appropriate dimensioned sketch(es)
- Estimate the Major Equipment Capital Cost (Capex)
- Estimate Operating Cost (Opex)
 - Select, with justification, an appropriate operating period of days in a year the plant will be on stream

- Use \$0.05/gal to estimate the annual water cost for cooling water
- For prices of steam and power contact your local utility company, but in the absence of such data from the local company, use data presented in Appendix B of “Plant Design and Economics for Chemical Engineers” by Peters, M.S., K.D. Timmerhaus and R.E. West. The annual power cost estimate should be obtained either as indicated above or based on the value \$0.05/Kwh, whichever is lower. All prices should be escalated with inflation over the life of the project.
- Estimate the Major Equipment Capital Cost (Capex)
- Estimate Operating Cost (Opex)
 - Assume an operating period of 8000 hours on stream
 - Use \$0.05/gal to estimate the annual water cost for cooling water
 - For prices of steam and power contact your local utility company, but in the absence of such data from the local company, use data presented in Appendix B of “Plant Design and Economics for Chemical Engineers” by Peters, M.S., K.D. Timmerhaus and R.E. West. The annual power cost estimate should be obtained either as indicated above or based on the value \$0.05/Kwh, whichever is lower. All prices should be escalated with inflation over the life of the project.
- Prepare a net present value and investor’s rate of return analysis for this investment over the life of the plant. Assume your company’s current capital hurdle rate is 15%.
- Prepare a project milestone schedule
- Prepare a control scheme to ensure safe operation of reactor(s) and absorption units
- Prepare a safety report: Indicate the safety measures required for the plant bearing in mind any toxic and flammable materials handled
- Recommendations

References:

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6. Chemical Market Reporter: Biweekly newspaper providing up-to-date prices on many chemicals



College of Engineering

Senior Design Project Manual

**Prairie View A&M University
Prairie View, Texas 77446**

Last Revision: 11/20/09

ACKNOWLEDGEMENT

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1. INTRODUCTION TO SENIOR DESIGN PROJECT

Senior Design Project is used to prepare students for professional practice through realistic application of mathematics, science and engineering to an open-ended major design problem in which students are required to design a system, component, or process to meet desired needs.

1.1 Importance of Senior Design

This course is important because it provides the student, an opportunity to practice design in a way that parallels what will be encountered in professional practice. Students are required to apply a systematic design process, incorporate engineering codes, standards, and realistic constraints that include economic; environmental; sustainability; manufacturability; ethical; health and safety; social; and political considerations in solving the design problem. In addition, Senior Design Project is the primary course used to satisfy ABET criterion 4 which requires students to be prepared for engineering practice through the curriculum culminating in a major design experience. The latter should be based on the knowledge and skills acquired in earlier course work and should incorporate appropriate engineering standards and multiple realistic constraints. Senior design is also used to satisfy outcome C of criterion 3. This outcome requires students to have the ability to design a system, component, or process to meet desired needs within realistic constraints such as economic, environmental, social, political, ethical, health and safety, manufacturability, and sustainability.

1.2 Purpose of Manual

The purpose of this manual is to inform students and faculty the importance of Senior Design Project and to clearly present the level of details required in the preparation and presentation of homework assignments, design, analysis, experimentation, presentations, intermediate reports, final oral presentation and final project report that may be required.

2. CAPSTONE DESIGN & DESIGN METHODOLOGY

The ABET accreditation criteria include a requirement that the various elements of each engineering curriculum be brought together in one or more capstone engineering design courses built around comprehensive, open-ended problems having a variety of acceptable solutions and requiring some economic analysis.

Teaching engineering design as a means of preparing students for the practice of engineering has been a tradition of all departments in the College of Engineering at Prairie View A&M University. The curricula have been designed to expose students to the process of engineering design, to integrate design activities throughout the curriculum, and culminate in a year of two-semester senior capstone design course sequence.

The open-ended engineering design projects used for the capstone design experience engage teams of students, drawing on their component-based design experiences, to solve contemporary, real world engineering design problems with exposure to the applicable social, global, environmental, safety and economic issues while demonstrating their oral and written communication skills.

Each team is required to submit a written technical report and to make a public presentation of its design solution. Typically, the projects selected involve corporate representatives as project consultants. Evaluation of the teams' products typically involves both corporate representatives and departmental faculty. The capstone design courses provide a broad, general engineering design experience as well as an in-depth design experience within the each relevant discipline.

3. REQUIREMENTS FOR SELECTION OF PROJECTS

The Senior Design and Professionalism courses are intended to provide capstone design experience. The Senior Design courses draw on the students' skills and knowledge gained from previous years of coursework's in mathematics, sciences, engineering science and design. The senior design project should be sufficient in scope and technical content to demonstrate the students' technical competence in their major area of study. The successful completion of senior design project is indicative of the students' preparedness to pursue professional practice of engineering.

The following guidelines are provided to help faculty and project sponsors identify suitable senior project topics:

- The project should emphasize design, experimentation and/or hands-on skills.
- The project should offer opportunity for creativity.
- The project should allow teamwork among seniors in one or more majors.
- The project should be of sufficient complexity to allow each team member to contribute about 150 hours in class time and 150 hours outside class.
- The project should draw on the students' skills and knowledge gained from previous years of coursework.
- The project should incorporate engineering standards and realistic constraints that include most of the following: economic; environmental; sustainability; manufacturability; ethical; health and safety; social; and political.
- The project schedule should be limited to eight months (Early September to End of April)
- The project should have concrete and measurable goals.

Projects involving only collection of published materials are unacceptable and projects involving classified materials should be avoided.

4. TEAM FORMATION AND MANAGEMENT

4.1 Team Formation

The instructors will form the teams. Self-selection of teams by students is not used to avoid students teaming with friends and roommates. Research indicates that instructor-formed teams perform better than self-selected teams [1].

Group sizes of 3-4 will be the goal, as this number of members work best. Two is too small because there is not enough diversity of ideas and more than four leads to some members of the group not actively participating. Also, groups larger than four become harder to coordinate and increase non-linearly the possible lines of internal communication.

Groups are intended to be heterogeneous with a mix of ability levels, experiences and skills. However, certain considerations for under represented populations, e.g., women in engineering, on a team to avoid situations where such students will feel outnumbered and then become passive on the project, as research indicates can occur.

The teams will remain intact throughout the capstone experience; certainly for the whole semester and, to the extent practicable, across both semesters.

4.2 Team Contract

Individual behavior as members of a team can raise problems and is often the greatest barrier to team success. For example, differing expectations about communication and meeting attendance can cause a team to miss key deliverables. Therefore, teams will operate under a team contract. Each team will formulate their own contract on team behavior that they will follow for the rest of the project. The instructors will provide resources with good ideas that the students must process to formulate their own contract (however, a sample contract will not be handed out). The process fosters shared ownership by the team.

4.3 Team Roles

Being familiar with team sports we know that individual players have specific roles. In American football, for example, the quarterback throws the ball—while blockers hold off rushing opponents—and a receiver catches it; and if a player fails in his or her role, the whole team suffers. The same principle applies with engineering teams, whether in industry or with student teams. Either way, it is important to learn that team roles are necessary for successful teams.

The instructor will assign different roles to team members, e.g., coordinator or leader, recorder/note taker, timekeeper, devil's advocate and consultant. Various sets of roles are possible, and students are encouraged to propose their own set of roles, with their project in mind. Teams will be encouraged to rotate the roles periodically or for particular assignments.

4.4 Team Management – The Five Tenets of Cooperative Learning

Cooperative learning is an instructor-designed framework for instruction that involves students working in teams to accomplish an assigned task (such as a problem solution or product design) and to produce a final product (such as a prototype or a design report), under particular conditions. The framework includes the following elements:

- *Positive interdependence.* Team members have to rely on one another to achieve the goal. If any team members fail to do their part, everyone on the team suffers adverse consequences.

- *Individual accountability.* Each team member is held accountable both for doing his or her share of the work and for understanding everything in the final product (not just the parts for which he or she was primarily responsible).
- *Face-to-face promotive interaction.* Although some of the group work may be done individually, the nature of the assignment/task is such that some work must be done interactively, with team members providing mutual feedback and guidance, challenging one another, and working toward consensus.
- *Appropriate use of teamwork skills.* Students are helped to develop and exercise leadership, communication, conflict management, and decision-making skills.
- *Regular self-assessment of team functioning.* Each team must set goals, periodically assess how well the team members are working together, and identify changes they will make to function effectively in the future [1].”

Following the above *five tenets*, which provide a good training ground for teamwork, students may expect to see assignments for individuals as well as teams, and be expected to critically evaluate the performance of their team, teammates, as well as themselves.

Information in this section was derived in part from portions of the *Practical Guide to Teamwork* [2]. Students are strongly encouraged to read this guide and use it to maintain excellent team functioning.

5. MAIN PARTS OF REPORTS

The senior project report is the main document that tells the whole story about the project. It should be detailed and well organized enough for a technical reader with no knowledge of the project to completely understand the design presented in the report. To ensure that the important details are included, the report should, in the least, contain the parts listed in this section, and in the order provided here. The initial part of the report should have the following:

- Title Page
- Letter of Transmittal
- Acknowledgements
- Project Summary or Abstracts
- Table of Contents
- List of Figures
- List of Table

The main body of the report should have the following major sections

- PROJECT SCOPE
- PROJECT PLANNING AND TASK DEFINITION
- LITERATURE REVIEW
- PRELIMINARY DESIGN
- DETAILED SYSTEM DESIGN
- RESULTS & DISCUSSION
- CONCLUSIONS
- RECOMMENDATIONS
- List of References
- Appendix

The details of the format and content of each part are provided in section 6 of this manual.

6. DETAILS AND FORMAT FOR PARTS OF REPORT

The details and the formats needed for the parts of the report listed in section 5 are provided in this section. Students are advised to strictly adhere to the information provided here in preparing the project reports. The following format should be used for all formal project reports. Project reports should be neat and accurate.

In general, a report is written in **the past tense and in the third person**. It should be impersonal throughout, personal pronouns (I, You, We) being avoided. The report should be written to enable a reader (who has a general science or engineering background) with no prior knowledge of the project to fully understand what has been designed. The report must be complete in itself. A good report is thorough, concise, orderly, neat, and grammatically correct.

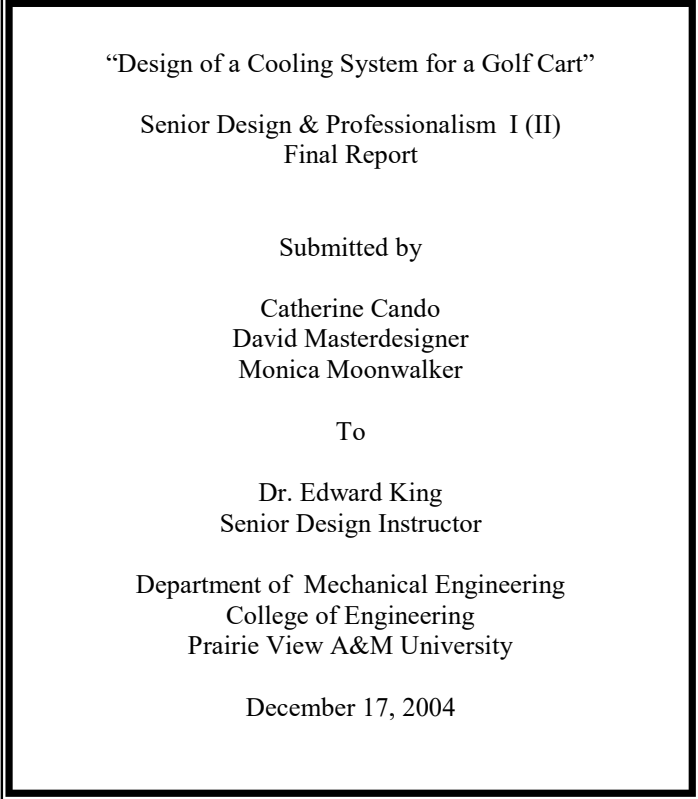
6.1 General Report Specifications

In order to observe the accepted rules of good writing form, the following specifications for the general makeup of the project report should be strictly used.

1. The report should be written in chapters as done in this document. The chapter headings should be capitalized, bolded, and of font size 14. The chapter headings should be centered unless when it covers more than one line in which case it should be left justified. The chapter heading should be preceded by the chapter number as demonstrated in this document.
2. The first letters of major headings should be capitalized except conjunctions, be of font size 11 or 12, bolded, and preceded by the subsection number, the first of which is the chapter number followed by a decimal point, followed by the major section sub-number, as demonstrated in this document
3. Use 8½ x 11 inch white paper.
2. Write the report with a word processor such as MS Word, Word Perfect
3. All equations should be typed using any equation editing feature within the word processor.
4. Use one side of the paper only.
5. Create all drawings and figures using computer drawing package and plotting programs. Scanned images are allowed where appropriate.
6. Use the same font style (Times New Roman recommended) in the report and on drawings. The recommended font size is 11 or 12 points for all text except chapter headings.
7. Use 1" margin on all sides (preferably, 1.5" margin on the left side)

6.2 The Title Page

The title page contains important information about the project including the name of your organization, title of the project, names of members producing the report, name of receiving person and organization, and date of submission. The format should follow that shown in Figure 6.1.



The figure shows a sample title page enclosed in a double-line rectangular border. The text is centered and reads as follows:

“Design of a Cooling System for a Golf Cart”

Senior Design & Professionalism I (II)
Final Report

Submitted by

Catherine Cando
David Masterdesigner
Monica Moonwalker

To

Dr. Edward King
Senior Design Instructor

Department of Mechanical Engineering
College of Engineering
Prairie View A&M University

December 17, 2004

Figure 6.1 Sample Details and Format for a Title Page

6.3 Letter of Transmittal

This is a cover letter used to officially inform the recipient (your boss, client, customer) of the completion of the project, and about the accompanying report. Within the company, it is usually a memorandum. In either case, it introduces the report to the person or group for whom it is intended. It may refer to a request or a contract that initiated the study but should not attempt to summarize the contents of the report. The letter of transmittal should be signed. A sample letter of transmittal is shown in the Appendix.

6.4 Table of Contents

The project report should have a Table of content page that lists all chapters and sections of the report, comparable to the table of content page you would normally see in a book.

In any event, be sure that the titles used in the table of content page match those in the text exactly and the page numbers indicated for each section match those in the report. A sample table of contents page is provided in Figure 6.2 All the major sections included in Figure 6.2 should appear in the Table of contents of all senior project reports. In addition to these major sections, each project should have appropriate sub-sections under Literature Review, Preliminary Design and the Detailed Design sections of the report.

TABLE OF CONTENTS

Letter of Transmittal	ii
Acknowledgement.....	iii
Project Summary or Abstracts.....	iv
Table of Contents	v
List of Figures	vi
List of Table	vii
1. PROJECT SCOPE	1
1.1 Problem Statement	1
1.2 Client identification and recognition of need	3
1.3 Project goals and objectives	3
1.4 Contemporary issues relevant to project	3
1.5 Potential impact of project on society (global, national ,local).	3
1.6 Initial Project constraints	4
2. PROJECT PLANNING AND TASK DEFINITION....	5
2.1 Task identification.....	8
2.2 Timeline	10
2.3 Gantt Chart	12
3. LITERATURE REVIEW	13
(Provide sub-sections based on project)	
4. PRELIMINARY DESIGN	25
4.1 Concept Generation	25
4.2 Concept Evaluation and selection	28
4.3 Design Constraints and Applicable Codes and Standards Used in the Design.....	30
4.4 Preliminary Analysis	33
(Provide additional sub-sections based on project)	
5. DETAILED SYSTEM DESIGN	40
5.1 (Provide sub-sections based on project)	40
5.4 Engineering Analysis and Simulation	47
5.5. Layout/Detailed Drawings/Equipment selection and specifications	48
5.6 Application of Engineering Codes and Standards in design .	49
5.7 Economic Analysis	55
6. RESULTS & DISCUSSION	60
6.1 Summary of Goals and Objectives	
6.2 Summary of Constraints and Codes met by Design (Provide additional sub-sections)	
7. CONCLUSIONS AND RECOMMENDATIONS.....	70
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Figure 6.2 Sample Details, Required Content and Format for Table of Content

6.5 List of Figures and List of Tables

The list of figures is a page that lists the titles of all figures exactly as used in the report and the page numbers for the format for the figures. A similar list is made for all the tables in the report. A sample list of Figures is given in Figure 6.3. The list of Tables is similar to the list of figures in format.

Each figure or table should be placed immediately after the page of first reference. This means that each figure or table included in the report should be referenced and described in the report. In addition, each figure should have a figure number, followed by two spaces, then the title of the figure (which should be centered) and placed one line space BELOW the figure as shown in Figure 6.4.

Each table should have a table number, followed by two spaces, then the title of the table (which should be centered) placed one line space ABOVE the table as shown in Figure 6.5.

If a figure or table does not have a number, title, and not cited and described in the report, then there is no need for that figure or table to be in the report.

6.6 Abstracts

This summarizes the report, including results, in one page so that readers can decide whether they want to read the report in detail. The abstract should contain a summary of the following:

- a brief statement of the problem
- the project definition, goals and objectives
- the method of solution within the stated constraints;
- the significant results; and
- the conclusions drawn from the results.

The abstract is placed on a separate page, single-spaced with no indentions.

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Figure 2.1 Pump Characteristic Curve used for Pump Selection.....	35
Figure 3.1 Effects of Heat Transfer Coefficient on Heat Exchanger Area Required	38

Figure 6.3 Sample Details and Format for List of Figures and Tables



Figure 2.13 Helium Mass Spectrometer Sample Holder

Figure 6.4 Sample Format for Labeling a Figure in Reports

Table 3.3. Baseline Mechanical Property for T650-35/HPPE-II-52 Material

Material Type	Stress (MPa)	Strain (%)	Modulus (MPa)	Max load (KN)
KC-X-80A-1	868.68	1.102	73049.04	28.807
KC-X-80A-2	852.92	1.116	79838.61	27.541
KC-X-80A-3	907.22	0.830	84347.52	29.382
KC-X-80A-4	958.67	0.907	97627.90	31.111
KC-X-80A-5	920.62	1.075	87055.10	29.816
Mean	901.62	1.006	84383.64	29.331
S. D.	42.1	0.129	9106.02	1.312

Figure 6.5 Sample Format for Labeling a Table in Reports

6.7 The Main Body of the Report

The main body of the report contains the introduction, project planning and task definition, the literature survey, the preliminary design, the detailed design, the conclusion and the recommendations.

This section should be written using active voice. The use of first person pronouns should be avoided, and correct grammar should be used. The detailed content of each section of the main body of the report are provided in Figure 6.2. It is required that each sub-section shown in Figure 6.2 be included in the report.

6.8 Literature Review

In the literature review section, you are required to find out what has been done by others in related areas of the project. To do a good literature review, it is necessary to have a complete understanding of the problem as described under the project scope. Material discussed in the literature review should be directly related to the project, provide advantages and disadvantages of various theoretical and practical concepts applicable to solving the problem.

6.9 Citation of References in a Report

When information is obtained from an external source and used in the report, it should be cited or referenced in the report to give credit to the original authors of the information and to enable readers of your report to directly access the source of the information.

There are several standards available for in text citation and listing references in a report including the American Psychological Association (APA), the Modern Language Association of America (MLA), and the Council of Biology Editors (CBE) standards. The method recommended for use in all project reports is the Council of Biology Editors (CBE) number system, in order of first mention. In this system the reference immediately follows the material that needs to be cited in the text using a reference number in square brackets. The first source cited will be [1], the second source will be [2] and so on as shown in the example in Figure 6.6. In the case of two citations, the numbers should be separated by a comma [1,2]. In the case of more than two reference citations, the numbers should be separated by a dash [5-7].

Each report should have references cited in the report and a complete list of such references should be listed at the section of the report titled “LIST OF REFERENCES” . Providing a list of references at the end of the report means the references have been cited by name and number in the report. All references should be cited in the report followed by the reference number in square brackets. Citations should always follow the example given in the sample in Figure 6.6.

In calculating the heat transfer coefficient, equations obtained from Chapman [1] were used. The manufacturer [2] has provided heat transfer coefficient for various shell side fluids as shown in Figure 1.1.

Figure 6.6 Method for citing and referencing a Reference source in Reports

6.10 List of References.

References cited in the report should be listed together at the end of the report in a section titled “List of References.” Footnotes should not be used for this purpose. References should be arranged in numerical order according to their order of appearance within the report.

The detailed format and examples for listing references from different sources are provided below.

6.10.1 Books.

The citation-sequence system shown below should be used to list book references.

Reference number in square brackets, followed by last name, first and middle initials, of each author separated by commas, followed by the title of the book (in italics or underline), followed by the name of the publisher, city of publication, the year of publication, and the inclusive pages preceded by pp.

Example

- [1] White, F.M., *Fluid Mechanics*, McGraw-Hill, New York, 1999, pp 120-135

6.10.2 Magazine and Journal Articles

The citation-sequence system shown below should be used to list magazine and Journal article references. Reference number in square brackets, followed by last name, first and middle initials, of each author separated by commas, followed by the title of the article in quotation marks, followed by the title of the Magazine or Journal (in italics or underline), followed by the volume number if available, followed by the date of issue of the magazine or journal the article occurs in, and the inclusive pages preceded by pp. If there are more than three authors, use the first one (last name first), followed by "et al.," which means "and others."

Example

- [15] Biney, P.O, Dong, W.G., and Lienhard, J.H., "The use of a cubic equation to predict surface tension and spinodal limits," *Journal of Heat Transfer*, 108, 1986, pp405-410.

6.10.3 Reports.

The citation-sequence system shown below should be used to list report references.

Reference number in square brackets, followed by last name, first and middle initials, of each author separated by commas or the group name, followed by the title of the report (in italics or underline), followed by report number, followed by the name of the publisher or publishing organization, followed by the date of publication of the report, and the inclusive pages preceded by pp.

Example:

- [11] Biney, P.O., *Effects of Service Conditions on the Morphology and Properties of Advanced Composites for Cryogenic Tank Applications*, NASA FAR NCC3-972-2004, PVAMU FAST Center, 2004, pp 25-30.

6.10.4 Personal interviews, correspondence, and other nonprint sources.

The citation-sequence system shown below should be used to list personal interviews, correspondence, and nonprint source references.

Reference number in square brackets, followed by last name, first and middle initials, the person interviewed or the information source, followed by the title and organization of the person interviewed, followed by location of the interview, followed by the type of information (personal interview, personal correspondence, etc.), followed by the date of interview.

Example

- [32] Lin. S.B., Department Head, Mechanical Engineering Department (PVAMU), Prairie View, Texas, personal interview, January 15, 2005.

6.10.5 Encyclopedia articles.

The citation-sequence system shown below should be used to list encyclopedia references.

Reference number in square brackets, followed by last name, first and middle initials of the article's author if shown, followed the title of the article in quotes followed by the name of the encyclopedia, then the date of the edition.

Example

[14] Kazumi, A.M., "Fusion Reactors," Encyclopedia Britannica, 1998 ed.

6.10.6 Product brochures.

The citation-sequence system shown below should be used to list product brochure references. Reference number in square brackets, followed by name of author or company, followed by the title of the brochure information, (in *italics* or underline), followed the type of brochure, followed by the name of publisher, city, and date of publication

Example

[22] PVAMU FAST Center, *Permeability Measurement System*, Research Equipment Brochure, PVAMU FAST Center, Prairie View, 2002.

6.10.7 Borrowed graphics and tables.

The source of the borrowed graphics or Table is indicated in the title of the Figure or the Table as shown in the example in Figure 6.7, and the reference is listed according to the source type described earlier.

Example

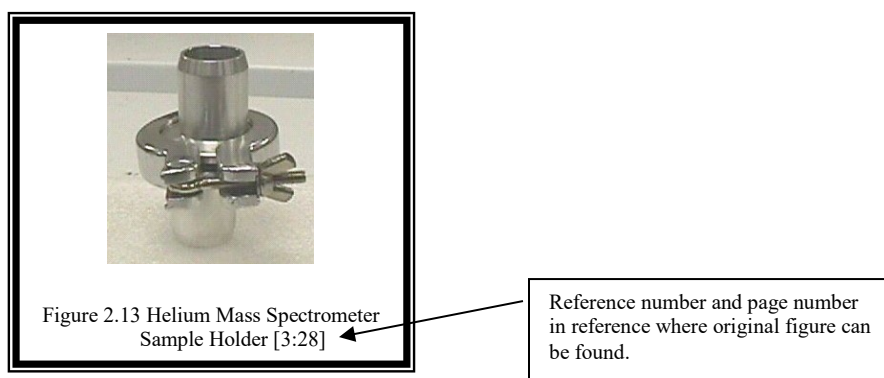


Figure 6.7 Sample Reference for a Borrowed Graphic

6.10.8 WWW Sites (World Wide Web)

Author's name, last name first; the full title of the work (capitalizing only the first word and any proper nouns in quotation marks); the date of the document or last revision in parenthesis. The protocol (e.g., "http") and the full URL, followed by the date of access in parentheses.

Example:

[9] McMurrey, David A; "Documentation: Citing Sources of Borrowed Information", <http://www.io.com/~hcexres/tcm1603/achtml/docu.html#numbersystem> (January 10, 2005)

Students are encouraged to consult David A. McMurrey article on Citing Sources of Borrowed Information [3].

Evaluation of the written communication component of the project report will be based on ability to organize, plan, and properly format a technical report; ability to compose original texts and properly apply the conventions of written language; and ability to provide appropriate discussion, conclusions and recommendations. The form shown in Table 8.2 provides the details of all items used for evaluating students' performance on the written communication under three performance criteria.

Table 8.2 Written Communication Evaluation Form

Outcome Performance Criteria Areas Assessed	MAX POINTS	POINTS RECEIVED
1. Ability to organize, plan and properly format a written technical report		
(i) Students are able to organize report by categorizing ideas for the report into well and logically organized chapters, major sections, subsections and paragraphs blended within the larger units.		
(ii) Students provide Title Page, Abstract, and Table of Contents, list of Figures, and List of Table formatted.		
(iii) Students provide figure number and title for each figure in the report, reference each figure discuss each figure in the report in accord with standards in the project manual.		
(iv) Students provide table number and title for each table in the report in accord with standards in the project manual, reference each table, and completely discuss each table in the report.		
(v) Students properly cite references in the report and provide well formatted reference list at the end.		
(vi) Students prepare the written report in accord with standard report formatting provided in the Senior Projects Report Manual.		
Total for PC1		
2. Ability to compose original texts and properly apply the conventions of written language.		
(i) Properly apply capitalization, punctuation, and penmanship, to communicate clearly		
(ii) Spell proficiently		
(iii) Apply standard grammar and usage to communicate clearly and effectively in writing including • using complete sentences, varying the types such as compound and complex to match meanings and purposes • properly employing standard English usage in writing for audiences, including subject-verb agreement, pronoun referents, and parts of speech • properly using adjectives (comparative and superlative forms) and adverbs appropriately to make writing vivid or precise • properly using prepositional phrases to elaborate written ideas • properly using conjunctions to connect ideas meaningfully		
(iv) Use available technology to support aspects of creating, revising, editing, spell checking, and publishing the report.		
3. Ability to provide appropriate discussion, conclusions and recommendations		
(i) Summarize the goals, objectives, and indicate whether they were met.		
(ii) Summarize the results.		
(iii) Summarize constraints and codes and indicate whether they were met.		
(iv) Provide logical conclusions and recommendations (including strengths and weaknesses).		

9. PROJECT REPORT EVALUATION

There will be at least two formal written reports in each Senior Design Project course consisting of the mid-semester and the final written project reports in addition to any intermediate reports that may be required. The technical/design content of the project will be evaluated based on ability to define/understand the problem and plan the project; ability to conduct relevant literature review, generate ideas and apply creativity; and ability to perform preliminary and detailed design leading to the realization of the system, component or process. Table 9.1 shows the details of all items used to evaluate the technical content of the final project report for Senior Design and Professionalism I and II.

Table 9.1 Project Design Content Evaluation Form

Outcome Performance Criteria Areas Assessed	MAX POINTS	POINTS RECEIVED
1. Ability to Define/Understand the Problem and then Plan the Project		
(i) Identify the customer and the needs.		
(ii) Identify and list the design objectives.		
(iii) Identify the design constraints.		
(iv) Define the design strategy and methodology.		
(v) Identify and break down work into tasks and subtasks and identify the personnel and deliverables for each.		
(vi) Develop a Gantt chart and critical path analysis for managing the project.		
(vii) Establish major milestones for tracking progress and define performance metrics to measure success		
2. Ability to Conduct a Review of the Literature, Generate Ideas and Apply Creativity		
(i) Identify the types of information needed for a complete understanding of all aspects of the project (Based on task described in the project planning).		
(ii) Gather information on relevant fundamentals, theory / concept (demonstrate technical competence) and relate them to the design.		
(iii) Provide the sources in a list of references properly cited in the literature review section and relevant sections of the report.		
(iv) Define functional requirements for design (Specific required actions needed to be performed for the design to be achieved).		
(v) Transform functional requirements into candidate solutions / mathematical modeling.		
(vi) Evaluate candidate solutions to arrive at feasible designs.		
3. Ability to Perform Preliminary and Detailed Design		
(i) Identify applicable codes and standards for the design		
(ii) Perform relevant detailed analysis (engineering, mathematical, economic) in accord with applicable codes and standards.		
(iii) Develop final design specifications		
(iv) Do the design within realistic constraints such as economic, environmental, social, political, ethical, health and safety, manufacturability, and sustainability		
(v) Select materials/components/software/test equipment.		
(vi) Fabricate a prototype or a model (physical, software, hardware) of the design.		
(vii) Test or simulate the design and make necessary changes to obtain optimum design.		

10. GENERIC TIMETABLE FOR MAJOR PROJECT EVENTS

The senior design project sequence begins in the Fall semester and ends by the end of April the following Spring semester. A guideline is, therefore, needed to ensure that the various sections of the project design sequence are on schedule. Table 10.1 is a generic time table for major events in the senior design project sequence. Separate schedules are provided for projects that begin in the Fall semester and in the Spring semester. The course instructors are strongly advised to ensure that the schedule in Table 10.1 is followed as closely as possible to ensure successful timely completion of the projects.

Table 10.1 Generic Timetable for Senior Design Project and Professionalism

ITEM NUMBER	MONTH	8-MONTH SCHEDULE FOR PROJECTS THAT BEGIN IN FALL SEMESTER (tentative)	8-MONTH SCHEDULE FOR PROJECTS THAT BEGIN IN SPRING SEMESTER (tentative)	BEGINNING SPRING MAJOR PROJECT EVENT
0	0			Project Identification
1	1	9/7	1/14	Project Selection and Team Formation
2	1	9/30	1/30	Project Definitions and Specifications and Background Research
3	2	10/15	2/15	Project Planning and Task Definition
4	2	10/31	2/28	Literature Review
5	3	11/21	3/21	Preliminary Design and Oral Presentations
6	4	12/1	4/30	Project Report
7	6	2/15	9/15	Detailed Design Development and Parts Acquisition
8	7	3/1	10/15	Mid-semester Design Review and Presentations
9	8	4/8	11/8	System Simulation & Optimization; Design Iteration; and Construction & Testing
10	8	4/15	11/15	Final Design Review (Oral Presentations and Draft Final Report)
11	8	4/30	11/30	Final Senior Design Report

LIST OF REFERENCES

- [1] Felder, R. M. and Rebecca Brent, "How to Improve Teaching Quality," *Quality Management Journal*, Vol. 6, No. 2, 1999, pp. 4-5.
- [2] Csemica, J. et. Al., *Practical Guide to Teamwork* (Version 1.1), Bucknell University, June 26, 2002.
- [3] Murrey, David A; "Documentation: Citing Sources of Borrowed Information", <http://www.io.com/~hcexres/tcm1603/achtml/docu.html#numbersystem> (January 10, 2005).
- [4] Hart, H., *Introduction to Engineering Communication*, Pearson Prentice Hall, 2005.
- [5] Lannon, J.M., *Technical Writing*, Harper Collins College Publishers, 6th Edition, 1994.

APPENDIX: LETTER OF TRANSMITTAL

FIRM IDEAS

100 East 51st

Austin, TX. 78705

(512) 400-3333

May 1, 2004

Mike Parker, Manger of EBC Properties
1000 Summit Lane
Austin, TX 78705

Dear Mr. Parker:

The attached technical report contains Firm Ideas' evaluation of wall designs that control airborne sound transmission. This report includes the descriptions of each wall design, the evaluation process, and the wall design that Firm Ideas recommends EBC Properties use in their new apartment complexes. We used the solution criteria established by EBC Properties and Firm Ideas to evaluate six wall designs:

- Single-Stud Wall with Resilient Channel
- Single- Stud Wall with Sound-Deadening Board
- Staggered-Stud Wall
- Staggered-Stud Wall with Sound-Deadening Board
- Double –Stud Wall
- Double-Stud Wall with Sound-Deadening Board

Firm Ideas recommends that EBC Properties use the Double-Stud Wall in their new apartment complexes. First, the Double-Stud Wall provides moderate performance with an STC value of 53 decibels. Second, the Double-Stud Wall has a relatively low materials cost \$11.98 per linear foot and a relatively low labor cost of \$8.74 per linear foot. Finally, the Double-Stud Wall can support the highest mountable object weight, 110 pounds per linear foot. This wall design best meets the needs of EBC Properties.

Firm Ideas is available to answer any questions you may have concerning this report or the project in general. You can contact Firm Ideas at (512) 400-3333 or by e-mail at engineers@mail-utexas.edu.

Sincerely,

Jeffrey Hunt
Project Engineer

**ABOVE AVERAGE
PROJECT REPORT**

Design Report for the Industrial Production of Penicillin G Potassium

Dr. Lealon Martin

Team 2

Tiarra Rodrigues, Caleb Myers, Katelynn Inman, Chiebuka Ejimadu

December 6th, 2021

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LETTER OF TRANSMITTAL

December 6, 2021

Dr. Lealon Martin
Professor, Roy G. Perry College of Engineering
Prairie View A&M University

Dear Dr. Martin,

Team 2, which comprises Tiarra Rodrigues, Caleb Myers, Katelynn Inman, and Chiebuka Ejimadu, has completed the Fall 2021 semester requirements for Senior Design & Professionalism I. This report includes details on a suggested plant design for the production of penicillin G potassium, or penicillin G K. After conducting research on the global and local markets for penicillin (supply and demand), an extensive literature analysis, and price estimates based on raw material and process costs, the team believes that this process is both feasible and profitable. From extensive economic research, the team has proposed a plant capacity of 6.86 million kg/yr in order to meet 20% of the U.S. demand for penicillin. Moreover, the team suggests building the plant in Magnolia, TX, to take advantage of extensive land for potential expansion, mild ambient temperatures, and due to its proximity to farms and necessary raw materials.

The team hopes that this design proposal will gain your approval, and is available to answer any questions about the project that you may have; please contact our team leader, Tiarra Rodrigues, @ trodrigues1@pvamu.edu.

Sincerely,

Tiarra Rodrigues
Caleb Myers
Katelynn Inman
Chiebuka Ejimadu

Caleb Myers *Katelynn*
Inman

Chiebuka Ejimadu *Tiarra*
Rodrigues

Acknowledgement *(Tiarra)*

We would like to acknowledge and express our utmost thanks and gratitude to each of the individuals who assisted in the completion of our plant design and report. A great thanks goes out to Dr. Martin and Dr. Gyamerah for their exceptional leadership and guidance throughout the design process. Their stewardship and advice played a pivotal role in the development of the proper plant design and report format.

We would also like to thank the staff within the Chemical Engineering Department of the Roy G. Perry College of Engineering. They assisted our team and made sure we had access to all the tools we needed in order to be successful. We would also like to thank our graduate student colleagues for not only paving the way for us to follow but showing us the necessary steps to be successful as we emerge from the department as alumni.

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Project Summary *(Tiarra)*

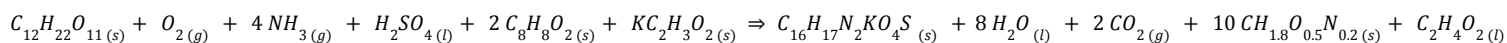
The purpose of this project is to design a plant that produces Penicillin G Potassium. There are various components that have contributed to our project success and semi-completion. Our team has completed an analysis to understand the Penicillin G Potassium market both domestically and internationally and have identified market trends to fulfil the product demand. After the plant's capacity was determined, we selected the production process. Alternate production routes are to be considered, but the highest yield and most economically viable process must be chosen. Once decided, the chosen process must be modeled within simulation software, in this case ASPEN Plus, to analyze process feasibility and steady-state process conditions. Doing so will display the efficiencies and deficiencies of the process in terms of what is necessary for plant capacity to be met and production to occur. Ultimately, our goal is to create a Penicillin G Potassium production plant that is up to date with modern chemical manufacturing plant regulations and standards

Project Scope

Problem Statement (Tiarra)

According to the Centers for Disease Control and Prevention (CDC), 101,567 cases of syphilis were reported in the U.S. in 2017, yielding a rate of 31.4 cases per 100,000 population as compared to previous years. The inception of the pandemic of 2020 is a prime case as well, that is projected to fuel the demand for penicillin antibiotics forecasted for 2026. The demand for medicinal penicillin in the U.S. is approximately 34.3 million kg per year based on the percentage of dependence on China's production. In response to this high demand for Penicillin G, our team will produce a preliminary design of a Penicillin plant to produce 20% of the U.S. demand. The sales department has conservatively estimated that they can sell 6.86 million kg of penicillin per year to various wholesalers and pharmaceutical companies in the United States.

Penicillin G potassium will be synthesized from *Penicillium Chrysogenum* and media containing lactose, ammonium sulfate as a nitrogen source, and an acidic precursor (phenylacetic acid) via aerobic fermentation:



Penicillin is a fungal antibiotic that is derived from the species *Penicillium chrysogenum*; it is used to treat many varieties of bacterial infections. The main two forms of first-generation penicillin – penicillin G and penicillin V – differ in that penicillin V is a derivative of penicillin G and is taken orally, unlike penicillin G, which is intravenous. Potassium acetate is introduced within the extraction phase to contribute potassium ions to the broth and further synthesize Penicillin G Potassium, which is the powder medicine used to treat various bacterial infections. Within the design parameters we have given the annual production, cost parameters, time horizon, thermodynamic properties, and performance models of the units. Our team will present a design proposition that includes equipment sizes and structural alternatives. The facility will present stable operating conditions that simultaneously maximizes the economic performance and minimize the environmental impact.

Client Identification and Recognition of Need (Caleb)

The widespread growth of bacteria with resistance to standard antibiotics has been a topic of concern over the past few decades. Figure 1a shows the growth in the percentage of infectious bacteria that possess this resistance since 2000. Based on the trend, although the data only extends to 2014, it reveals a 2% increase in the concentration of resistant bacteria about every 6-7 years; based on this assumption, it is safe to expect over 12% of infectious bacteria to be resistant to standard antibiotics by 2022. This phenomenon has undoubtedly increased the demand for higher-level penicillins that are able to eradicate these evolved bacteria. Figure 1b shows the expected growth in the demand for amoxicillin over the course of the next 6 years. Amoxicillin is a penicillin antibiotic that specifically treats stomach ulcers. It is assumed that the market for other high-level penicillins will see similar increases within the decade. The primary goal of the plant is to supply its pharmaceutical clients an adequate amount of penicillin G potassium to synthesize enough high-level penicillins that can reverse this trend.

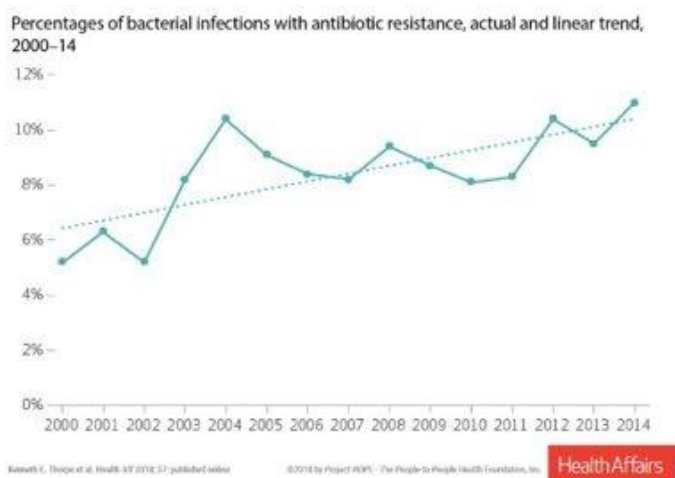


Figure 1a. Growth of bacterial infections with resistance to antibiotics from 2000-2014

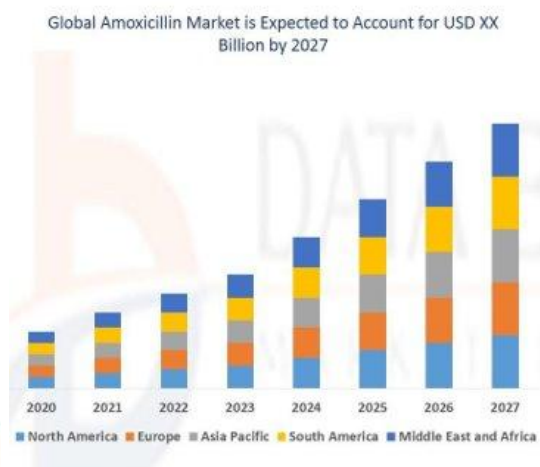


Figure 1b. Expected Growth of the Amoxicillin Market by 2027

The plant's clientele mainly consists of pharmaceutical companies, specifically Pfizer, Baxter, King Pharmaceuticals, and Sandoz. After being dried and grinded, the final penicillin G potassium recovered is in the form of crystal powder which allows for easier and more efficient handling and distribution. The powder is sent to a solid hopper via conveyor belt, and is dispensed into bulk bags that will be transported to clients by road. Once shipped to pharmaceutical buyers, the penicillin G potassium may be diluted with solution to form intravenous benzylpenicillin, or, in most cases, used to synthesize higher-level penicillins that are specialized to treat specific bacterial infections.

Project Goals and Objectives (Tiarra)

1. Determining an optimal process design simultaneously maximizes the economic performance and minimizes the environmental impact.

2. We will be selling biomass which is one of the byproducts from the process. It is created within our production and is great for outsourcing agriculturally. This will be explained further in the report.
3. Our process will also produce a purity of 99.5% Penicillin G Potassium.

Contemporary issues and impact of project on society (Tiarra)

1. Contemporary issues relevant to project

The Center for Disease Control and Prevention, more commonly known as CDC, is an American government-based organization that helps stabilize the infrastructure of public health and aid in stopping the spread of diseases. From their statements, antimicrobial resistance is the leading issue concerning antibiotics[8]. The resistance occurs when bacteria evolve and develop counterattacks to withstand the drugs designed for them. These evolved bacteria continue to grow and spread and are very difficult to maintain. In more severe cases, they are impossible to kill. In the United States every year, there are 2.8 million people who become infected with antimicrobial resistant bacteria and they most likely will have to be admitted into hospitals and receive stronger doses of toxic medications.[8] Even still more than 35,000 individuals will die each year from the 2.8 million people infected.[8] Even during the COVID-19 pandemic, the CDC monitors what possible effects antimicrobial resistance could have on the nation. Below is a chart provided by the CDC of antibiotics and their resistant bacteria that evolved over time.

Table 1. List of Antibiotics and their Identified Resistant Bacteria since the Creation of each Antibiotic [8]

Antibiotic Approved or Released	Year Released	Resistant Germ Identified	Year Identified

Penicillin	1941	Penicillin-resistant <i>Staphylococcus aureus</i>	1942
		Penicillin-resistant <i>Streptococcus pneumoniae</i>	1967
		Penicillinase-producing <i>Neisseria gonorrhoeae</i>	1976
Vancomycin	1958	Plasmid-mediated vancomycin-resistant <i>Enterococcus faecium</i>	1988
		Vancomycin-resistant <i>Staphylococcus aureus</i>	2002
Methicillin	1960	Methicillin-resistant <i>Staphylococcus aureus</i>	1960
Extended-spectrum cephalosporins	1980 (Cefotaxime)	Extended-spectrum beta-lactamase- producing <i>Escherichia coli</i>	1983
Azithromycin	1980	Azithromycin-resistant <i>Neisseria gonorrhoeae</i>	2011
Imipenem	1985	<i>Klebsiella pneumoniae</i> carbapenemase (KPC)-producing <i>Klebsiella pneumoniae</i>	1996

Ciprofloxacin	1987	Ciprofloxacin-resistant <i>Neisseria gonorrhoeae</i>	2007
Fluconazole	1990 (FDA approved)	Fluconazole-resistant <i>Candida</i>	1988
Caspofungin	2001	Caspofungin-resistant <i>Candida</i>	2004
Daptomycin	2003	Daptomycin-resistant methicillin-resistant <i>Staphylococcus aureus</i>	2004
Ceftazidime-avibactam	2015	Ceftazidime-avibactam-resistant KPC-producing <i>Klebsiella pneumoniae</i>	2015

2. Potential impact of project on society

Since our company's goal is to decrease the United States dependency of Penicillin G from China, our impact will come from how much product is created. The United States in theory should buy from our company to save money on import cost and support local businesses. The most damaging greenhouse gas, carbon dioxide, is released into the atmosphere from the burning of fossil fuels. Factory emissions contribute greatly to the release of carbon dioxide into the atmosphere. Industry and electrical generating factories contribute slightly more than 50 percent of greenhouse gases.[11] To combat this epidemic, our company will be implementing a carbon capture system (CCS) in place. There are three steps to this process:

1. **Capture:** the CO₂ is separated from other gases produced in industrial processes, such as those at coal and natural-gas-fired power generation plants or steel or cement factories.[11]
2. **Transport:** the CO₂ is then compressed and transported via pipelines, road transport or ships to a site for storage.[11]
3. **Storage:** finally, the CO₂ is injected into rock formations deep underground for permanent storage.[11]

The mycelium biomass from our process is captured and sold as a byproduct for animal feed. Due to our location, Magnolia, TX, this will play a major role in our economic breakdown. There is a lot of agriculture related businesses that we will sell to. To support a large production scale, the design team must take into account the effect of the production process on the environment while utilizing inexpensive substrates and achieving high production yields. The development of a plant will provide a moderate amount of jobs for engineers, contractors and operators alike, be they local or outsourced from different locations.

Project Planning and Task Identification

Task Identification (Caleb)

Team 2 began its project on September 6, 2021. The final fall semester presentation and evaluation was set to November 20, 2021, and the fall semester report will be due December 6, 2021; consequently, the group had roughly three months to complete tasks for the fall semester. In order to effectively and efficiently meet the demands of this design project, it was divided into three phases, each requiring its own set of tasks and most tasks requiring sub-tasks. Given the three-month time constraint and identified deliverables, the group was able to develop a long-term schedule based on assumptions of how much time each deliverable was believed to have required.

Project Phases:

- Phase 1 - Project Initiation & Conceptual Design
- Phase 2 - Flow Sheet Development
- Phase 3 - Project Term Assessments and Reporting

Timelines (Caleb)

As previously mentioned, the major tasks outlined on the gantt chart were further divided into sub-tasks to ensure all parts of each major task were satisfied. The timeline below lists the required tasks for the fall semester and the amount of time allocated for each one:

1. Process Initiation & Conceptual Design

- a. Project Overview & Market Data: 24 days (9/6/21 - 9/29/21)
- b. Process Parameters: 32 days (9/10/21 - 10/11/21)
- c. Process Safety: 21 days (10/29/21 - 11/19/21)

2. Flow Sheet Development

- a. Process Description: 13 days (9/21/21 - 10/3/21)

- b. Block Flow Diagram: 10 days (9/24/21 - 10/3/21)
 - c. Preliminary Process Flow Diagram: 13 days (9/29/21 - 10/11/21)
 - d. Material Energy Balances: 11 days (10/1/21 - 10/11/21)
 - e. ASPEN Simulation: 17 days (10/3/21 - 10/19/21)
 - f. Final Process Flow Diagram: 9 days (10/11/21 - 10/19/21)
- 3. Project Term Assessments & Reporting**
- a. Weekly Meetings with Dr. Lealon Martin (9/9/21 - 11/25/21)
 - b. Assessments/Homework Assignments (9/21/21 - 11/30/21)
 - c. Midterm Presentation: 23 days (9/27/21 - 10/19/21)
 - d. End of Term Presentation: 30 days (10/22/21 - 11/20/21)
 - e. End of Term Report: 46 days (10/22/21 - 12/6/21)

Gantt Chart (Caleb)

The gantt chart shown below was constructed to show the team's plan for executing deliverables during the fall semester (Figure 2). Detailed views of the individual sections of the gantt chart are provided below the full view.

FALL 2021 SEMESTER GANTT CHART

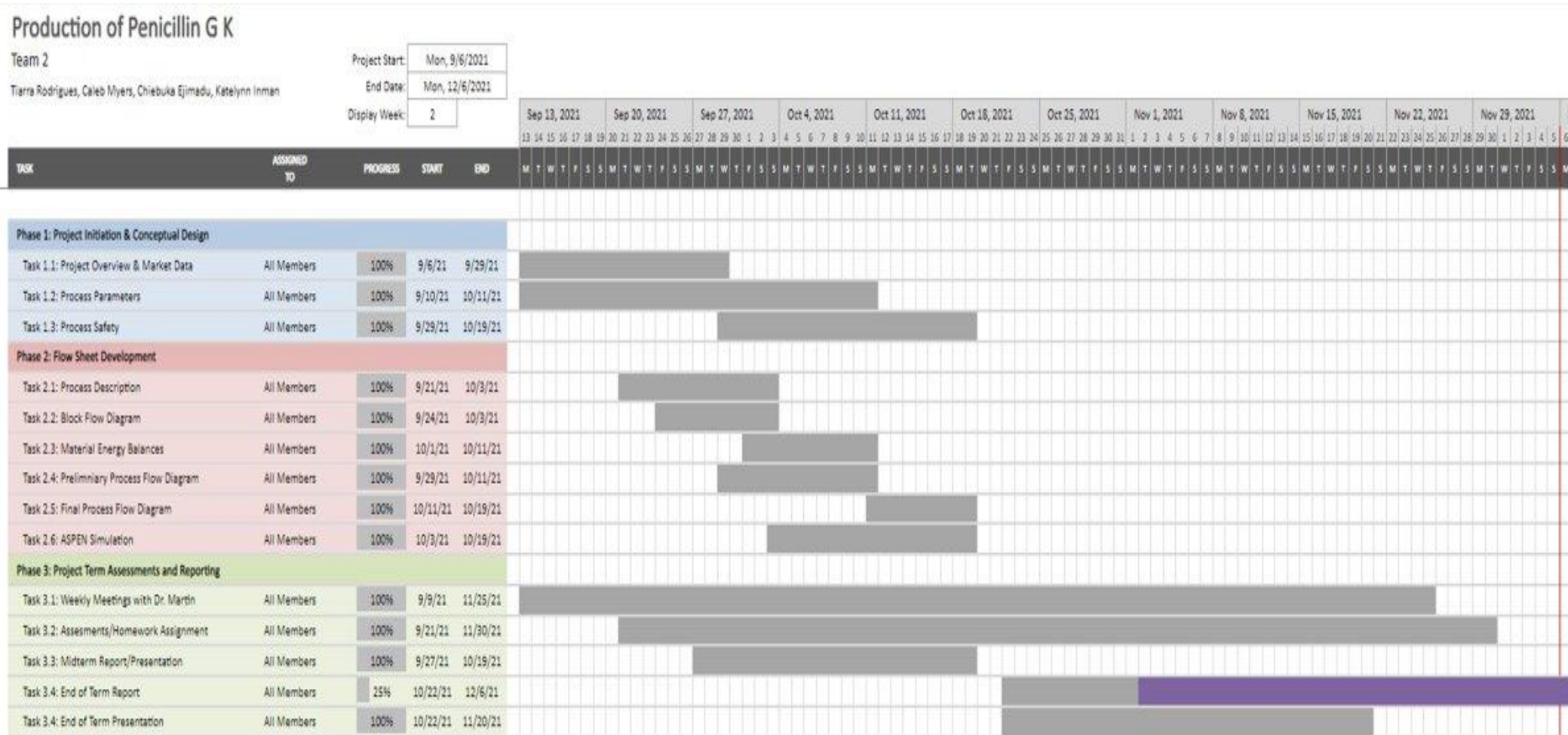


Figure 2. Fall Semester Gantt Chart

Literature Review

Penicillin G was first synthesized as..... (Tiarra)

Before the creation of antibiotics, there were no effective treatments for infections like pneumonia, and gonorrhea. Someone could contract a serious disease from a simple cut/scratch. In 1928, Professor Alexander Fleming accidentally discovered the first strain of penicillium notatum within his staphylococcus petri dishes. This penicillium was capable of killing a wide range of harmful bacteria. Now that scientists were able to separate the strain and cultivate it, they wanted to increase their yield to a large-scale production to be used during WWII. Penicillin was named the “wonder drug” that saved millions of lives. By 1949, the US successfully industrialized penicillin production to be distributed to pharmacies throughout the nation. After the rise of resistant bacteria, in 1961, scientists sought out alternatives to the original antibiotics. The idea of synthetic drugs formulated from the original properties was executed and this was only the beginning. Modern day penicillin is derived from a newer fungal bacteria strand penicillium chrysogenum. Today, penicillin is still used to treat various bacterial infections like syphilis, strep throat, meningitis and so on. Higher level penicillins are used to combat the evolved bacterias.

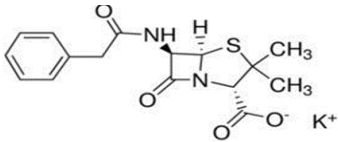
Production Route (Katelynn)

The production of Penicillin G is done through fermentation. All penicillin G is derived from the fermentation of a microorganism, *Penicillium chrysogenum*, with an addition of a precursor, phenylacetic acid. The fermentation process starts with a cell culture, a pure strain of *Penicillium chrysogenum*. In a lab the cells are added to a petri dish to increase their size, from there they are put in a flask with more medium to multiply. Once the cells have reached the max growth phase in the flask, they are transferred to the inoculum. From the inoculum into the fermenter where penicillin is produced. Then the penicillin G is sent to the extraction phase.

Physical and Chemical Properties (Tiarra)

Table 2. List of Chemical and Physical Properties of the Product Penicillin G Potassium [5]

Chemical Properties	Physical Properties

Chemical Formula	C ₁₆ H ₁₇ KN ₂ O ₄ S	Color	White
Drug Class	Penicillin	Odor	Odorless
pH	6.5	Phase	Solid powder
Stability	Stable	Molecular Weight	372.5 kg/kmol
Solubility	Soluble in Water	Density	1.36 kg/L
Structure		Melting Point	214-217 °C
Flammability	This material is combustible, but will not ignite readily	Particle Size	10 microns
Reactivity	High accumulation results in combustion (dust explosion)	Flash Point	335 C

Handling, Storage and Safety (Tiarra)

1. Handling

- When handling, use appropriate personal protective equipment (ppe listed in safety). Individuals with direct exposure to the product should avoid inhalation and contact with skin, eye, and clothing. This is to ensure that there is no contamination transferred from the individual to the product. Individuals should wash their hands before and after leaving the facility post PPE removal.
- When handling the product, it would be optimal to minimize dust generation and accumulation by regularly maintaining the facility, equipment, and storage of any exposed areas.

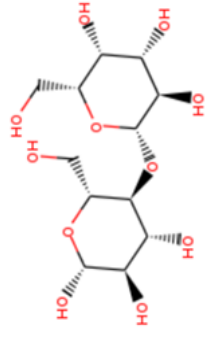
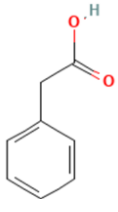
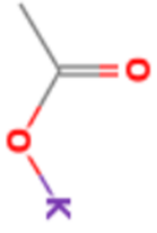
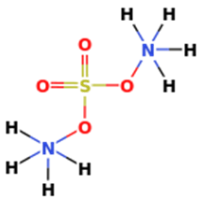
Accidental spills

- **Health and Safety Precautions:** Personnel involved in clean-up should wear appropriate personal protective equipment (listed in Safety) to limit their exposure.
- **Measures To Take for Cleaning / Collecting:** Contain the source of spill if it is safe to do so. Collect spilled material by a method that controls dust generation such as a damp cloth or a filtered vacuum. These ways are great for thoroughly cleaning spills of dry solids.
- **Additional Consideration for Large Spills:** Non-essential personnel should be evacuated from affected areas. Report emergency situations immediately. Clean up operations should only be undertaken by trained personnel.

2. Storage

Table 3 : Raw Process Materials

	Lactose	Phenylacetic Acid	Sulfuric Acid	Potassium Acetate	Ammonium Sulfate
Molecular Weight	342.3 kg/kmol	136.15 kg/kmol	98.079 kg/kmol	98.142 kg/kmol	132.14 kg/kmol
Chemical Formula	$C_{12}H_{22}O_{11}$	$C_8H_8O_2$	H_2SO_4	$C_2H_3KO_2$	$(NH_4)_2SO_4$

Chemical Structure					
Boiling Point	668.9 °C	265 °C	337 °C	117.1 °C	330 °C
Freezing Point	202.8 °C	76.5 °C	10 °C	292 °C	235 °C
Flash Point	357.8 °C	132 °C	-	> 250 °C	-
Critical Temperature	-	-	654 °C	-	250 °C
Density	1.76 kg/L	1.081 kg/L	1.83 kg/L	1.57 kg/L	1.77 kg/L

- Lactose
 - This material should be stored in a cool and ventilated place to replicate dry conditions. This material should avoid any heat source and oxidizing agents. Similar to Penicillin G Potassium, this is a white crystalline powder that if accumulated can become combustible.[4] This will be stored with materials that have similar storage requirements. This material will be transported in bulk and it is classified as not dangerous.[4]
- Phenylacetic Acid
 - This material will be stored in an airtight container with a ventilated and cooled room. This material should be kept away from incompatible substances like strong bases.[10] This will be stored with materials that have similar storage

requirements.[10] This material will be transported in bulk and it is classified as not dangerous.

- **Sulfuric Acid**
 - This material is a level 8 transport hazard and will be handled as such. Sulfuric acid is typically transported within an high-density polyethylene (HDPE) tank car. When arriving at the facility, this material will be placed in a cool dry room.
- **Potassium Acetate**
 - This material will be stored in an airtight container with a ventilated and cooled room.[12] This material should be kept away from incompatible substances. This will be stored with materials that have similar storage requirements. This material will be transported in bulk and it is classified as not dangerous.
- **Ammonium Sulfate**
 - This material should be stored in a cool and ventilated place to replicate dry conditions. This material should avoid any heat source and oxidizing agents. This will be stored with materials that have similar storage requirements. This material will be transported in bulk and it is classified as not dangerous.

3. *Safety*

Personal Protective Equipment:

- **Hands:** Wear suitable protective gloves according to EN 374. It is recommended to test the chemical resistance of the gloves with the supplier. The gloves should be made of nitrile rubber (NBR) and have a 0.11 mm layer thickness. There should be a minimum level 6 permeation of breakthrough.
- **Eyes:** Wear safety glasses or goggles if eye contact is possible.
- **Skin:** Wear protective clothing when working with large quantities.
- **Respiratory protection:** If airborne exposures are within or exceed the Occupational Exposure Band (OEB) range, wear an appropriate respirator with a protection factor sufficient to control exposures to the bottom of the OEB range. Respiratory protective gear is necessary when dust formation is visible. At this point the individual should wear a respirator with a particulate filter (P2) meeting EN 143 standards. The filters should be able to combat 94% of airborne particles.

First Aid Measures:

- **Eye Contact:** If contact is made, the individual must immediately flush their eyes with water for at least 15 minutes. If the irritation occurs or persists, they will need to receive medical attention.[7]
- **Skin Contact:** Any articles of contaminated clothing must be removed. Flush area where the product came in contact with with large amounts of water and use soap (wash clothing).[7]

- **Ingestion:** One should never give anything by mouth to an unconscious person. Rinse out the individual's mouth with water. Lastly, do not induce vomiting unless directed by medical personnel.[7]
- **Inhalation:** The individual should remove themselves from the contaminated environment and move to fresh air and rest. Also they should seek medical attention immediately.[7]

Reactivity: Initially, the state of the product at delivery is not explosive, however, when there is a large accumulation of fine particles this will lead to a dangerous dust explosion.[9] A dust explosion is defined as a combustion of suspended particles in the air within an enclosed area. These dangerous situations can happen where there is a powdered combustible material in high concentrations within the air and another oxidizing gas (i.e., pure oxygen).[9]

Measures for Environmental Protections: Place waste in an appropriately labeled, sealed container for disposal to avoid environmental release. The product should be kept from drains, ground and surface water as well. We are choosing to implement appropriate technical and procedural waste water and waste disposal measures to prevent occupational exposure or environmental releases. Potential points of process emissions of this material to the atmosphere should be controlled with dust collectors, HEPA filtration systems, or other equivalent controllers.

Uses (Tiarra & Caleb)

The two main uses of Penicillin G Potassium are to treat various bacterial infections like pneumonia, strep throat, and syphilis, and to serve as a precursor to high-level penicillins that may be resistant to natural antibiotics. Because antimicrobial resistance has become one of the greatest global health threats in recent years, new synthetic strains of antibiotics are created to eradicate the bacteria entirely rather than simply inhibiting growth.

Penicillin G in its natural state, is a white powder. The powder can be dissolved in water and injected into a muscle or vein, but the solution may also be administered directly into the lining of the chest cavity, into the fluid surrounding the spinal cord, or into a joint. Conventional antibiotics are derived from natural sources, typically from certain fungi or soil bacteria, and therefore rely on timely fermentation processes that require large-scale bacterial cultures and several subsequent purification stages. They are not designed to avoid resistance. In contrast, synthetic antibiotics are exclusively synthesized in labs to be potent enough to mitigate the threat posed by these evolved bacteria. Unlike their precursor, penicillin G, many synthetic penicillins, such as amoxicillin, may be administered orally.

Product Specification (Tiarra & Katelynn)

Table 4: Product Specification

Purity	99.5% Penicillin G Potassium
Product Recovery	78%

Our product Penicillin G Potassium is a white crystalline powder which is odorless and moderately hygroscopic.[6] Penicillin G potassium is very soluble in water. The pH of the reconstituted product is between 6.0–8.5.[6] The particle size of the will be around 10 microns which is not visible to the naked eye. We chose this size because we wanted a fine particle that is able to be produced consistently and easily stores away. Our product purity is specified as 99.5% Penicillin G Potassium.

Process Selection

Market Analysis and Trends (BUKA)

Natural Penicillin like Penicillin G or V, are major active ingredients for higher-level synthetic penicillin that combat more aggressive bacterial infections/diseases. The global market of penicillin is a very dynamic space, but the demand is forecasted to increase in the coming years due to the increase of drug-resistant bacterial infections. For this project, Penicillin G is our focus. Due to limited market data because most were restricted since it's mostly under China's control, we made a few educational assumptions based on literature study and various historical data that we found. The world production of penicillin was about 105,000 metric tons/year, which is equivalently 95.3 million kg/yr. Based on literature study, China is the main manufacturer of Penicillin G. They produce nearly all of the Penicillin G globally so we assumed a basis of 90 %. Also, the United States is a major importer of Penicillin G from China and they receive about 40-45% of the production.[2] As a desired plant capacity, we assumed 20 % of US demand to fulfill the lack of Penicillin G manufacturing in the United States and to relinquish some percentage of dependence from China in terms of major ingredients to make higher-level penicillin. The calculation to find the desired plant capacity is shown below:

World Production – 105,000 Tons/yr (95.3 million kg/yr)

Nearly all of Penicillin G Production is in China (Assumed 90%)

US demand from China (40% Import)

Desired Plant Capacity (Assumed 20% of US Demand)

To find Plant Capacity ...

$$(95.3 \text{ million kg/yr} * 0.9 * 0.4 * 0.2) = \textbf{6.86 million kg/yr}$$

Medium routes to producing products (Katelynn)

- 1. Penicillin G industrial process and lab/patent routes have been reported to be used for producing Penicillin***

The production process to produce penicillin G has two parts, fermentation and extraction. The Fermentation process starts with a cell culture, a pure strain of *penicillium chrysogenum*. The cell culture is freeze dried and transferred with viable spores of the microorganism. In a lab the microorganism is introduced to a medium that will provide nutrients for it to grow. Once the cells have reached maximum growth it will be transferred to the inoculum tank to start the production of penicillin G. Once the cells have reached peak production of penicillin G it will be transferred to a fermenter. In the fermenter it will continue to produce penicillin G at its peak production rate, allowing the cells to produce the highest yield possible of Penicillin G. The medium was chosen due to it producing the highest yield of Penicillin G compared to others. A carbon source is needed in the medium most being some type of sugar. A simple sugar is best to use as it is easily absorbed by microorganisms allowing a higher number of primary metabolites to be produced. In figure 3 it shows the relation of 5 mediums, one being potato dextrose broth and the other various carbon sources contain, glucose, lactose, maltose, and sucrose; to the concentration of penicillin G those mediums produce. From figure 3 it shows that the potato dextrose medium broth and lactose medium broth produced the highest concentration of penicillin G.

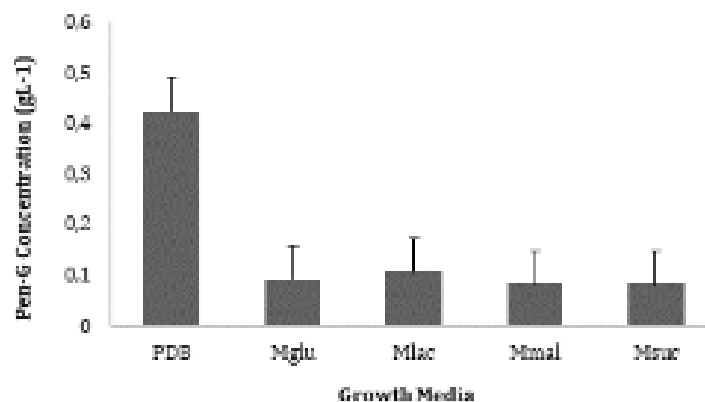


Figure 3. Penicillin G production from *Penicillium chrysogenum* in Various Mediums

In the industry of penicillin G production, a precursor is needed. The precursor allows a higher change of microbes to produce a specific penicillin depending on the precursor. The precursor, phenylacetic acid, acts as a hydrophobic side chain of benzylpenicillin allowing *P. chrysogenum* to specifically produce Penicillin G. The mediums with an addition of a precursor, phenyl acetic acid, give a significantly different result. The penicillin G produced with varied carbon sources have a much lower concentration than the mediums with an addition of PAA. With proper doses the PAA allows optimum Pen G production. The mediums that produced the highest concentration of Pen G without PAA were potato dextrose broth and lactose medium broth. Figure 4 shows the comparison of the 2 mediums with various concentrations of phenylacetic acid and the concentration amount of pen g that they produced. From the graph the Lactose Medium F produced the highest concentration of penicillin G with a PAA concentration of 0.6g/L to be used to derive a relationship in order to find the scaled up concentration for our industrial-size plant.

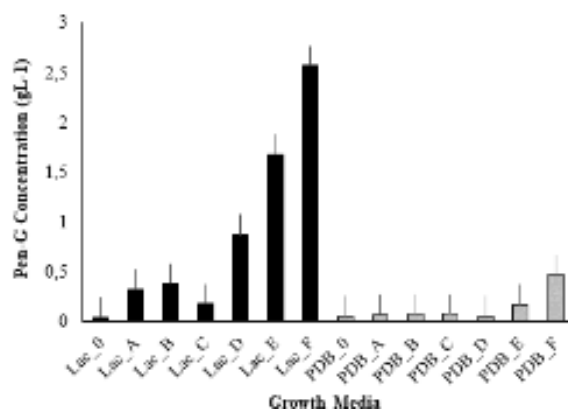


Figure 4. Penicillin Production from *Penicillium chrysogenum* with Various Concentrations of Phenylacetic Acid

2. Medium route 1

The medium is the nutrition factor that governs growth and production of penicillin G by *P. chrysogenum*. The penicillin G medium is first introduced as lab-scale of the process. The medium broth is a standard medium with a lactose carbon source and phenyl-acetic acid precursor. The medium is composed of the following components shown in figure 5. In figure 5 the carbon source chosen is lactose and the composition of the precursor, phenyl-acetic acid, is 0.6g/L. The *penicillium chrysogenum* is inoculated in the medium at room temperature for 48 hours. The medium is then incubated for 10 days with agitation at room temperature. Phenyl acetic acid is added 3 days after the bio production of fungi takes place. Once inoculation is complete the medium produces a 2.46 g/L yield of penicillin G (Sari 2020).

No.	Production medium	Weight (g)
1	KH ₂ PO ₄	0.4
2	(NH ₄) ₂ SO ₄	0.45
3	MgSO ₄ ·7H ₂ O	0.05
4	Na ₂ SO ₄ ·7H ₂ O	0.15
5	ZnSO ₄ ·7H ₂ O	0.2
6	Yeast Extract	0.5
7	Phenylacetic Acid (PAA)	0-0.6
8	Carbon Source Variation (Lac, Glu, Suc, Mal) and PDB	1.5

Notes: Lac= Lactose, Glu= Glucose, Suc= Sucrose, Mal= Maltose and PDB as standard medium. PAA concentration variation (0, A, B, C, D, E, F). 0= 0 gL⁻¹; A= 0.1 gL⁻¹; B= 0.2 gL⁻¹; C= 0.3 gL⁻¹; D= 0.4 gL⁻¹; E= 0.5 gL⁻¹; F= 0.6 gL⁻¹

Figure 5. Penicillin G Production Medium Composition with Various Carbon Sources

The information from this article was utilized to derive a relationship to create an industry scaled process. The composition of the components in the medium were scaled up to find the mass fractions needed to produce penicillin G in a process plant.

3. Medium route 2

Another medium that was reflected upon was a potato dextrose broth medium. This broth is created by the fermentation of potato skins in distilled water. This medium was economically cheaper than the lactose medium selected. The reason this medium was eliminated from the process was due to it producing a smaller yield of penicillin g compared to the lactose medium once the precursor, phenyl-acetic acid, was added. As well the potato dextrose broth medium contains complex sugars that would need to be hydrolyzed by enzymes into simple sugars (Sari 2020). In order for the fungus to hydrolyze these sugars it would have to produce the enzymes to break down the complex sugar into a simple sugar making the fungus work harder.

Process Economy of Overall Reaction (Katelynn)

Overall Reaction Path:

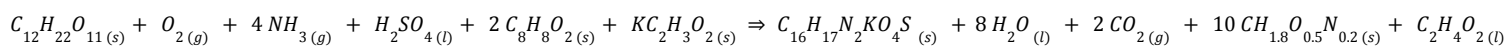


Table 5. Overall Reaction Component Cost

Components	kg-mole	Molecular Weight (g/mol)	kg	kg/kg of Penicillin G Potassium	\$/kg
------------	---------	--------------------------	----	---------------------------------	-------

Lactose	1	342.3	0.342	0.917	
Oxygen	1	16	0.016	.043	
Ammonia	4	17.031	3200 kg/h of ammonium sulfate		
Sulfuric Acid	1	98.079	0.098	0.263	
Potassium Acetate	2	98.15	0.098	0.263	
Penicillin G Potassium	1	372.5	0.373	1	
Water	8	18.01528	0.018	0.048	
Carbon Dioxide	2	44.01	0.044	0.118	
Biomass	10				
Acetic Acid	1	60.052	0.060	0.161	

Theoretical Profit = [Cost of Products] - [Cost of Reactants]

$[\$(1) + \$(1) + \$(4) + \$(1) + \$(2) + \$(1)] - [\$(1) + \$(8) + \$(2) + \$(10)] =$

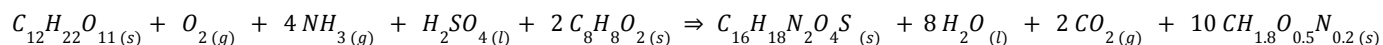
The theoretical profit indicator is about... showing that our process is profitable.

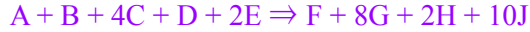
Process Chemistry

In the creation of penicillin, there are two main reactions that occur within the process. Reaction (1) is the fermentation process occurring with the presence of a carbon source, nitrogen source, oxygen and other components to produce Penicillin G. Reaction (2) is the crystallization reaction that occurs with the addition of potassium acetate to form Penicillin G Potassium crystals from Penicillin G. Each reaction has a letter that corresponds to each component. It has been shown below:

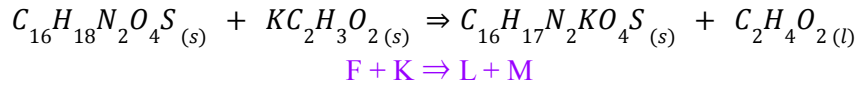
Reaction Mechanisms (BUKA)

Reaction 1: Fermentation

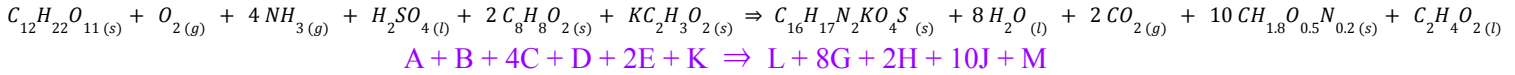




Reaction 2: Crystallization of Penicillin G Potassium



Overall Reaction:



Overall Mass Balance (Buka)

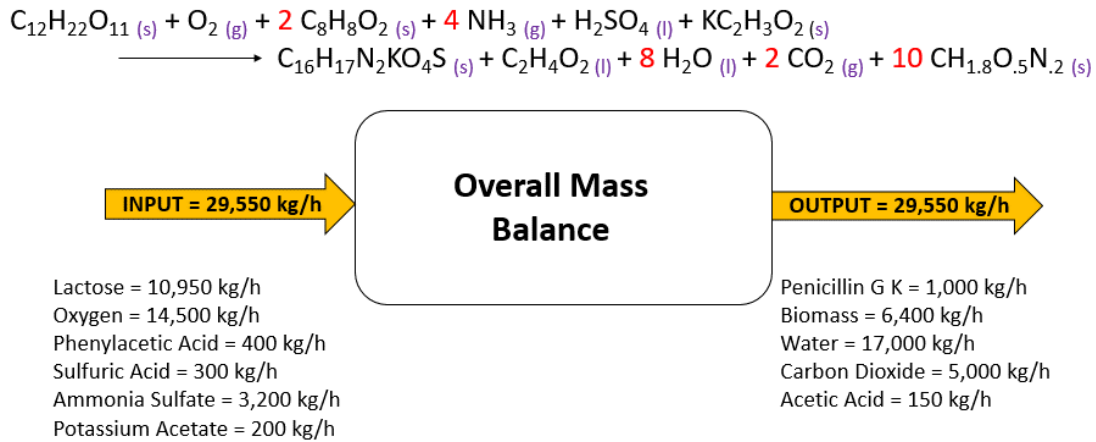


Figure 6. Overall Mass Balance across the Entire Process

Stoichiometry of Overall Reaction (BUKA)

The stoichiometry table depicts the relationship between the reactants and products. The overall reaction is based on the production of one mole of Penicillin G Potassium.

Table 6. Stoichiometry Table

Component	Stoichiometry
Lactose (A)	-1
Oxygen (B)	-1

Ammonia (C)	-4
Sulfuric Acid (D)	-1
Phenylacetic Acid (E)	-2
Potassium Acetate (K)	-1
Penicillin G K (L)	+1
Water (G)	+8
Carbon Dioxide (H)	+2
Biomass (J)	+10
Acetic Acid (M)	+1

Kinetics and Rate Law Equations (BUKA)

This process will be using a semi-batch process fermenter. Semi-batch equation is shown below:

$$v_{in} C_{i.in} + r_i V_R = V_R \left(\frac{dC_i}{dt} \right) + C_i \left(\frac{dV_R}{dt} \right)$$

It shows the input flow with a generation factor coming from the reaction giving us accumulation that factors when there's a change in both reactor volume and concentration of species i. The rate laws for each component is found below in regards to the overall reaction equation:

Table 7. Rate Law Equations

Component	Rate Law Equation
Lactose (A)	$r_A = -k C_A C_B C_C^4 C_D C_E^2 C_K$
Oxygen (B)	$r_B = r_A = -k C_A C_B C_C^4 C_D C_E^2 C_K$
Ammonia (C)	$r_C = 4 r_A = -4 k C_A C_B C_C^4 C_D C_E^2 C_K$
Sulfuric Acid (D)	$r_D = r_A = -k C_A C_B C_C^4 C_D C_E^2 C_K$
Phenylacetic Acid (E)	$r_E = 2 r_A = -2 k C_A C_B C_C^4 C_D C_E^2 C_K$

Potassium Acetate (K)	$r_K = r_A = -kC_A C_B C_C^4 C_D C_E^2 C_K$
Penicillin G K (L)	$r_L = -r_A = kC_A C_B C_C^4 C_D C_E^2 C_K$
Water (G)	$r_G = -8r_A = 8kC_A C_B C_C^4 C_D C_E^2 C_K$
Carbon Dioxide (H)	$r_H = -2r_A = 2kC_A C_B C_C^4 C_D C_E^2 C_K$
Biomass (J)	$r_J = -10r_A = 10kC_A C_B C_C^4 C_D C_E^2 C_K$
Acetic Acid (M)	$r_M = -r_A = kC_A C_B C_C^4 C_D C_E^2 C_K$

Process Description

Raw Material Preparation (Caleb)

Raw Materials

- ***P. chrysogenum* cells**
 - Obtained in a freeze-dried state from a laboratory. Cell culture will ultimately be grown to a concentration of 66 g/L before entering the bioreactor.
- **Lactose**
 - Pure lactose solids in powder form. Exists as a solid at room temperature. Being the carbon source for biomass, lactose has a much higher concentration in the medium than the other minerals.
- **Phenylacetic acid**
 - Highly concentrated powder (54.8 g/L). Exists as a solid at room temperature. Is necessary for the growth of penicillin G, but fed at a considerably low concentration to avoid inhibiting fungal growth.
- **Sulfuric acid**
 - Highly concentrated sulfuric acid. Exists as a liquid at room temperature. Centrifugally pumped to tank V-202 to substantially decrease the pH of the agitated mixture.
- **Potassium acetate**
 - Used in powder form. Exists as a hygroscopic solid at room temperature. Potassium ion is necessary to deprotonate penicillin G within the crystallizer.
- **Ammonium Sulfate**

- Powder that is very soluble in water. Exists as a solid at room temperature. Because it serves as the nitrogen source for biomass, ammonium sulfate is the second-most concentrated species within the design medium, behind lactose.
- **Butyl acetate**
 - Serves as the solvent for the penicillin extraction process. Exists as a colorless liquid at room temperature. Supplied in large amounts for liquid-liquid extraction and in many instances of crystal washing.
- **Air**
 - Approximately 78% N₂ and 22% O₂. Enters with a massive flow rate to satisfy the needs of the aerobic fermentation.

Utilities

- **Cooling water**
 - Used to maintain a steady fermentation temperature within the jacketed bioreactor. Also used as a heat transfer medium to reduce the temperature of penicillin G broth from the bioreactor before passing through the rotary vacuum filter.
- **Chilled water**
 - Used to reduce the temperature of the penicillin G broth from the first rotary vacuum filter before entering the mixing tank. Also used in the jacketed heat sterilizers to reduce the streams back to their inlet temperatures after sterilization.
- **Steam**
 - Used to sterilize inlet air and medium impurities before they enter the bioreactor. Also used to slightly increase the temperature of the air and medium to the fermentation temperature after sterilization.

Reaction and Fermenter Operation (BUKA & Caleb)

Prior to the bioreaction, in which *P. chrysogenum* cells will undergo fermentation within bioreactors to produce penicillin G, the raw materials must first be properly prepared. The inlets of the bioreactor include the inoculum and the fermentation medium, which will be fed to the reactor separately from each other.

The growth and multiplication of *P. chrysogenum* cells occurs in four phases: the lag phase, growth phase, stationary phase, and decline phase. In the lag phase, the cells become acclimated to the medium they have been introduced to and undergo the necessary metabolic processes for eventual cell multiplication. After this, they enter the growth phase and the concentration of cells in the inoculum increases exponentially. At a certain point, the cells will have absorbed most of the nutrients in the medium and the concentration will converge to a certain range

(stationary phase) before eventually decreasing again due to the absence of adequate carbon and nitrogen sources within the broth. This fungal cell growth from the growth to stationary phase occurs in logarithmic fashion.

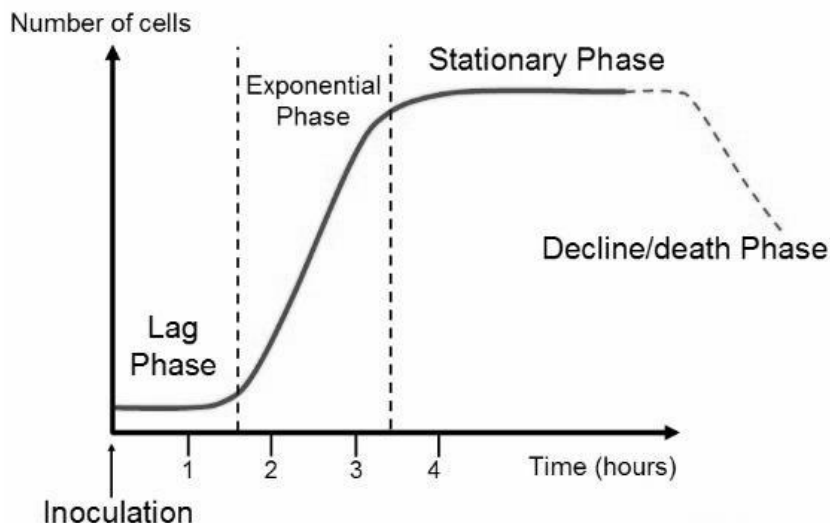


Figure 7. Phased Fungal Cell Growth Curve

In order to thoroughly explain the processes preceding fermentation, both the inoculum and fermentation medium will be discussed independently.

Inoculum

The inoculum, which is a conglomerate of both fungal cell biomass and fermentation medium minerals, must undergo preparation prior to being ready for admission into the bioreactor. The goal of the preceding process is to increase the concentration of cells in broth to a value sufficient enough for a resulting yield of penicillin G by introducing the cells to “food sources” (primarily sources of carbon and nitrogen) that will promote rapid cell growth. Initially, stock cultures of freeze-dried *P. chrysogenum* cells are obtained via laboratory. These cells are then extracted from their stock container and brought to an agar plate, which will serve as the site for the cells’ initial introduction to the fermentation medium. Before the cells can multiply, they must first enter the *lag phase*, in which they may become accustomed to their new environment before being able to multiply. A small amount of medium must be added to the agar plate containing these fungal cells in order to initiate this process. During the lag phase, cells synthesize enzymes necessary for growth; although the cell concentration does not yet increase, the cells do increase in size.

Following the conclusion of the lag phase is the *growth phase*, in which the cells use nutrients from the fermentation medium to increase in concentration. The new cells, having increased in size after exiting the lag phase, are transferred from the agar plate to a flask and reintroduced to

fermentation medium. By this time, the cells have adapted to these conditions and the concentration of cells begins to increase. This process will have to be repeated various times to increase the cell concentration to a level sufficient enough for the full-scale bioreactor. For this specific design, a cell concentration of 66 g/L and temperature of 30 degrees Celsius within the agitated inoculum tank (V-103) are desired before releasing it into the bioreactor. Once this concentration is reached, the contents are pumped to the fermenter (V-104) to eventually coexist with a high concentration of fermentation medium.

The overall material balance across the fermenter is shown below. Because this fungal fermentation is an aerobic process, an inlet stream of air is required to provide an adequate supply of O_2 for the biochemical reaction. The extracted air first enters a compressor (C-101) in order to increase its pressure to 2.04 atm, and is then passed across a heat sterilizer (E-103) to destroy lingering microorganisms. Afterwards, the air reaches a heater (E-104) and its temperature raised from ambient conditions to 30 degrees Celsius before entering the fermenter from the bottom. Another stream to consider is that of the exhaust gas leaving from the top of the fermenter, which is composed of O_2 and N_2 (from inlet air) and CO_2 (fermentation byproduct).

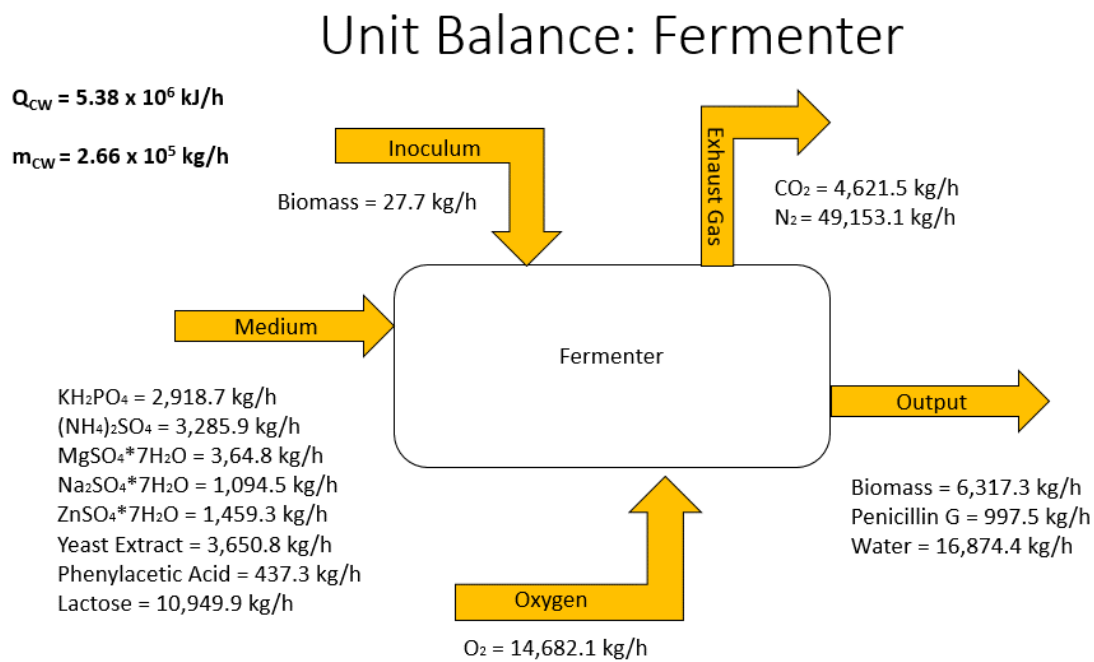


Figure 8. Material Balance across Fermenter

Medium

Because the growth of fungal cells primarily requires an abundance of a carbon source (lactose), it is initially stored separately from the rest of the minerals and phenylacetic acid in the medium, which are stored together.

Lactose will be in solid form stored in a hopper (TK-101) before being transported to an agitated medium tank (V-102) via conveyor belt. The rest of the medium components, before entering the agitated mineral tank (V-101), must be stored in their respective tanks or hoppers; liquid constituents will be pumped through pipes to V-101, while solid constituents, like lactose, must also be stored in solid hoppers and transported via conveyor. The mineral solution will then be pumped into the agitated medium tank. The design will feature multiple batch medium tanks in parallel to compensate for time required for solids to dissolve into the broth. After exiting the medium tank, the complete medium will be pumped to a heat sterilizer (E-101) to eliminate any impurities from the solution and then heated (E-102) to 30 degrees Celsius prior to entering the fed-batch fermenter (V-104). At the same time, the biomass will be entering in the fermenter from the inoculum tank (V-103). The fermentation process will be conducted at 30 degrees Celsius and 1.02 atm. The fermentation time will be 120 hours, which includes the growth phase, production phase, cleaning and so on. The design includes multiple fermenters in parallel to maintain a continuous process, as certain fermenters will undergo cleaning at different times. The fermenter's output stream includes the intermediate product penicillin G, high amounts of water and lots of biomass. The full fermentation phase of the *P. chrysogenum* is shown below:

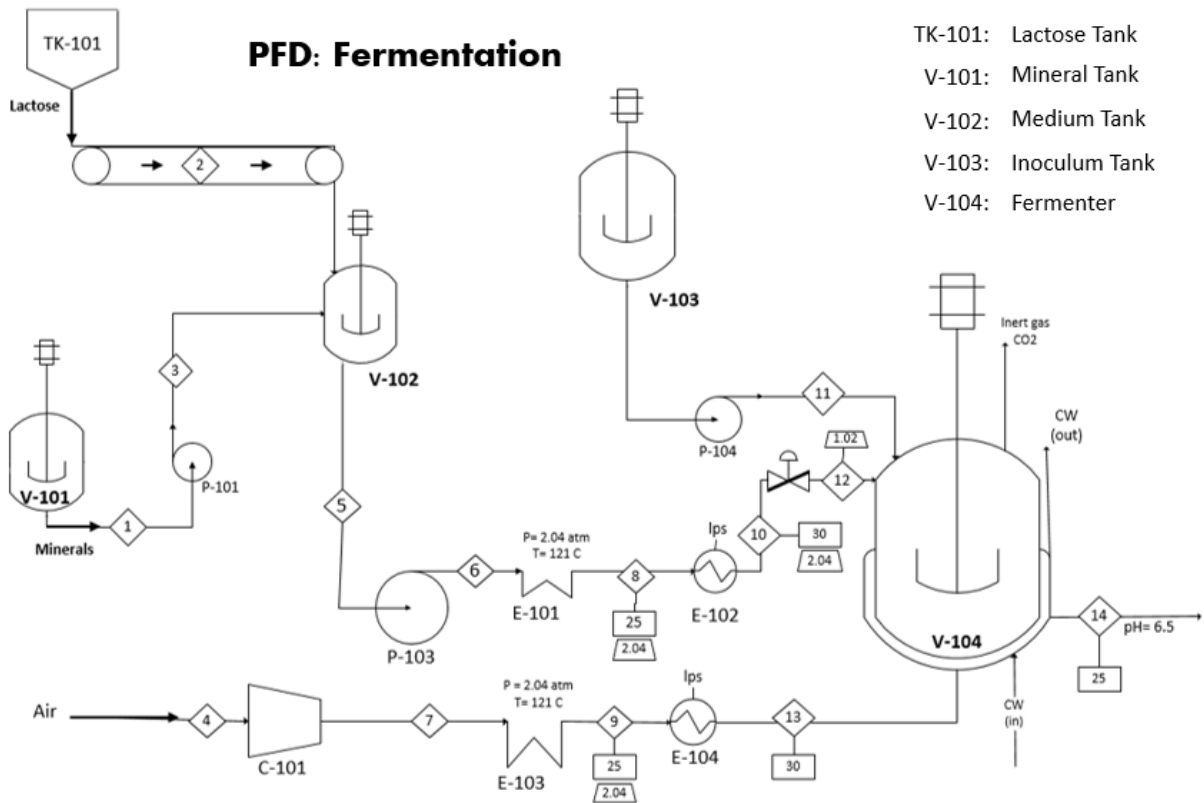


Figure 9. Process Flow Diagram of the Fermentation of *P. chrysogenum* to Produce Penicillin G

Separation Units (BUKA)

The extraction process begins after the fermentation process. The main purpose is to stabilize and isolate our final product at a high purity to be sold to our various clients. This process involves various units and equipment that performs different separations of solids from liquid like rotary vacuum filters, and liquid-liquid extraction like solvent extractor, that can transfer mass based on solubility of desired component from one liquid to liquid. As a result of fermentation, a mixture of biomass, water and Penicillin G goes through a rotary vacuum filter (V-201) to remove the biomass, which will be sold for agricultural purposes and animal feed. It will be cooled with a cooler (E-202) to 2 degrees celsius to prevent the product intermediate to degrade. Next, the mixing tank (V-202) is introduced to add sulfuric acid and butyl acetate (solvent) together, which results in penicillin G being soluble in solvent to be extracted in the solvent extractor (V-201). The carbon adsorption tower (T-201) removes the color and odor for a pure, colorless hue for the broth. Next step is to introduce it in the crystallizer to form crystals of Penicillin G Potassium with the presence of potassium acetate. It will go through the first crystal filter (V-205), re-washed in a crystal washing tank (V-206) and filtered again in another crystal filter (V-207). Finally, it is sent to a vacuum dryer (E-203) to dry off the product crystals before being sent to a grinder (V-208). It is stored in a hopper (TK-206) and then packaged in bulk bags.

The image below shows the process of the Penicillin G broth going through each separation unit until it is ready for product storage:

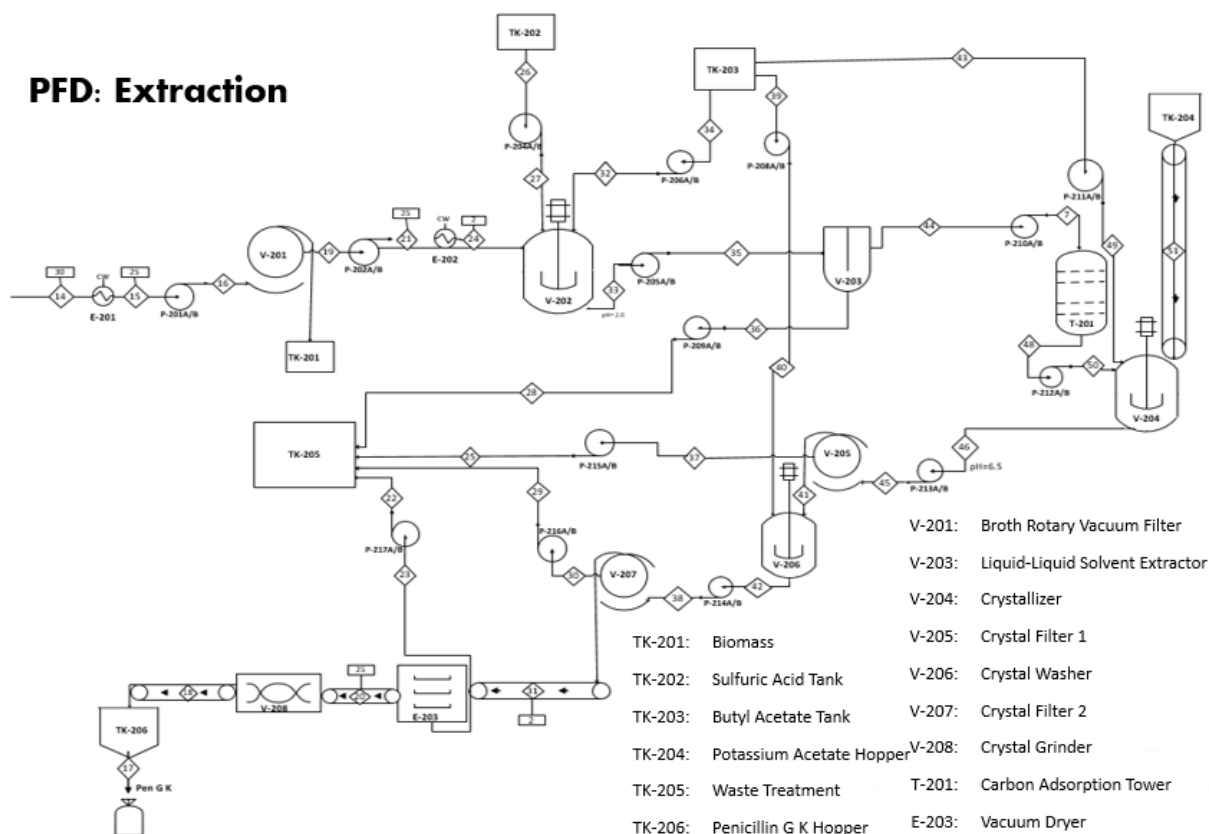


Figure 10. Process Flow Diagram of the Extraction of Penicillin G Potassium

Product Storage (Tiarra & Buka)

The product will be stored in super sacks (bulk bags) post-process and placed in a dry refrigerated room awaiting transportation to our clients. Our product, Penicillin G Potassium, has a 7-day maximum life expectancy at room temperature before it degrades. However, the product will be stored in a refrigerated room at 4 °C. This condition helps extend the shelf life of the product for up to 3 months.

Basis of Calculations and Major Assumptions (Buka & Caleb)

Based on the previously discussed global market analysis conducted by the team of engineers, a production capacity of 6.86 million kg/yr was determined to be feasible to satisfy 20% of the U.S. demand for penicillin. Our plant will have about 90% uptime, based on the fact that it will operate for 330 days (7,920 hours) out of the year; the other 35 days will be used as a buffer for

unscheduled downtime. The plant efficiency was also determined to be 78%, which was obtained from literature analysis for general penicillin processes. Lastly, a feasible specific production rate of 0.15g penicillin G/Lhr was obtained from literature and used to determine the necessary working volume.

The team's basis calculations were obtained for a period of 1 year for simplification purposes. A molar mass ratio of 1.11 was derived from the division of penicillin G potassium's molar mass by that of penicillin G. Dividing the plant capacity by this ratio revealed that 6.18 million kg penicillin G is required as a fermenter output. Because the plant is 78% efficient, it became apparent that more than 6.18 million kg penicillin G is required in order to satisfy the resulting losses of penicillin G potassium. Dividing the plant capacity by 0.78 yields a temporary capacity of 8.80 million kg penicillin G potassium that was solely used to calculate the required production rate of penicillin G. Dividing this plant capacity by the molar mass ratio (1.11) once more yielded a production rate of 7.90 million kg penicillin G, which is the required capacity of the fermenter. Next, dividing this penicillin G by the plant's operating time of 7,920 hours resulted in a required flow rate of 1 million g penicillin G/hr from the fermenter. Finally, the team manipulated the specific production rate of penicillin G (0.15g/Lhr) to obtain a mass flow rate on the basis of 1 L working volume (0.15g penicillin G/hr/1L). A proportional relationship between this production rate and the required flow rate of penicillin G out of the fermenter (1 million g/hr) was used to solve for the required working volume of the full-scale process, which was determined to be about 6.65 million liters.

The extraction process recovers 78% of the desired product output. The extraction process includes various equipment like rotary vacuum filters for both removal of biomass and crystal filtration, mixing tanks, solvent extractor, carbon adsorption tower, crystallizer, and vacuum drying. Based on literature, the product recovery percentage for each major unit was obtained. The first major unit, solid-liquid separator called rotary vacuum filter, recovers 93% of the penicillin G while the rest leaves with the majority of biomass. Following, the solvent extractor recovers 80% - 90% of penicillin G based on current process research so we assumed 86% for our process. The rotary vacuum filters for both of the crystal filters were assumed to have a product recovery of 99%. For the rest of the units being used for the extraction process, we assumed the output was 100%. Our basis with the crystallizer was assumed that all of the penicillin G is converted to penicillin G potassium when introduced to potassium acetate.

Based on these calculations for the required production rate of penicillin G and total working volume, the team worked backwards to find required feed conditions for the fermenter and eventually find material balances across each unit using their product recoveries as well.

Material Balance of each Unit (Buka)

After exiting the fermenter, the resulting mixture of Penicillin G, water and biomass will be heading towards the extraction process. There are several units used to transform the product intermediate of Penicillin G to our desired product of Penicillin G Potassium to be stored and sold to our clients. The units are shown below:

Rotary Vacuum Filter (RVF)

A rotary vacuum filter is used to separate solids from liquids. In this case, we are trying to remove biomass in order to concentrate the Penicillin G in the broth solution. We assumed that the large amount of biomass removed will be 93%, but also small amounts of Penicillin G (7%) and water (8%) are lost at this stage as well.

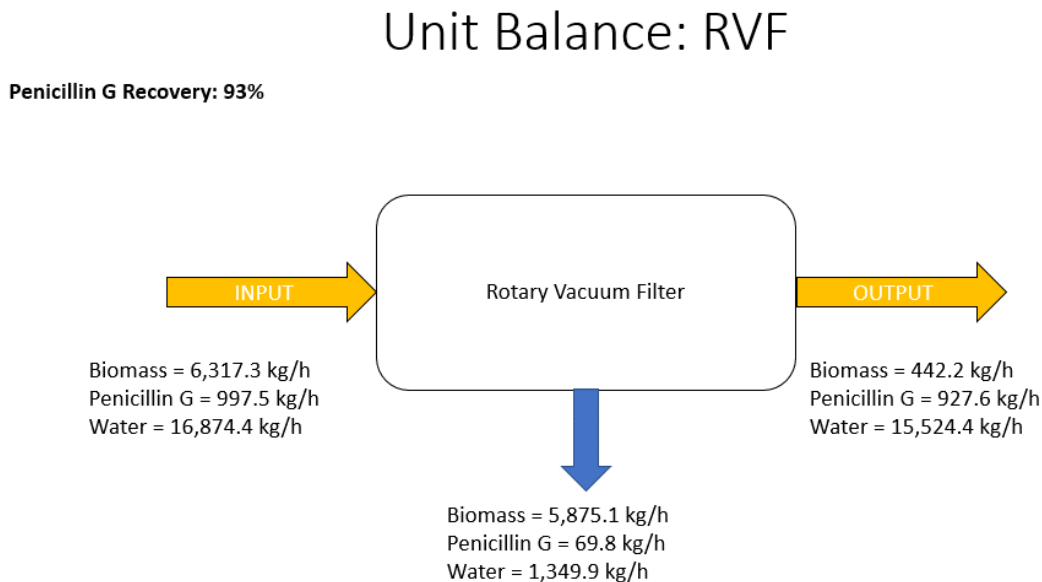


Figure 11. Material Balance across Broth Rotary Vacuum Filter

Mixing Tank

The purpose of this mixing tank is to agitate the combination of Penicillin G broth with the newly added components of sulfuric acid and butyl acetate, which is the solvent. Sulfuric acid was added based on the relationship between itself and Penicillin G produced on Reaction (1). Based on literature review, butyl acetate is added at 0.25 g butyl acetate/ g broth. Adding sulfuric acid is for adjusting the pH level down to 2, which is when Penicillin G exists as an undissociated acid making it soluble in organic solvents like butyl acetate.

Unit Balance: Mixing Tank

Penicillin G Recovery: 100%

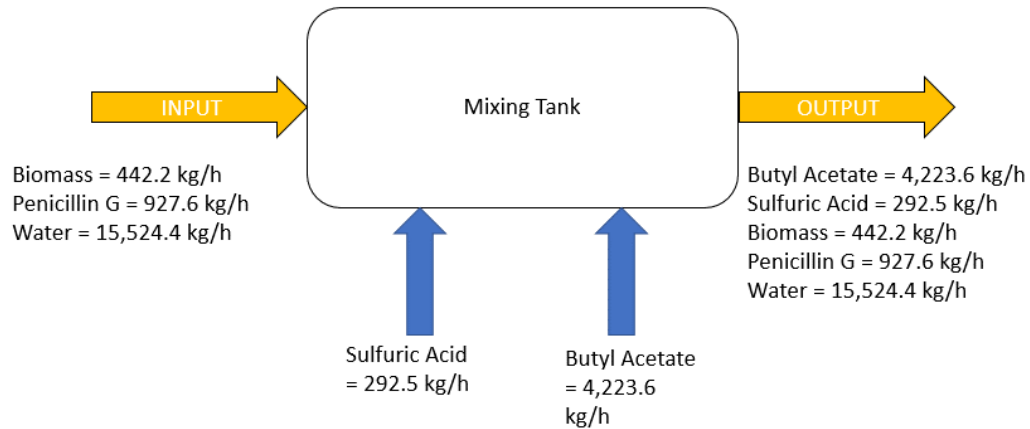


Figure 12. Mass Balance across Mixing Tank

Solvent Extractor

The purpose behind the solvent extractor is to conduct a liquid-liquid extraction which transfers some constituents of one liquid into the other one. In this process, the constituent will be Penicillin G being moved from the broth to the solvent, which will be extracted while the rest is sent to a waste treatment to recover the lost butyl acetate of 10% for reuse. Penicillin G recovery in this unit will be 86% based on literature parameters. However, we made assumptions that 95% of water is lost and all of the sulfuric acid is lost as well because it's very soluble in water. Also, we assumed that 96% of biomass that was left after the rotary vacuum filter is removed at this step.

Unit Balance: Solvent Extractor

Penicillin G Recovery: 86%

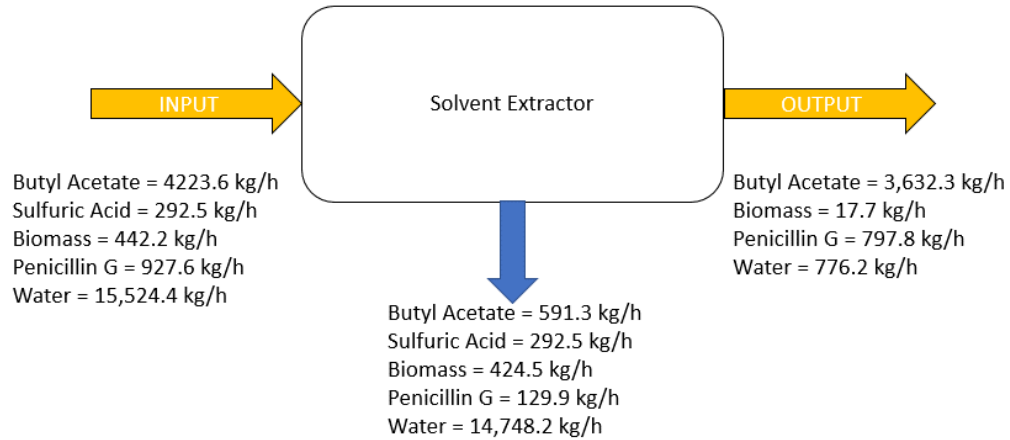


Figure 13. Mass Balance across Solvent Extractor

Carbon Treatment

Carbon treatment is done in an adsorption tower with carbon trays with carbon particle sizes between 10-20 microns. This step focuses on removing the color and odor of the solution coming from the solvent extractor. It also removes impurities like the remaining biomass. Solution particles and impurities stick or adhere to the surface of the carbon molecules on the trays, which can be replaced when the trays are overused. We assumed that there was a 5% loss on butyl acetate and 3% of remaining water. No Penicillin G was lost at this stage.

Unit Balance: Carbon Treatment

Penicillin G Recovery: 100%

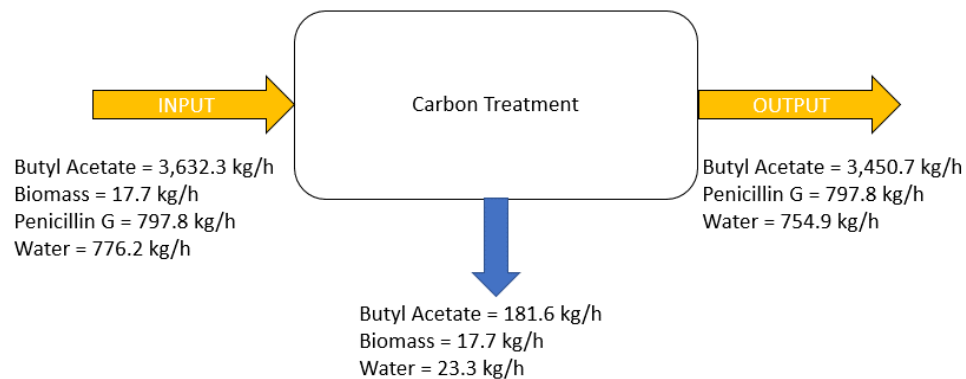


Figure 14. Material Balance across Carbon Adsorption Tower

Crystallizer

This stage is for creating the crystals. Penicillin G broth is sent into the crystallizer with the addition of butyl acetate and potassium acetate. As Penicillin G is in contact with potassium acetate, Reaction 2 comes into effect making penicillin G a negative ion which also makes it insoluble in butyl acetate. This process is by the deprotonation of penicillin G molecule by the strong base of potassium acetate, which removes the hydrogen atom from penicillin G, and then protonated with the potassium atom to form Penicillin G Potassium crystals. Then, the free-floating hydrogen atoms will bond with the negatively-charged remainder of potassium acetate to form acetic acid.

Unit Balance: Crystallizer

Penicillin G K Recovery: 100%

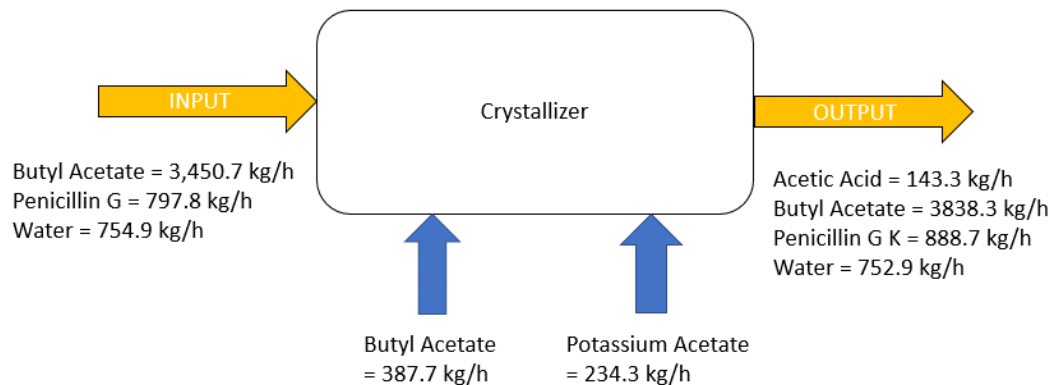


Figure 15. Material Balance across Crystallizer

Crystal Filter 1

Following the crystallizer, the crystal filter is another rotary vacuum filter that separates solids from liquid solution. In this case, we are separating the Penicillin G Potassium crystals from the solvent solution. The solvent solution will be heading off to a waste treatment to re-extract the butyl acetate for re-use in the process. We assumed that 88% of butyl acetate is removed with 95% of water content and all of the acetic acid is gone because it's soluble and fully miscible in water. We assumed that we will experience a 99% recovery of Penicillin G Potassium.

Unit Balance: Crystal Filter 1

Penicillin G K Recovery: 99%

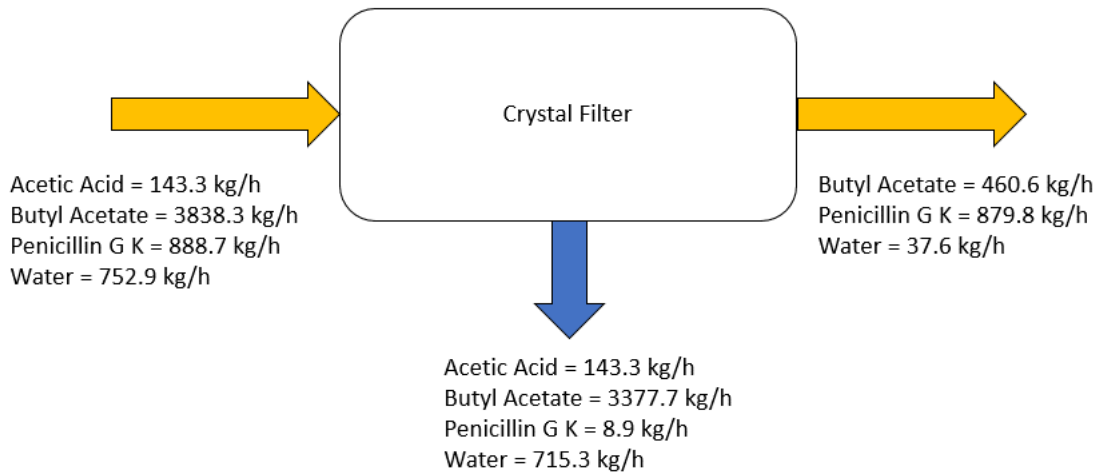


Figure 16. Material Balance across Crystal Rotary Vacuum Filter 1

Crystal Washing

At this stage, the crystals need to be rewashed with more solvent while still using the 0.25 g butyl acetate/ g broth ratio.

Unit Balance: Crystal Washing

Penicillin G K Recovery: 100%

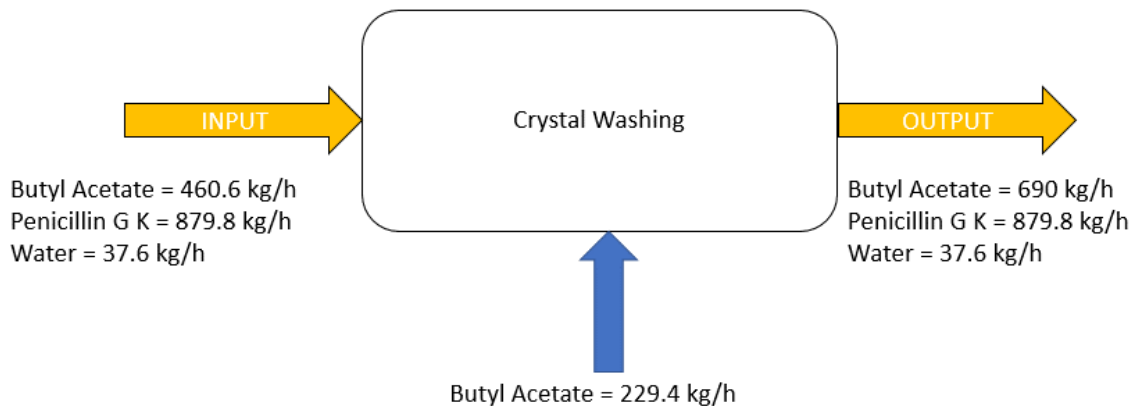


Figure 17. Material Balance across Crystal Washer

Crystal Filter 2

The crystals are re-filtered with the same assumed parameters from the first crystal filter since both equipment are the same.

Unit Balance: Crystal Filter 2

Penicillin G K Recovery: 99%

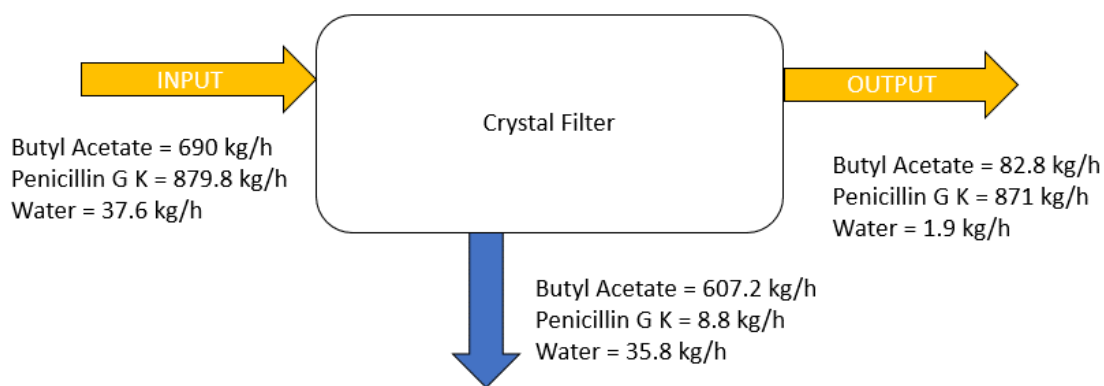


Figure 18. Material Balance across Crystal Rotary Vacuum Filter 2

Vacuum Drying

Finally, the crystals are dried at an ambient temperature with a pressure slightly below atmospheric. Butyl acetate is assumed to be retained at 5% of its content and water is retained at 4 % of its content. At the end, the product is at a purity of 99.5% before being transported to the grinder to be converted to a fine powder.

Unit Balance: Vacuum Drying

Penicillin G K Recovery: 100%

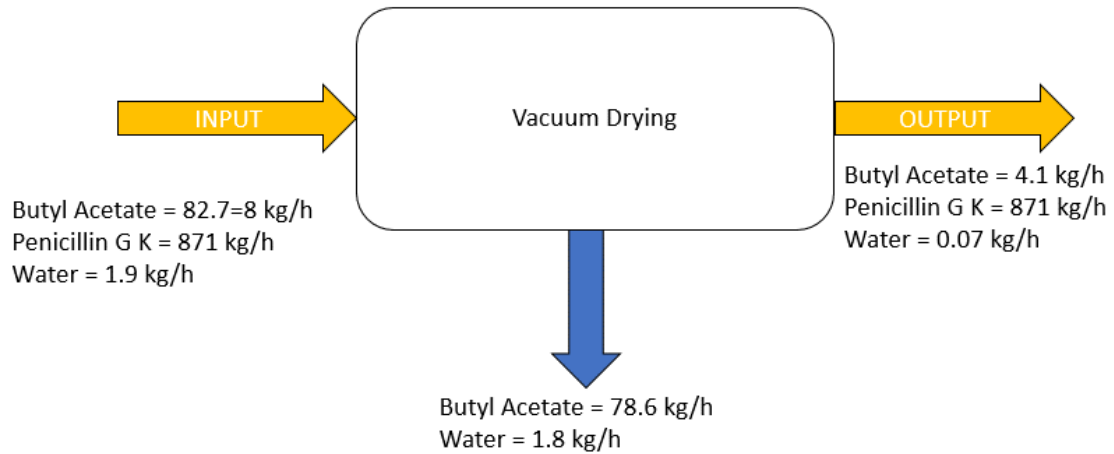


Figure 19. Material Balance across Vacuum Dryer

Degree of Freedom Analysis (Caleb)

According to Gibbs's Phase Rule, the number of degrees of freedom can be calculated using the following relationship:

$$F = C - P + 2$$

Where F = # degrees of freedom; C = # of components; P = # of phases

The following table shows the number of degrees of freedom corresponding to each process unit in the team's design:

Table 8. Degrees of Freedom for all Major Process Units

Process Unit	C [# of components]	P [# of phases]	F [C - P + 2]
V-104	10	2	10
V-201	3	2	3
V-202	5	2	5

V-203	5	2	5
T-201	4	2	4
V-204	4	2	4
V-205	4	2	4
V-206	3	2	3
V-207	3	2	3
E-203	3	3	2

Energy Balance (Caleb)

Figure 16 shows the specifications for all heat exchangers used in the team's design. Each exchanger requires a utility/requires utilities that serve as mediums for heat transfer. The heat duties of the exchangers and the flow rate of the inlet utilities for each exchanger are shown below:

Energy Balance: Utility Equipment Table

Exchanger	Inlet Temp [°C]	Outlet Temp [°C]	Pressure [atm]	Utility	Heat flow [kJ/h]	Utility flow rate [kg/h]
E-101 (jacketed)	25	25	2.04	Steam	-1.33 x 10 ⁷	74,324.9
				Chilled water	1.33 x 10 ⁷	33,112.3
E-102	25	30	-	Steam	-6.02 x 10 ⁵	64,592.3
E-103 (jacketed)	25	25	2.04	Steam	-1.2 x 10 ⁷	67,060.1
				Chilled water	1.2 x 10 ⁷	29,875.7
E-104	25	30	-	Steam	-6.23 x 10 ⁵	66,845.5
E-201	30	25	-	Cooling water	9.44 x 10 ⁵	45,124.3
E-202	25	2	-	Chilled water	3.03 x 10 ⁶	31,486.4

Figure 20. Utility Equipment Table

According to the table, steam utilities all have negative heat flow values, while those of cooling and chilled water are all positive. This is a reasonable occurrence due to the fact that both steam and liquid water serve opposite purposes as utilities for the heat exchangers. Because the steam is supplying the process stream with the heat it needs to see a temperature increase, heat is being transferred from the steam to the process stream. For this reason, heat flow values for steam

should be negative because the steam is losing heat while serving as the heat flow medium; conversely, the purpose of cooling/chilled water is to remove heat from the process streams, thus decreasing their temperatures. Moreover, heat flow values for cooled and chilled water should be positive because heat is being transferred from the process streams to the water.

After calculating the heat duties of each heat exchanger unit, utility flow rates were determined by the equation

$$Q = mc_p\Delta T$$

Solving for m ,

$$m = Q/c_p\Delta T$$

It is important to note that mass, m , in this situation represents a mass flow rate, not simply a mass. This is true because the calculated heat duty, Q , is in units of [kJ/hr] or [kW]. C_p represents the specific heat capacity of the water utility (liquid water or steam, depending on the exchanger) and ΔT is the temperature difference between the utility and the inlet stream. The mass flow rates of the utilities in the heat exchangers appear considerably high, but this is because a large flow of water is needed to facilitate the transfer of so much heat.

In-depth calculations concerning the derived heat flow and utility flow rate values can be found within the appendix of this report.

Aspen Simulation (Buka)

After all process parameters and designing the Process Flow Diagram, the Aspen Simulation was created. Due to the fact that some equipment wasn't available in Aspen, we simulated our process using closely related equipment that was applicable which resulted in our process converging and having practical values close to our hand calculations. Also, our process was a bioprocess which requires a bio-simulator with the correct raw material component and accurate fluid package as well. Aspen Model is visible below:

Aspen Simulation

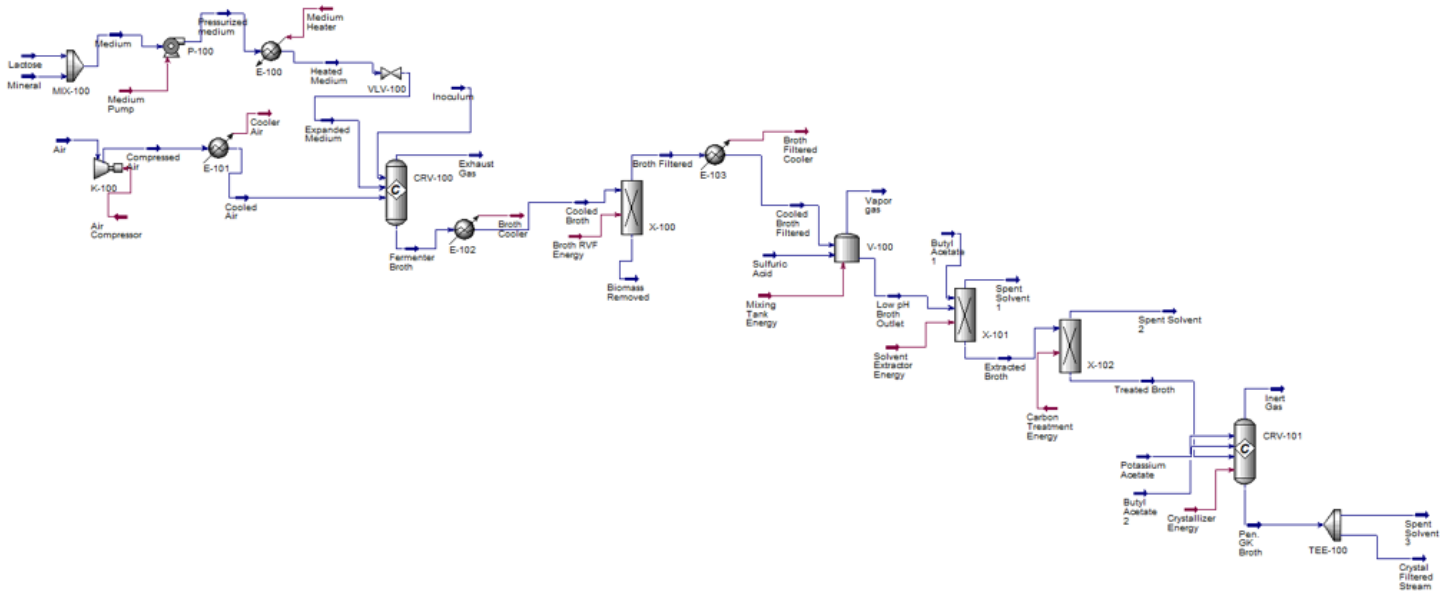


Figure 21. Aspen Simulation

Conclusion and Recommendations *(Buka & Caleb)*

All in all, the design project satisfied all objectives and revealed itself to be feasible. According to the growth profit indicator, the total cost of necessary raw materials (excluding transportation costs) is less than the total value of products manufactured for sale (penicillin G potassium and biomass), indicating that this plant is profitable and thus worth constructing. Although this analysis does not take into account transportation and utility costs, it is useful in determining the validity of a premature design plan. Regardless, the proximity of the plant to its raw material suppliers on either side of the country significantly reduces the effect of transportation costs on overall profit.

One recommendation the Team has to ultimately increase profit in the long run is to utilize multiple liquid-liquid extractors in series, rather than one extractor for the whole process. As mentioned earlier in the report, the plant has an overall efficiency of 78%, meaning that the remaining 22% represents the extra amount of penicillin G potassium that could be produced in the event of a theoretically seamless process. By attempting to minimize these potential losses and make the process more efficient, less raw materials will be required and more penicillin G potassium can be manufactured with minimal extra effort. The liquid-liquid extractor in the design has an efficiency of 86%, meaning that 86% of incoming penicillin G is admitted onward

to the next unit in the process. By placing multiple liquid-liquid extractors in series, the design will permit for the process stream to be more penicillin G-rich. Adding multiple extractors will lead to a 92% - 96% efficient extraction process, which is around an 8% higher efficiency. While adding multiple extraction units does initially cost, that cost will pale in comparison to the total operating cost because it will maximize the amount of penicillin G potassium that can be made from the same amount of raw materials.

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Appendix

E-101
Energy Balance across ~~Heat Exchanger~~ (Heat Sterilizer)

25°C → 201 mol/min → 121°C → 25°C

$C_{12}H_{22}O_{11}(s)$:
 $C_6H_6O_2(s)$:
 $NH_3(g)$:
 $H_2SO_4(l)$:

$C_{12}H_{22}O_{11}(s)$:
 $C_6H_6O_2(s)$:
 $NH_3(g)$:
 $H_2SO_4(l)$:

A
B
C
D

similar velocities
no elevation
no moving parts

$$\dot{n}(\hat{H} + \hat{E}_k + \hat{E}_p)_{in} - \dot{n}(\hat{H} + \hat{E}_k + \hat{E}_p)_{out} + \dot{Q} + \dot{W}_s = 0$$

$$\dot{Q} = \dot{n}\hat{H}_{out} - \dot{n}\hat{H}_{in}$$

$$\dot{Q} = \dot{n}\Delta\hat{H}$$

$$= \dot{n}[\sum \hat{H}_{products} - \sum \hat{H}_{reactants}] \text{ or } \dot{n}\sum \Delta\hat{H}$$

$$\dot{Q} = \dot{n} \sum_i C_p^i \left(\frac{121^\circ C - 25^\circ C}{25^\circ C - 121^\circ C} \right)$$

where $\dot{Q}$ = J/s of heat required from sterilizer to bring temp up to 121°C

$T_M^* = 202.8^\circ C$; $T_0^* = 337^\circ C$; $T_u^* = 76.5^\circ C$; $T_b^* = 2105.5^\circ C$

Phenylacetic acid ($C_8H_8O_2$) will phase chg
s → l

$$\Delta\hat{H}_a = \int_{25^\circ C}^{121^\circ C} C_p^a dT$$

$$\Delta\hat{H}_b = \int_{25^\circ C}^{76.5^\circ C} C_p^b dT + \Delta\hat{H}_{fus} + \int_{76.5^\circ C}^{121^\circ C} C_p^l dT$$

$$\Delta\hat{H}_c = \int_{25^\circ C}^{121^\circ C} C_p^c dT$$

$$\Delta\hat{H}_d = \int_{25^\circ C}^{121^\circ C} C_p^d dT$$

* $C_p^a = 417.6 \text{ J/mol}\cdot K$

* $C_p^b = 36.8 \text{ J/mol}\cdot K$

* $C_p^c = 131.4 \text{ J/mol}\cdot K$

* $C_p^d = 35.5 \text{ J/mol}\cdot K$

$C_p^a = (417.6 \text{ J/mol}\cdot K) \left(\frac{1 \text{ mol}}{166.17 \text{ g}} \right) \left(\frac{1000 \text{ J}}{1 \text{ kJ}} \right)$

$C_p^b = (36.8 \text{ J/mol}\cdot K) \left(\frac{1 \text{ mol}}{166.17 \text{ g}} \right) \left(\frac{1000 \text{ J}}{1 \text{ kJ}} \right)$

$C_p^c = (131.4 \text{ J/mol}\cdot K) \left(\frac{1 \text{ mol}}{166.17 \text{ g}} \right) \left(\frac{1000 \text{ J}}{1 \text{ kJ}} \right)$

$C_p^d = (35.5 \text{ J/mol}\cdot K) \left(\frac{1 \text{ mol}}{166.17 \text{ g}} \right) \left(\frac{1000 \text{ J}}{1 \text{ kJ}} \right)$

$\Delta\hat{H}_{fus} = 97.3 \text{ J/mol}$

$\Delta\hat{H}_{fus} = 97.3 \text{ J/mol} \left(\frac{1 \text{ mol}}{166.17 \text{ g}} \right) \left(\frac{1000 \text{ J}}{1 \text{ kJ}} \right)$

$\Delta\hat{H}_{fus} = 0.585 \text{ kJ/mol}$

$\Delta\hat{H}_{fus} = 0.585 \text{ kJ/mol} \left(\frac{1 \text{ mol}}{166.17 \text{ g}} \right) \left(\frac{1000 \text{ J}}{1 \text{ kJ}} \right)$

$\Delta\hat{H}_{fus} = 0.585 \text{ kJ/mol}$

$$\Delta \hat{H}_A = (129.99 \text{ J/kg}^\circ\text{C})(121^\circ\text{C} - 25^\circ\text{C}) = 117.12 \text{ kJ/kg}$$

$$\begin{aligned} \Delta \hat{H}_B &= \cancel{(260.74 \text{ J/kg}^\circ\text{C})(121^\circ\text{C} - 25^\circ\text{C})} \\ &= (260.74 \text{ J/kg}^\circ\text{C})(76.5^\circ\text{C} - 25^\circ\text{C}) + 71509.36 \text{ J/kg} \\ &\quad + (260.74 \text{ J/kg}^\circ\text{C})(121^\circ\text{C} - 76.5^\circ\text{C}) \\ &= 96.54 \text{ kJ/kg} \end{aligned}$$

$$\Delta \hat{H}_C = (2160.77 \text{ J/kg}^\circ\text{C})(121^\circ\text{C} - 25^\circ\text{C}) = 207.43 \text{ kJ/kg}$$

$$\Delta \hat{H}_D = (1339.83 \text{ J/kg}^\circ\text{C})(121^\circ\text{C} - 25^\circ\text{C}) = 128.62 \text{ kJ/kg}$$

$$\Delta \hat{H}_T = \Delta \hat{H}_A + \Delta \hat{H}_B + \Delta \hat{H}_C + \Delta \hat{H}_D$$

$$\begin{aligned} &= 117.12 \text{ kJ/kg} + 96.54 \text{ kJ/kg} + 207.43 \text{ kJ/kg} + 128.62 \text{ kJ/kg} \\ &= 549.72 \text{ kJ/kg} \end{aligned}$$

$$\dot{n} = 24161.4 \text{ kg/hr}$$

$$\begin{aligned} \dot{Q} &= \dot{n} \Delta \hat{H}_T = (24161.4 \text{ kg/hr})(549.72 \text{ kJ/kg}) \\ &= 1.33 \times 10^7 \text{ kJ/hr} = \text{heat input required from E-JT} \end{aligned}$$

$$\begin{aligned} \dot{Q}_s &= \text{Heat brought in by steam} \\ \dot{Q}_{cw} &= \text{Heat absorbed by cooling water} = -1.33 \times 10^7 \text{ kJ/hr} \end{aligned}$$

$$\dot{Q} = -\dot{Q}_s$$

$$\dot{Q}_s = \dot{n}_s C_{p,H_2O} (25^\circ\text{C} - 121^\circ\text{C})$$

$$\dot{n}_s = \frac{\dot{Q}_s}{C_{p,H_2O} [25^\circ\text{C} - 121^\circ\text{C}]} = \frac{-1.33 \times 10^7 \text{ kJ/hr}}{(4.184 \text{ kJ/kg}^\circ\text{C})(-96 \text{ K})}$$

$$\dot{n}_s = \text{flow rate of incoming steam} = \boxed{31926.2 \text{ kg/hr}} \quad \boxed{74324.93 \text{ kg/hr}}$$

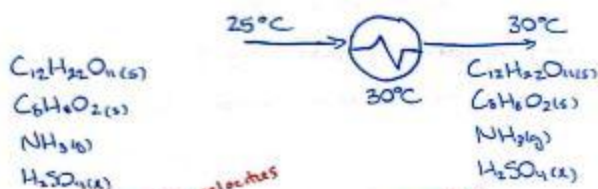
Cooling mechanism:

$$\dot{Q}_{cw} = \dot{Q} = 1.33 \times 10^7 \text{ kJ/hr} = \dot{n}_{cw} C_{p,H_2O} (121^\circ\text{C} - 25^\circ\text{C})$$

$$\dot{n}_{cw} = \frac{\dot{Q}_{cw}}{C_{p,H_2O} [121^\circ\text{C} - 25^\circ\text{C}]} = \frac{1.33 \times 10^7 \text{ kJ/hr}}{(4.184 \text{ kJ/kg}^\circ\text{C})(96 \text{ K})}$$

$$\dot{n}_{cw} = \text{flow rate of incoming cooling water} = \boxed{33112.25 \text{ kg/hr}}$$

Energy Balance across E-102 (Heat Exchanger)



$$\dot{n}(\hat{H} + \hat{E}_k + \hat{E}_p)_{in} - \dot{n}(\hat{H} + \hat{E}_k + \hat{E}_p)_{out} + \dot{Q} + \dot{W}_s = 0$$

similar velocities (crossed out)
no elevation (crossed out)
no moving parts (crossed out)

$$\dot{Q} = \dot{n}\hat{H}_{out} - \dot{n}\hat{H}_{in} - \dot{W}_s$$

$$\dot{Q} = \dot{n}\Delta\hat{H}$$

$$= \dot{n} \sum \Delta\hat{H}$$

$$\dot{Q} = \dot{n} \sum c_p (30^\circ\text{C} - 25^\circ\text{C})$$

where $\dot{Q}$ = % of heat required from sterilizer to bring temp up to 30°C

$$T_H^* = 202.8^\circ\text{C}, T_B^* = 337^\circ\text{C}; T_H^* = 76.5^\circ\text{C}; T_B^* = 265.5^\circ\text{C}$$

$$\Delta\hat{H}_H = \int_{25^\circ\text{C}}^{30^\circ\text{C}} c_p^H dT \quad \Delta\hat{H}_B = \int_{25^\circ\text{C}}^{30^\circ\text{C}} c_p^B dT \quad \Delta\hat{H}_C = \int_{25^\circ\text{C}}^{30^\circ\text{C}} c_p^C dT$$

no phase change

$$\Delta\hat{H}_D = \int_{25^\circ\text{C}}^{30^\circ\text{C}} c_p^D dT$$

$$c_p^H = 1219.99 \text{ J/kg}\cdot\text{K} \quad \Delta\hat{H}_H = (1219.99 \text{ J/kg}\cdot\text{K})(30^\circ\text{C} - 25^\circ\text{C}) = 6.10 \text{ kJ/kg}$$

$$c_p^B = 240.74 \text{ J/kg}\cdot\text{K} \quad \Delta\hat{H}_B = (240.74 \text{ J/kg}\cdot\text{K})(30^\circ\text{C} - 25^\circ\text{C}) = 1.30 \text{ kJ/kg}$$

$$c_p^C = 2160.77 \text{ J/kg}\cdot\text{K} \quad \Delta\hat{H}_C = (2160.77 \text{ J/kg}\cdot\text{K})(30^\circ\text{C} - 25^\circ\text{C}) = 10.80 \text{ kJ/kg}$$

$$c_p^D = 1339.83 \text{ J/kg}\cdot\text{K} \quad \Delta\hat{H}_D = (1339.83 \text{ J/kg}\cdot\text{K})(30^\circ\text{C} - 25^\circ\text{C}) = 6.70 \text{ kJ/kg}$$

$$\Delta\hat{H}_T = \Delta\hat{H}_H + \Delta\hat{H}_B + \Delta\hat{H}_C + \Delta\hat{H}_D$$

$$= 6.1 \text{ kJ/kg} + 1.3 \text{ kJ/kg} + 10.8 \text{ kJ/kg} + 6.7 \text{ kJ/kg}$$

$$= 24.9 \text{ kJ/kg}$$

$$\dot{n} = 24161.4 \text{ kg/hr}$$

$$\dot{Q} = \dot{n}\Delta\hat{H}_T = (24161.4 \text{ kg/hr})(24.9 \text{ kJ/kg})$$

$$= 6.02 \times 10^6 \text{ kJ/hr} = \text{heat absorbed by broth}$$

$$\dot{Q}_S = -\dot{Q} = \text{heat brought in by steam}$$

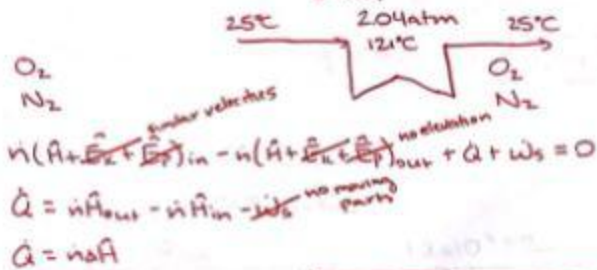
* c_p of water vapor @ 300 K

$$\dot{Q}_S = \dot{n}_s c_{p,s} [25^\circ\text{C} - 30^\circ\text{C}]$$

$$\dot{n}_s = \frac{\dot{Q}_S}{c_{p,s} [25^\circ\text{C} - 30^\circ\text{C}]} = \frac{-6.02 \times 10^6 \text{ kJ/hr}}{(1.8641 \text{ kJ/kg}\cdot\text{K})(-5 \text{ K})}$$

$$= \text{flow rate of incoming steam} = 64592.27 \text{ kg/hr}$$

Energy Balance across ~~H-103~~ (Heat Sterilizer) E-101



$$\dot{Q} = n \sum_i c_{pi} (121^\circ\text{C} - 25^\circ\text{C})$$

where $\dot{Q}$ = % of heat required from sterilizer to bring temp up to 121°C

$$\Delta\hat{H}_{O_2} = \int_{25^\circ\text{C}}^{121^\circ\text{C}} C_{p,i} dT \quad \Delta\hat{H}_{N_2} = \int_{25^\circ\text{C}}^{121^\circ\text{C}} C_{p,i} dT$$

$$C_{p,i}^{O_2} = (29.1 \text{ J/mol}\cdot\text{K}) \left(\frac{1 \text{ mol}}{31.998 \text{ g}} \right) = 0.91 \text{ J/g}\cdot\text{K}$$

$$C_{p,i}^{N_2} = (1.042 \text{ J/g}\cdot\text{K}) = 1.042 \text{ J/g}\cdot\text{K}$$

$$\Delta\hat{H}_{O_2} = (0.91 \text{ J/g}\cdot\text{K}) \left(\frac{1000 \text{ g}}{1 \text{ kg}} \right) (121^\circ\text{C} - 25^\circ\text{C}) = 87.36 \text{ kJ/kg}$$

$$\Delta\hat{H}_{N_2} = (1.042 \text{ J/g}\cdot\text{K}) \left(\frac{1000 \text{ g}}{1 \text{ kg}} \right) (121^\circ\text{C} - 25^\circ\text{C}) = 100.03 \text{ kJ/kg}$$

$$\Delta\hat{H}_T = \Delta\hat{H}_{O_2} + \Delta\hat{H}_{N_2}$$

$$= 87.36 \text{ kJ/kg} + 100.03 \text{ kJ/kg}$$

$$= 187.39 \text{ kJ/kg}$$

$$\dot{n} = 63655.2 \text{ kg/hr}$$

$$\dot{Q} = n\Delta\hat{H}_T$$

$$= (63655.2 \text{ kg/hr}) (187.39 \text{ kJ/kg}) = 1.2 \times 10^7 \text{ kJ/hr} = \text{heat absorbed by incoming air}$$

$$\dot{Q}_s = \text{heat leaving steam} = -\dot{Q} = -1.2 \times 10^7 \text{ kJ/hr}$$

$$\dot{Q}_s = \dot{n}_s c_{p,s}^{(9)} [25^\circ\text{C} - 121^\circ\text{C}]$$

$$\dot{n}_s = \frac{\dot{Q}_s}{c_{p,s}^{(9)} [25^\circ\text{C} - 121^\circ\text{C}]} = \frac{-1.2 \times 10^7 \text{ kJ/hr}}{(1.864 \text{ kJ/kg}\cdot\text{K}) (-96 \text{ K})}$$

= flow rate of incoming steam = 67060.1 kg/hr

Cooling mechanism:

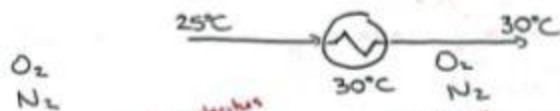
$$\dot{Q}_{cw} = \dot{Q} = 1.2 \times 10^7 \text{ kJ/hr}$$

$$\dot{Q}_{cw} = \dot{n}_{cw} c_{p,cw}^{(4)} [121^\circ\text{C} - 25^\circ\text{C}]$$

$$\dot{n}_{cw} = \frac{\dot{Q}_{cw}}{c_{p,cw}^{(4)} [121^\circ\text{C} - 25^\circ\text{C}]} = \frac{1.2 \times 10^7 \text{ kJ/hr}}{(4.184 \text{ kJ/kg}\cdot\text{K}) (96 \text{ K})}$$

$$= \text{flow rate of incoming cooling water} = \text{29875.72 kg/hr}$$

Energy Balance across ~~E-104~~ (Heat Exchanger)



$$\dot{n}(\hat{H} + \cancel{\hat{E}_k} + \cancel{\hat{E}_p})_{in} - \dot{n}(\hat{H} + \cancel{\hat{E}_k} + \cancel{\hat{E}_p})_{out} + \dot{Q} + \dot{W}_s = 0$$

similar velocities *no calculation*

$$\dot{Q} = \dot{n}\hat{H}_{out} - \dot{n}\hat{H}_{in} - \cancel{\dot{W}_s}$$

no moving parts

$$\dot{Q} = \dot{n}\Delta\hat{H}$$

$$= \dot{n}\sum\Delta\hat{H}$$

$$\boxed{\dot{Q} = \dot{n}\sum_i c_p(30^\circ\text{C} - 25^\circ\text{C})}$$

Where $\dot{Q} = 3/5$ of heat required from exchanger to bring temp up to 30°C

$$\Delta\hat{H}_{O_2} = \int_{25^\circ\text{C}}^{30^\circ\text{C}} c_p^{O_2} dT \quad \Delta\hat{H}_{N_2} = \int_{25^\circ\text{C}}^{30^\circ\text{C}} c_p^{N_2} dT$$

$$c_p^{O_2} = 0.91 \text{ J/gK}$$

$$c_p^{N_2} = 1.042 \text{ J/gK}$$

$$\Delta\hat{H}_{O_2} = (0.91 \text{ J/gK}) \left(\frac{1000 \text{ g}}{1 \text{ kg}} \right) (30^\circ\text{C} - 25^\circ\text{C}) = 4.55 \text{ kJ/kg}$$

$$\Delta\hat{H}_{N_2} = (1.042 \text{ J/gK}) \left(\frac{1000 \text{ g}}{1 \text{ kg}} \right) (30^\circ\text{C} - 25^\circ\text{C}) = 5.21 \text{ kJ/kg}$$

$$\Delta\hat{H}_T = \Delta\hat{H}_{O_2} + \Delta\hat{H}_{N_2}$$

$$= 4.55 \text{ kJ/kg} + 5.21 \text{ kJ/kg}$$

$$= 9.76 \text{ kJ/kg}$$

$$\dot{Q} = \dot{n}\Delta\hat{H}_T, \dot{n} = 63835.2 \text{ kg/hr}$$

$$= (63835.2 \text{ kg/hr}) (9.76 \text{ kJ/kg}) = \underline{6.23 \times 10^6 \text{ kJ/hr}} = \text{heat absorbed by incoming air}$$

$$\dot{Q}_s = -\dot{Q} = \text{heat brought in by steam} = -6.23 \times 10^6 \text{ kJ/hr}$$

$$\dot{Q}_s = \dot{n}_s c_{p,H_2O}^{(g)} (25^\circ\text{C} - 30^\circ\text{C})$$

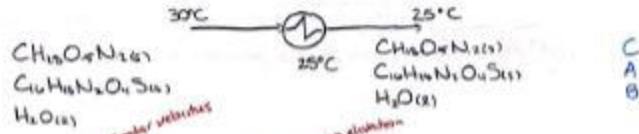
$$\dot{n}_s = \frac{\dot{Q}_s}{c_{p,H_2O}^{(g)} [25^\circ\text{C} - 30^\circ\text{C}]} = \frac{-6.23 \times 10^6 \text{ kJ/hr}}{(2.01 \text{ kJ/kgK}) (5 \text{ K})}$$

18.4

$$\dot{n}_s = \text{flow rate of incoming steam} = \underline{\underline{61940.5 \text{ kg/hr}}}$$

$$= \underline{\underline{61940.5 \text{ kg/hr}}}$$

Energy Balance across E-201 (Heat Exchanger)



$$n(\hat{H} + \hat{E}_k + \hat{E}_p)_{in} - n(\hat{H} + \hat{E}_k + \hat{E}_p)_{out} + \dot{Q} + \dot{W}_s = 0$$

$$\dot{Q} = n\hat{H}_{out} - n\hat{H}_{in} - \dot{W}_s$$

$$\dot{Q} = n\hat{H}$$

$$= n\sum o\hat{H}$$

$$\dot{Q} = n\sum_i c_p (25^\circ\text{C} - 30^\circ\text{C})$$

where $\dot{Q}$ = % of heat that the exchanger must remove to bring temp down to 25°C

$$n\hat{H}_A = \int_{30^\circ\text{C}}^{25^\circ\text{C}} C_p dT \quad n\hat{H}_B = \int_{30^\circ\text{C}}^{25^\circ\text{C}} C_p dT \quad n\hat{H}_C = \int_{30^\circ\text{C}}^{25^\circ\text{C}} C_p dT$$

$$C_p = 4.184 \text{ kJ/kg}\cdot\text{K} \quad C_p^A = C_p^B = C_p^C = 1.81 \text{ kJ/kg}\cdot\text{K} \quad \text{Assumption that } C_p \text{ of } C_p^A \text{ of } C_p^B \text{ of } C_p^C \text{ found via literature}$$

$$n\hat{H}_A = (1.81 \text{ kJ/kg}\cdot\text{K})(25^\circ\text{C} - 30^\circ\text{C}) = -9.05 \text{ kJ/kg}$$

$$n\hat{H}_B = (4.184 \text{ kJ/kg}\cdot\text{K})(25^\circ\text{C} - 30^\circ\text{C}) = -20.92 \text{ kJ/kg}$$

$$n\hat{H}_C = (1.81 \text{ kJ/kg}\cdot\text{K})(25^\circ\text{C} - 30^\circ\text{C}) = -9.05 \text{ kJ/kg}$$

$$n\hat{H}_T = n\hat{H}_A + n\hat{H}_B + n\hat{H}_C = 2(-9.05 \text{ kJ/kg}) - 20.92 \text{ kJ/kg}$$

$$= -39.02 \text{ kJ/kg}$$

$$\dot{Q} = n\hat{H}_T; \dot{n} = 24189.1 \text{ kg/hr} \quad \dot{Q} = (24189.1 \text{ kg/hr})(-39.02 \text{ kJ/kg}) = -9.44 \times 10^5 \text{ kJ/hr} = \text{heat absorbed from brass by cooling water}$$

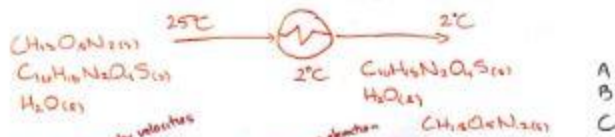
$$\dot{Q}_{cw} = -\dot{Q} = \text{heat absorbed by cooling water}$$

$$= 9.44 \times 10^5 \text{ kJ/hr}$$

$$\dot{Q}_{cw} = \dot{n}_{cw} C_{p,cw} (30^\circ\text{C} - 25^\circ\text{C})$$

$$\dot{n}_{cw} = \frac{\dot{Q}_{cw}}{C_{p,cw} (30^\circ\text{C} - 25^\circ\text{C})} = \frac{9.44 \times 10^5 \text{ kJ/hr}}{(4.184 \text{ kJ/kg}\cdot\text{K})(5 \text{ K})} = \text{flow rate of incoming cooling water} = 45124.28 \text{ kg/hr}$$

Energy Balance across E-202 (Heat Exchanger)



$n(\hat{H}_A + \hat{H}_B + \hat{H}_C)_{in} - n(\hat{H}_A + \hat{H}_B + \hat{H}_C)_{out} + \dot{Q} + \dot{W}_s = 0$
 $\dot{Q} = n\hat{H}_{out} - n\hat{H}_{in}$ (no mixing parts)
 $\dot{Q} = n\Delta\hat{H}$
 $= n\sum \Delta\hat{H}$

$\dot{Q} = n\sum c_p(2^\circ C - 25^\circ C)$

Where $\dot{Q}$ = % of heat that the exchanger must remove to bring temp down to 2°C

$\Delta\hat{H}_A = \int_{25^\circ C}^{2^\circ C} c_p^A dT$ $\Delta\hat{H}_B = \int_{25^\circ C}^{2^\circ C} c_p^B dT$ $\Delta\hat{H}_C = \int_{25^\circ C}^{2^\circ C} c_p^C dT$

$c_p^A \approx 4.184 \text{ kJ/kg} \cdot ^\circ C$

$c_p^B = (4.184 \text{ kJ/kg} \cdot ^\circ C) \left(\frac{1.17}{1000} \right) (2^\circ C - 25^\circ C) = 4.184 \text{ kJ/kg} \cdot ^\circ C$

$\rho_A = \left(\frac{1.17 \text{ g/cm}^3}{1000} \right) \left(\frac{1 \text{ kg}}{1000 \text{ g}} \right) = 1.17 \text{ kg/m}^3$
 $\rho_C = (1.095 \text{ g/cm}^3) \left(\frac{1000 \text{ g}}{1 \text{ m}^3} \right) \left(\frac{1 \text{ kg}}{1000 \text{ g}} \right) = 1.095 \text{ kg/m}^3$

$c_p^A = c_p^B = 1.81 \text{ kJ/kg} \cdot ^\circ C$ - Assumption that $c_p^A = c_p^B$, c_p^C found via literature

$\Delta\hat{H}_A = (1.81 \text{ kJ/kg} \cdot ^\circ C) (2^\circ C - 25^\circ C) = \Delta\hat{H}_C = -41.63 \text{ kJ/kg}$

$\Delta\hat{H}_B = (4.184 \text{ kJ/kg} \cdot ^\circ C) (2^\circ C - 25^\circ C) = -96.23 \text{ kJ/kg}$

$\Delta\hat{H}_T = \Delta\hat{H}_A + \Delta\hat{H}_B + \Delta\hat{H}_C$
 $= 2(-41.63 \text{ kJ/kg}) + (-96.23 \text{ kJ/kg})$
 $= -179.49 \text{ kJ/kg}$

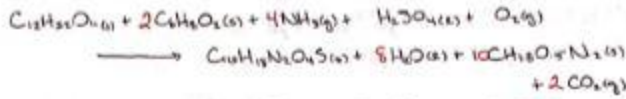
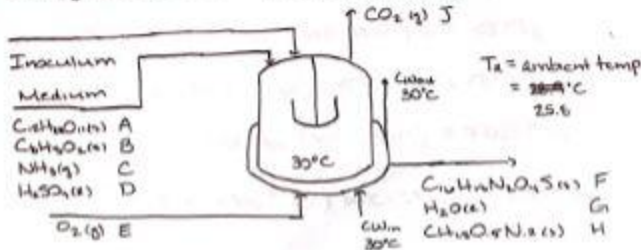
$\dot{Q} = n\Delta\hat{H}_T$, $n = 168943 \text{ kg/hr}$
 $= (168943 \text{ kg/hr}) (-179.49 \text{ kJ/kg})$
 $= -3.03 \times 10^7 \text{ kJ/hr}$ = heat lost from broth

$\dot{Q}_{CW} = -\dot{Q}$ = heat absorbed by cooling water
 $= 3.03 \times 10^7 \text{ kJ/hr}$

$\dot{Q}_{CW} = n_{CW} c_p^{in} [25^\circ C - 2^\circ C]$

$n_{CW} = \frac{\dot{Q}_{CW}}{c_p^{in} [25^\circ C - 2^\circ C]} = \frac{3.03 \times 10^7 \text{ kJ/hr}}{(4.184 \text{ kJ/kg} \cdot ^\circ C) (23^\circ C)}$
 $= \text{Flow rate of incoming cooling water} = 31486.41 \text{ kg/hr}$

Energy Balance across V-104 (Fermenter)



$$\dot{n}(\hat{H} + \hat{E}_k + \hat{E}_p)_{in} - \dot{n}(\hat{H} + \hat{E}_k + \hat{E}_p)_{out} + \dot{Q} + \dot{W}_s = 0$$

$$\dot{Q} + \dot{n}\hat{H}_{in} - \dot{n}\hat{H}_{out} + \dot{W}_s = 0$$

$$\dot{Q} = \dot{n}\hat{H}_{out} - \dot{n}\hat{H}_{in}$$

$$\hat{H}_{out} = \hat{H}_F + 2\hat{H}_B + 4\hat{H}_C + \hat{H}_D + \hat{H}_E, \quad \hat{H}_{in} = \hat{H}_A + 2\hat{H}_B + 4\hat{H}_C + \hat{H}_D + \hat{H}_E$$

$$C_p^A = 1.22 \text{ kJ/kg}\cdot\text{K}; \quad C_p^B = 0.261 \text{ kJ/kg}\cdot\text{K}; \quad C_p^C = 2.161 \text{ kJ/kg}\cdot\text{K}$$

$$C_p^D = 1.341 \text{ kJ/kg}\cdot\text{K}; \quad C_p^E = 0.91 \text{ kJ/kg}\cdot\text{K}; \quad C_p^F = 1.81 \text{ kJ/kg}\cdot\text{K}$$

$$C_p^G = 4.184 \text{ kJ/kg}\cdot\text{K}; \quad C_p^H = 1.81 \text{ kJ/kg}\cdot\text{K}; \quad C_p^J = 0.844 \text{ kJ/kg}\cdot\text{K}$$

$$\dot{n}\hat{H}_A = \int_{25.5}^{30} C_p^A dT = (1.22 \text{ kJ/kg}\cdot\text{K})(30^\circ\text{C} - 25.5^\circ\text{C}) = 5.124 \text{ kJ/kg}$$

$$\dot{n}\hat{H}_B = \int_{25.5}^{30} C_p^B dT = (0.261 \text{ kJ/kg}\cdot\text{K})(30^\circ\text{C} - 25.5^\circ\text{C}) = 1.071 \text{ kJ/kg}$$

$$\dot{n}\hat{H}_C = \int_{25.5}^{30} C_p^C dT = (2.161 \text{ kJ/kg}\cdot\text{K})(30^\circ\text{C} - 25.5^\circ\text{C}) = 9.05 \text{ kJ/kg}$$

$$\dot{n}\hat{H}_D = \int_{25.5}^{30} C_p^D dT = (1.341 \text{ kJ/kg}\cdot\text{K})(30^\circ\text{C} - 25.5^\circ\text{C}) = 5.125 \text{ kJ/kg}$$

$$\Delta \hat{H}_E = \int_{25.8^\circ\text{C}}^{30^\circ\text{C}} C_p^E dT = (0.91 \text{ kJ/kgK})(30^\circ\text{C} - 25.8^\circ\text{C}) = 3.822 \text{ kJ/kg}$$

$$\Delta \hat{H}_F = \int_{25.8^\circ\text{C}}^{30^\circ\text{C}} C_p^F dT = (1.81 \text{ kJ/kgK})(30^\circ\text{C} - 25.8^\circ\text{C}) = 7.602 \text{ kJ/kg}$$

$$\Delta \hat{H}_A = \int_{25.8^\circ\text{C}}^{30^\circ\text{C}} C_p^A dT = (4.184 \text{ kJ/kgK})(30^\circ\text{C} - 25.8^\circ\text{C}) = 17.573 \text{ kJ/kg}$$

$$\Delta \hat{H}_n = \int_{25.8^\circ\text{C}}^{30^\circ\text{C}} C_p^n dT = (1.81 \text{ kJ/kgK})(30^\circ\text{C} - 25.8^\circ\text{C}) = 7.602 \text{ kJ/kg}$$

$$\Delta \hat{H}_S = \int_{25.8^\circ\text{C}}^{30^\circ\text{C}} C_p^S dT = (0.846 \text{ kJ/kgK})(30^\circ\text{C} - 25.8^\circ\text{C}) = 3.55 \text{ kJ/kg}$$

$$\begin{aligned} \Delta \hat{H}_T &= \sum_i \Delta \hat{H}_i \\ &= 5124 \text{ kJ/kg} + 1.076 \text{ kJ/kg} + 9.08 \text{ kJ/kg} + 5.126 \text{ kJ/kg} + 3.822 \text{ kJ/kg} \\ &\quad + 2(7.602 \text{ kJ/kg}) + 17.573 \text{ kJ/kg} + 3.55 \text{ kJ/kg} \\ &= 61.077 \text{ kJ/kg} \end{aligned}$$

$$\begin{aligned} \dot{m} &= \dot{m}_{\text{mech}} + \dot{m}_{\text{med}} + \dot{m}_{\text{water}} \\ &= 27.7 \text{ kg/hr} + 24461.4 \text{ kg/hr} + 63835.2 \text{ kg/hr} \\ &= 88024.3 \text{ kg/hr} \end{aligned}$$

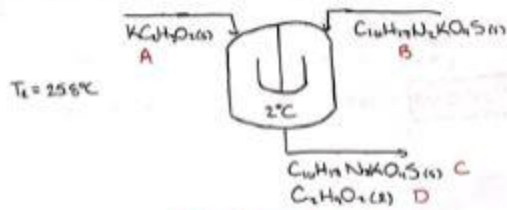
$$\begin{aligned} \dot{Q} &= \dot{m} \Delta \hat{H}_T \\ &= (88024.3 \text{ kg/hr})(61.077 \text{ kJ/kg}) \\ &= 5.38 \times 10^6 \text{ kJ/hr} = \text{heat absorbed by broth during rxn} \end{aligned}$$

$$\begin{aligned} \dot{Q}_{\text{cw}} &= -\dot{Q} = \text{heat that must be removed by water} \\ &= -5.38 \times 10^6 \text{ kJ/hr} \end{aligned}$$

$$\dot{Q}_{\text{cw}} = \dot{m}_{\text{cw}} C_p^{\text{cw}} [25.8^\circ\text{C} - 30^\circ\text{C}]$$

$$\begin{aligned} \dot{m}_{\text{cw}} &= \frac{\dot{Q}_{\text{cw}}}{C_p^{\text{cw}} [25.8^\circ\text{C} - 30^\circ\text{C}]} = \frac{-5.38 \times 10^6 \text{ kJ/hr}}{(4.184 \text{ kJ/kgK})(-4.2\text{K})} \\ &= \text{flow rate of incoming cw} = \boxed{2.6 \times 10^5 \text{ kg/hr}} \end{aligned}$$

Energy Balance across V-205 (Crystallizer)



$$\dot{n}(\hat{H} + \hat{E}_k + \hat{E}_p)_{in} - \dot{n}(\hat{H} + \hat{E}_k + \hat{E}_p)_{out} + \dot{Q} + \dot{W}_s = 0$$

Similar velocities no elevation

$$\dot{n}\hat{H}_{in} - \dot{n}\hat{H}_{out} + \dot{Q} + \dot{W}_s = 0$$

neglect kinetic

$$\dot{Q} + \dot{n}\hat{H}_{in} - \dot{n}\hat{H}_{out} = 0$$

$$\dot{Q} = \dot{n}\hat{H}_{out} - \dot{n}\hat{H}_{in} = \dot{n}\Delta\hat{H}$$

$$\dot{Q} = \dot{n} \sum c_p (2^\circ\text{C} - 25.8^\circ\text{C})$$

$$C_p^A = 1.11 \text{ kJ/kgK}; C_p^B = 181 \text{ kJ/kgK}; C_p^C = 181 \text{ kJ/kgK}; C_p^D = 2.05 \text{ kJ/kgK}$$

$$\Delta\hat{H}_A = \int_{25.8^\circ\text{C}}^{2^\circ\text{C}} C_p^A dT; \Delta\hat{H}_B = \int_{25.8^\circ\text{C}}^{2^\circ\text{C}} C_p^B dT; \Delta\hat{H}_C = \int_{2^\circ\text{C}}^{25.8^\circ\text{C}} C_p^C dT; \Delta\hat{H}_D = \int_{25.8^\circ\text{C}}^{2^\circ\text{C}} C_p^D dT$$

$$\Delta\hat{H}_A = (1.11 \text{ kJ/kgK})(2^\circ\text{C} - 25.8^\circ\text{C}) = -26.418 \text{ kJ/kg}$$

$$\Delta\hat{H}_B = \Delta\hat{H}_C = \int_{25.8^\circ\text{C}}^{2^\circ\text{C}} (181 \text{ kJ/kgK})(2^\circ\text{C} - 25.8^\circ\text{C}) = -43.076 \text{ kJ/kg}$$

$$\Delta\hat{H}_D = (2.05 \text{ kJ/kgK})(2^\circ\text{C} - 25.8^\circ\text{C}) = -46.79 \text{ kJ/kg}$$

$$\Delta\hat{H}_T = \Delta\hat{H}_A + \Delta\hat{H}_B + \Delta\hat{H}_C + \Delta\hat{H}_D$$

$$= -26.418 \text{ kJ/kg} - 2(43.076 \text{ kJ/kg}) - 46.79 \text{ kJ/kg}$$

$$= -161.364 \text{ kJ/kg}$$

$$\dot{Q} = \dot{n}\Delta\hat{H}_T; \dot{n} = 5235.7 \text{ kg/hr}$$

$$= (5235.7 \text{ kg/hr})(-161.364 \text{ kJ/kg})$$

$$= -8.45 \times 10^5 \text{ kJ/hr}$$

$$\dot{Q}_{cw} = -\dot{Q} = 8.45 \times 10^5 \text{ kJ/hr}$$

$$\dot{Q}_{cw} = \dot{m}_{cw} C_{p,cw} [25.8^\circ\text{C} - 2^\circ\text{C}]$$

$$\dot{m}_{cw} = \frac{\dot{Q}_{cw}}{C_{p,cw} [25.8^\circ\text{C} - 2^\circ\text{C}]} = \frac{8.45 \times 10^5 \text{ kJ/hr}}{(4184 \text{ kJ/kgK})(23.8^\circ\text{C})}$$

$$= \text{flow rate of incoming cooling water} = 8485.71 \text{ kg/hr}$$

AVERAGE
PROJECT REPORT



Senior Design & Professionalism

CHEG 4247 P02

Dr. Martin Team #3

The Production of Single Cell Protein

Kaylon Atkinson

Shanelle Bryant

Chad Gardner

Oluwatoyosi Idowu

December 3, 2021

Letter of Transmittal

Prairie View A&M University
Department of Chemical Engineering
100 University Dr.
Prairie View, TX 77446

December 3, 2021

Dear Dr. Martin,

The following report details a design process that utilizes *Methylococcus capsulatus*, a methanotrophic bacteria, to produce single-cell protein. The process yields 150,000 MT of single-cell protein per year. This design process includes a batch operation, extraction, purification, and packaging of the final product.

The economic analysis and the feasibility for the process indicate very favorable results, especially given the high quality and purity of the final product. With a global market for SCP production predicted to reach US\$ 27.3 billion by the end of 2027, with a CAGR (Compound Annual Growth Rate) of 7% and global demand of 600 million pounds each year, we recommend the implementation of the design detailed in this report. Additional research should be performed to guarantee the safe implementation of the design, as well as analyzing a wider range of market applications for greater financial success.

Thank you for the guidance given throughout the duration of this project.

Sincerely,

Oluwatoyosi Idowu

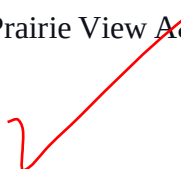
Kaylon Atkinson

Chad Gardner

Shanelle Bryant

Acknowledgement

We would like to express our sincerest gratitude to our advisors Dr. Martin and Dr. Gyamerah and the chemical engineering faculty at Prairie View A&M University for their invaluable guidance, comments, and suggestions throughout the course of this project. Finally, we would like to say thank you to the Prairie View A&M Industrial Council for their advice and inputs during this presentation.



Project Executive Summary

The purpose of this project was to design a Single Cell Protein plant to produce high-quality protein. Single-cell protein (SCP) is a microbial protein that is extracted from unicellular organisms such as bacteria, yeast, fungi, and algae. With a broad amino acid profile and an ability to produce essential organic compounds and vitamins, SCP is a promising alternative to classical protein. SCP is commonly used in animal feedstocks, food additives, and the pharmaceutical industry. With an increase in the demand for SCP for use in feedstock for aquaculture and farming for fish, the process outlined in this report produces 150,000 MT of SCP per year using *Methylococcus capsulatus*, a methanotrophic bacteria with Methanol and Nitric Acid as the carbon and nitrogen sources, respectively. The final product of SCP is sold at an average of \$1,650/MT. As the global market for SCP production is predicted to reach US\$ 27.3 billion by the end of 2027, with a CAGR (Compound Annual Growth Rate) of 7% and global demand of 600 million pounds each year, the profitability of the process is promising.

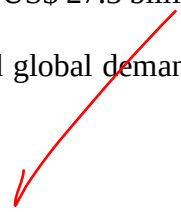


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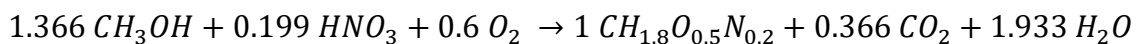
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1. Project Scope

1.1 Problem Statement

There is a growing awareness and popularity in today's world for single cell protein (SCP) as an alternative source of protein due to malnutrition being more prevalent. Prominent countries such as the United States, China, India, Indonesia, Vietnam, and Bangladesh are projecting an increase in SCP production by 2050. According to a recent report conducted by Transparency Market Research (TMR), the global market for SCP production is to reach US\$ 27.3 billion by the end of 2027, with a CAGR (Compound Annual Growth Rate) of 7% and global demand of 600 million pounds each year.

Consumers today demand nutritious foods with higher protein content, and high quality to encourage good health practices such as lowering overall body weight and cholesterol. There is also an increased demand for protein in aquaculture and animal feed, which require this specimen for the preservation of their stock to support market growth. Due to the increased demand for (SCP) in the United States and these nations, a new company has been established in Austin, Texas, to generate (SCP) through the bacteria cultivation of the *Methylococcus capsulatus* strand. The chosen method of production utilizes a methanotrophic bacteria, *Methylococcus capsulatus*, as the strain of choice, methanol as the carbon source, and nitric acid as the nitrogen source. The chemical reaction for this highly exothermic reaction is as follows:



Our goal is to establish a reliable supply of cost-effective, high-quality SCP that will successfully generate the much-needed protein to address the growing problem of malnutrition and protein deficit by operating a plant at a capacity of 150,000 metric tons per year.

REFERENCES/CITATIONS

1.2 Client Identification and Recognition of need

From our research of various literature reviews, we gathered that the global protein scarcity is at an all-time high, and the agricultural sector is being overwhelmed by the demand of meat and dairy it has to produce per year to maintain the growing population of people. Much of the recent interest in SCP is centered on the use of microbes to boost the protein content of side streams, which may then be used in animal feed and food additives. Countries like the United States, India, and China are interested in developing healthier foods with an optimal composition of low but high-quality amino acids and fats, combined with ethically sustainable production.

We will be providing Tyson (Houston, Texas) and Bluehouse Salmon (Sparks Nevada or Florida) our SCP products. Tyson is most known for its chicken, beef, and pork. They have one of the largest protein portfolios in their industry. In 2020 their net revenues were 43.2 billion which is a 2 percent increase from 2019. The seafood industry will always be a popular and growing industry, therefore, with Bluehouse salmon's main location being on the coast of Florida, there will not be a lack of resources. Although they are somewhat in the early stage of being in the fish industry, they supply about 400 thousand tons of salmon consumed each year. Their revenue increased from 5.5 million in 2019 to 6.3 million in 2020. This increase in revenue for both clients highlight the increased need for SCP in the market.

1.3 Project Goals and Objectives

Focus on the project activities

Our goal is to produce a reliable supply of cost-effective, high-quality SCP that will solve the growing problem of hunger and protein deficiency by providing much-needed protein. To achieve this goal, we came up with some objectives. We needed to research information about SCP; what it is, what it can be used for or what it is used in. We also thought about the location of our plant, what our feedstock would consist of and what the process is of producing single cell protein.

1.4 Contemporary Issues and Impact project society

1.4.1 Contemporary issues relevant to project

REFS

In previous years, finding alternative ways of providing food for people did not become such a concern until the population began to double unexpectedly and global protein scarcity became a growing issue. Research done by many concluded that if options are not thought of to take the pressure off the agricultural sector in providing various other protein options, then the growing malnutrition and protein deficiency will become worse. We hope that by producing high-quality and protein-rich SCP, we can contribute to lowering the global malnutrition problem that is safe and cost-effective for all.

How does this relate to SCP plants?

1.4.2 Potential impact of project on society

With a broad amino acid profile, a high protein content, and the ability to produce essential organic compounds and vitamins, SCP is a promising alternative to other classical sources of animal feed. Aquaculture and farming of fish are one of the fastest-growing food markets that heavily rely on the manufacturing of SCP. When used as a feed supplement for farmed salmon, one of the largest sectors of aquaculture, SCP serves as a nutritional additive and ensures that the salmon possesses its expected pigmentation. By implementing this project, we will be tackling 0.05% of the global demand for needed SCP to help tackle the increasing protein deficiency and the gap being created from the inability of classical protein sources to keep up with the growing populations' demand.

1.5 Project Constraints

capacity
economics
environmental
purity
safety

Since our research on SCP began, we have come across several constraints. Firstly, we considered yeast as our working microorganism from which SCP would be extracted, but we ran into difficulties finding detailed steps on the processes that could be used as a reference. After

consulting with our professor, we decided to use bacteria as our microorganism. Secondly, when choosing bacteria, we contemplated the raw materials that would be best suitable to efficiently grow our bacteria. Since the bacterial strain we decided on, *Methylococcus capsulatus* requires an adequate carbon source for optimum growth, extensive research was executed before concluding on the appropriate carbon source. Thirdly, we had to decide where our plant would be located. We debated whether it was more beneficial to be near our raw materials, or near our consumers. After much research, a decision was made that addressed both options. With a heat-sensitive product such as SCP, the different unit operating parameters we use can also have an impact on the quality of the final product. If we use an elevated temperature in our spray dryer to dry our product, then we risk damaging our product. After careful consideration, we concluded on our location, raw materials, and our unit operating parameter as they can have adverse effects on our process and final product.

2. Project Planning and Task Identification

2.1 Task Identification

The following is a detailed guide that lists the major tasks that we needed to achieve in order to complete this project.

Table 1. Task Identification list for project planning

Task Identification
Project Definition
Business Analysis and Cost Estimation
Safety and Environmental Regulations
Preliminary Process Design / simulation
End of semester presentation
End of semester report

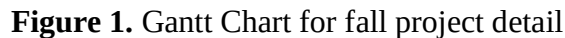
2.2 Timelines

The main tasks were also broken down into subtasks along with their durations to obtain optimal planning toward the completion of the project.

Table 2. Detailed task identification table with included timeline

Task Identification Timeline	
Outlined Task	Timeline (Weeks)
• Project Definition ○ Literature Review ○ Microorganism and Process Research/Selection	10
• Business Analysis and Cost Estimation ○ Market and consumer interest ○ Raw material/production source ○ Plant Location	7
• Safety and Environmental Regulations ○ Storage & Handling ○ Packaging & Waste Disposal ○ OSHA, FDA, EPA Regulations	10
• Preliminary Process Design ○ Preliminary BFD & PFD/ Visio / Process Flow Sheet Development ○ Material and Energy Balances ○ Process Chemistry ○ Preliminary Simulation	6
• End of semester presentation	2
• End of semester report ○ Submission of fall report	2.5

The organization of this fall semester project can be seen in the ~~Gantt~~ chart below in figure



What are the spots?

was brought to this issue, a

Table 3. Macromolecular composition and general properties of Microorganisms

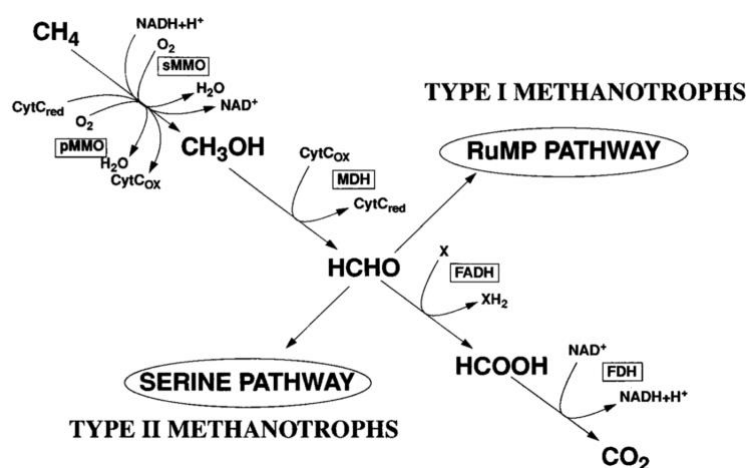
PARAMETERS	BACTERIA	YEAST	FUNGI	ALGAE
Doubling time (hours)	1-3	2-6	5-12	6-24
Crude protein (% dry cell weight)	40-80	40-60	30-45	40-50
Nucleic acids (%)	8-20	5-15	6-13	45-51 ^a
Carbohydrates and fats (%)	10-30	10-40	10-45	34.6-45
Ash content (%)	4-10	4-10	4-10	5-8
Temperature range (°C)	22-55	25-40	25-50	25-32
pH range	5-7	3-5	6-8	6.9-9.6

After careful consideration of the options given, we decided on using a bacterial strand as our choice of unicellular microorganism.

3.1.1 Methanol as carbon source

Written in wrong person.

With further research, we selected a methanotrophic bacteria known as *Methylococcus capsulatus*. Methanotrophic bacteria employ the use of methanol as a carbon source, and we chose nitric acid as our nitrogen source. The chemistry for methanotrophic bacteria using methane as a carbon source and converting it to carbon dioxide, one of the byproducts of the reaction, is outlined below in Figure 2. In this reaction, it is seen that methane is first converted to methanol. Methanol is then converted to formaldehyde and formic acid before being released as carbon dioxide.

Figure 2. Chemical pathway of methane converted to methanol as a carbon source

The decision to use methanol rather than methane as the source of carbon was made for several reasons. Methanol is easier to prepare and handle than methane, which helps in safety considerations. The cooling requirement for methanol when compared to methane is much lower as methane produces more heat than methanol. This is because the heat of conversion of methane to methanol is highly exothermic, therefore, contributing to the overall heat in the reaction. The overall cost of handling methanol is also much lower when compared to that of methane. Methane requires a greater amount of oxygen to be fed into the process. By doing so, there is a greater concern for flammability and explosivity. As methane is a natural gas product, it is much more difficult and expensive to handle gas. Methanol on the other hand can be handled as a liquid. As a large quantity of methanol is needed for this process, the storage and delivery of methanol are more economical and convenient.

3.1.2 Nitric acid as nitrogen source

Nitric acid was selected as the source of nitrogen for this process. It is a highly corrosive and strong mineral acid. Ordinary nitric acid has a concentration of 68% with water occupying the other 32%. This percentage causes the acid to be readily safer for usage. Nitric acid is often used as the starting material in industrial processes that require nitrogen sources for things such as fertilizers. They are also excellent neutralizers when mixed with ammonia to form ammonia nitrate. Nitric acid in this concentration is readily available in bulk quantities and is cheaper due to its common usage. The decomposition of nitric acid results in water, nitrogen dioxide, and oxygen. This contributes to the increased amount of water being generated in this reaction.

IMPROPER VOICE
FOR Technical Report.

3.2 Physical and chemical properties

Below is the physical and a chemical property of our raw materials.

Table 4. Physical and Chemical Property of Methanol

Parameters	Value
Molecular Weight	32 g/mol
Chemical Formula	CH ₄ O or CH ₃ OH
Color	Colorless
Physical State	Liquid
Odor	Slight alcoholic when pure
Boiling Point	64.7°C
Melting Point	-97.6°C
Vapor Pressure	18.7 Kpa @ 27°C
Solubility	Miscible with water @ 20°C

Table 5. Physical and Chemical Properties of Nitric Acid

Parameters	Value
Molecular Weight	63 g/mol
Chemical Formula	HNO ₃
Color	Transparent
Physical State	Liquid
Odor	Sweet
Boiling Point	83°C
Melting Point	-41.6°C
Vapor Pressure	6.4 Kpa
Solubility	Miscible with water

3.3 Handling, storage, and safety

Handling, storage, and safety is unarguably the most important aspect of this design process. Not only is it essential to adequately handle the raw materials involved in the production

of SCP, but the final product must also be carefully handled because it is being consumed/ingested by living organisms.

3.3.1 Handling

Correctly handling methanol and nitric acid are very vital in ensuring that we have a safe environment for everyone. Both chemicals are considered highly flammable, toxic if swallowed, and corrosive. They can cause severe damage to the skin and eyes. Safe work practices include avoiding ignition sources and ensuring that all personnel are equipped with the proper protective equipment (PPE).

3.3.2 Storage

Methanol, Nitric Acid, and SCP storage are overly critical in ensuring safety for everyone. Highly flammable methanol has to be stored at 20°C in 300 series stainless steel alloy tanks and ventilated to prevent accumulation of oxygen vapors. Additionally, the use of proper electrical grounding and bonding is essential when storing methanol. Nitric acid also has similar storing requirements. It must be stored below 0°C in a tightly closed stainless steel container in a cool, dry, and well-ventilated location away from light. Our product SCP must be stored in an airtight bin with less than 10% of moisture to prevent spoilage. Our bacteria *Methylococcus capsulatus* must be stored in a freezer that is -80°C or lower.

3.3.3 Safety

Exposure to methanol can cause severe and sometimes acute toxic effects even from a single exposure. General symptoms can include irritation of eyes, skin, respiratory tract, dizziness, headaches, and vomiting. Even though methanol is poisonous, it is consumed unknowingly in trace amounts by humans in some foods and beverages. As a result, when handling methanol, it is best to wear the appropriate personal protective equipment to prevent contact with the skin and other organs. Nitric acid can also cause severe issues to the body if it ever encounters it. It is

recommended that in the workplace, chemical safety glasses should be always worn, splash protection shield, gloves, and a vapor respirator to further prevent any respiratory issues.

3.3.3.1 EPA, OSHA regulations and environmental impact

The Hazardous Air Pollutant (HAP) identifies methanol as being hazardous. It is dangerous to aquatic life in concentrations but can be biodegradable in soil and water very rapidly. Methanol is also listed in the US Toxic Substance Control Act but is only hazardous when it is above 5000lbs. The Occupational Safety and Health Administration (OSHA) has nitric acid exposure limit set to 5mg/m³, if there is exposure above that level then it causes serious health issues for life. Nitric Acid is also considered highly corrosive by the Center for Disease Control and Prevention (CDC). Our Single Cell Protein process gives off copious amounts of CO₂. According to OSHA, it is considered hazardous and 40,000 is considered dangerous to life. Our biomass and water that is given off from various equipment, can be used as fertilizer in the agricultural sector.

3.4 Uses

Single Cell Protein can be used in a variety of products and can also be used to make a variety of products. Some of those products include animal feed to fatten cattle, chicken, pigs, and fish. Pharmaceutical companies as well use SCP in supplements for hair and the face. We plan to make SCP that can be used in food additives such as vitamins and to enhance foods such as soups and ready-made meals.

3.5 Product specification

Single Cell Protein derived from a unicellular microorganism such as bacteria, yeast, fungi, and algae are a high protein content alternative to plant-based proteins for animal feed and aquaculture. According to the literature, SCP has the potential to replace approximately 50% of

AWKWARD

fish meals. The market for SCP is globally growing to meet the increasing demand. The utilization of bacteria to produce our SCP results in a minimum to 20% more protein content when compared to the other alternatives. With the processes selected for harvesting our cells, further concentrating them, extracting the protein from the cell biomass, and purifying it, the expected purity for our SCP is 99.9% in its final and solid-state with a plant operating with a capacity of 150,000 MT per year operating for 340 days.

4. Process selection

4.1 Market analysis and trends

Single Cell Protein production is vastly growing over the years and is expected to continue increasing. The Transparency Market Research (TMR) team stated that the market for SCP production is projected to cross US\$ 27.3 billion by the end of 2027. We also have a Compound Annual Growth Rate (CAGR) that provided the rate of return to be 9.3% annually and estimated global demand for SCP to be 600 million pounds per year.

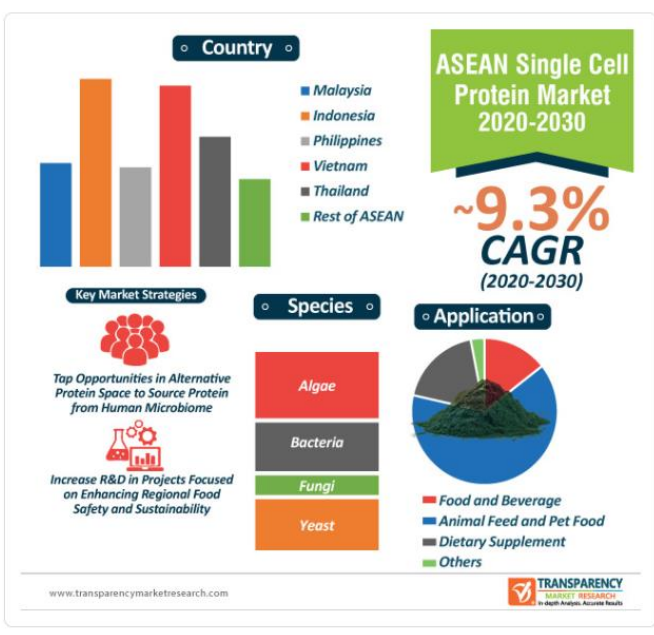


Figure 3. Compound Annual Growth Rate (CAGR) graphs

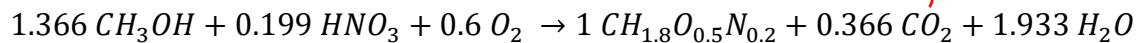
The above figure displays the CAGR of SCP's rate of return annually and the estimated global demand per year.

4.2 Reaction routes to producing the product

Awkward language

Even though Single Cell Protein can be extracted from different microorganisms, the reaction routes are similar for all of them because the products are the same for all reactions.

Below is the formula for production of SCP. As shown, the products are biomass where we extract protein from carbon dioxide and water. This process does not produce other reactions other than the products.



Really?

4.2.1 Industrial process and lab/patent routes have been reported to be used for producing Single-Cell Protein

Several patents for the production of SCP utilizing a methanotrophic bacteria is existent. U.S Patent 4,048,013, titled Process for producing single-cell protein from methanol using methylomonas sp. DSM 580, was established in 1976. The patent describes a process for preparing single cell protein from methanol. The process utilizes the bacteria Methylomonas sp. DSM 580 as the obligate methanol-assimilating bacterium for the extraction of single cell protein. Several companies like Cargill and Calysta have highly effective processes in place for producing high quality SCP from either methanol or methane.

4.2.2 Reaction route 1

The production of Single Cell Protein does not produce any side reactions.

Really?

4.3 Process screening by comparing the process economy of the reaction routes (the monetary difference between the value of the products and costs of the raw materials)

Reaction	1.366CH ₃ OH + 0.199HNO ₃ + 0.6O ₂ → CH _{1.8} O _{0.5} N _{0.2} + 0.366CO ₂ + 1.933H ₂ O					
lb.mol	1.366	0.199	0.6	1	0.366	1.933
Molecular weight	32	63	16	24.6	44	18
Lb.	32	63	16	24.6	44	18
\$/gal	50		0	402 each	0	0

4.4 Process comparison and selection

In order to achieve cost efficient single cell protein, the prices of each raw material needed for production have an extraordinarily strong impact. Since we are specifically producing single cell protein from our bacteria strand "*Methylococcus capsulatus*," that it will be affordable and worth the amount that will be given. From one of our sellers the American Type Culture Collection (ATCC) we are able to get the strand for \$402. The microorganism competitor to bacteria is yeast, in which with their most commonly used strand being the *Saccharomyces cerevisiae*, we would have been charged over \$140 more that could have gone to another area that needed more attention.

Our process specifically uses a batch reactor instead of a continuously stirred reactor or CSTR as our fermenter. This plays an important role in ensuring the purity of our production so that no contamination can be found. With the CSTR reactor, our process would continue to be running the contaminant through our equipment which we will as a result, we will need to stop each individual system in order to clean it out. This will take more time out of our scheduled production day and will cost us money that could have been made. All of the raw materials that was used in that contamination incident would have just gone to waste, and more labor work will have to be done for the cleaning process. However, with our batch reactor if a similar case was to occur, there would not be much stress. The batch reactor, like in its name, is only used to create one batch which allows us to clean and sterilize the reactor before the next production is set to

run. During this process, less raw materials will be wasted if there is contamination and will only be a minor setback.

phase review and revise

5. Process description

Many raw materials must be introduced into our bioreactor systems that will enable pH control, protein creation and aerobic cell growth of our choice of bacteria. The raw materials consist of methanol, nitric acid, and oxygen must be carefully prepared and stored in appropriate conditions to enhance maximum growth of cells and ensure safety. There will be storage tanks for nitric acid and methanol along with minerals, the design specification that are described in section 3.3.2. Air will be compressed and filtered before use of oxygen source for fermentation, which will require careful handling to avoid contamination and prepare the gas for inlet to the bioreactors. With the use of air instead of pure oxygen, a significant amount of nitrogen gas will be introduced into the system and will have vented for release to the atmosphere.

5.1 Process chemistry

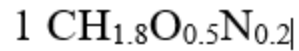
nothing else produced?!

Since there is only one reaction for the production of single cell protein, the following reaction occurs:



5.1.1 Reaction stoichiometry

The balanced single cell protein reaction (1) shows that for every mole of methanol, 1 mole of biomass along with carbon dioxide and water will be formed. This stoichiometric relationship can be shown below as:



5.1.2 Kinetics and rate equations

The Batch model constitutes a liquid phase in the bioreactor, where oxygen from compressed air is transferred from a gas to the liquid phase which is therefore sufficient to model the liquid phase. From this we were able to develop reactor designs for our process which are displayed below:

$$dN_x/dt = r_x \cdot V \text{ (Biomass)}$$

$$dN_s/dt = r_s \cdot V \text{ (Methanol)}$$

$$dN_o/dt = r_o \cdot V \text{ (Oxygen)}$$

$$dN_n/dt = r_n \cdot V \text{ (Nitrogen)}$$

use equation editor

5.2 Process (Block) flow diagram and process description

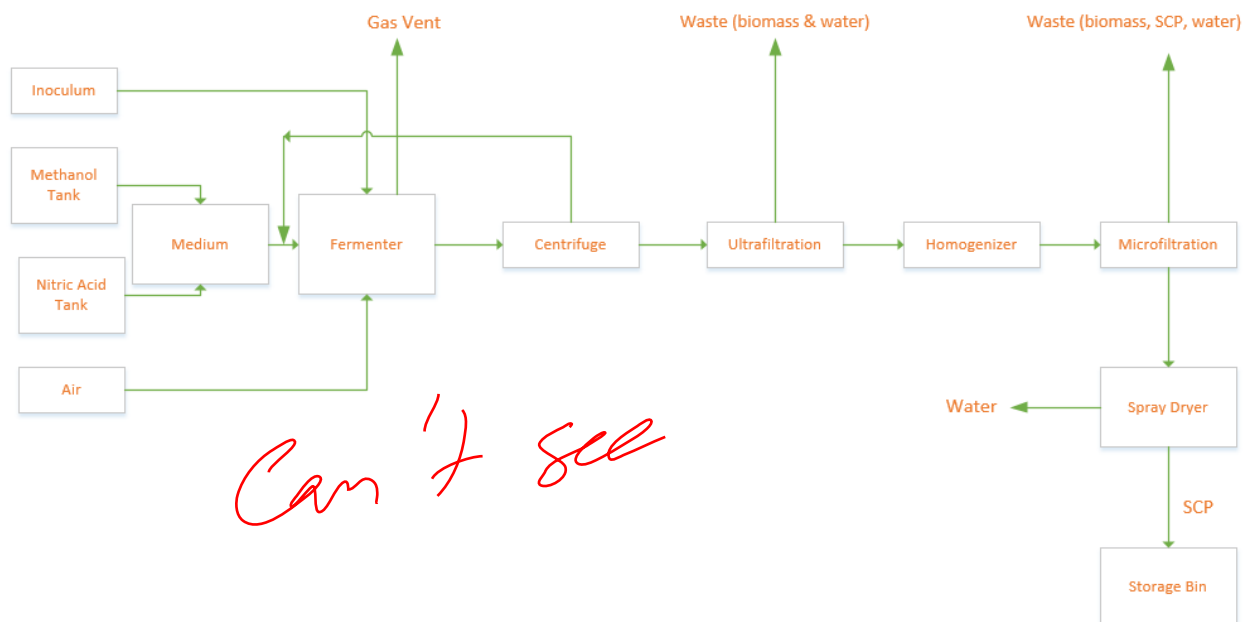


Figure 4. Block Flow Diagram for the production of Single Cell Protein

This block flow diagram gives a clear overview of the production of Single Cell Protein in a plant. In this block flow diagram, only the major units are represented in order to show the important process functions.

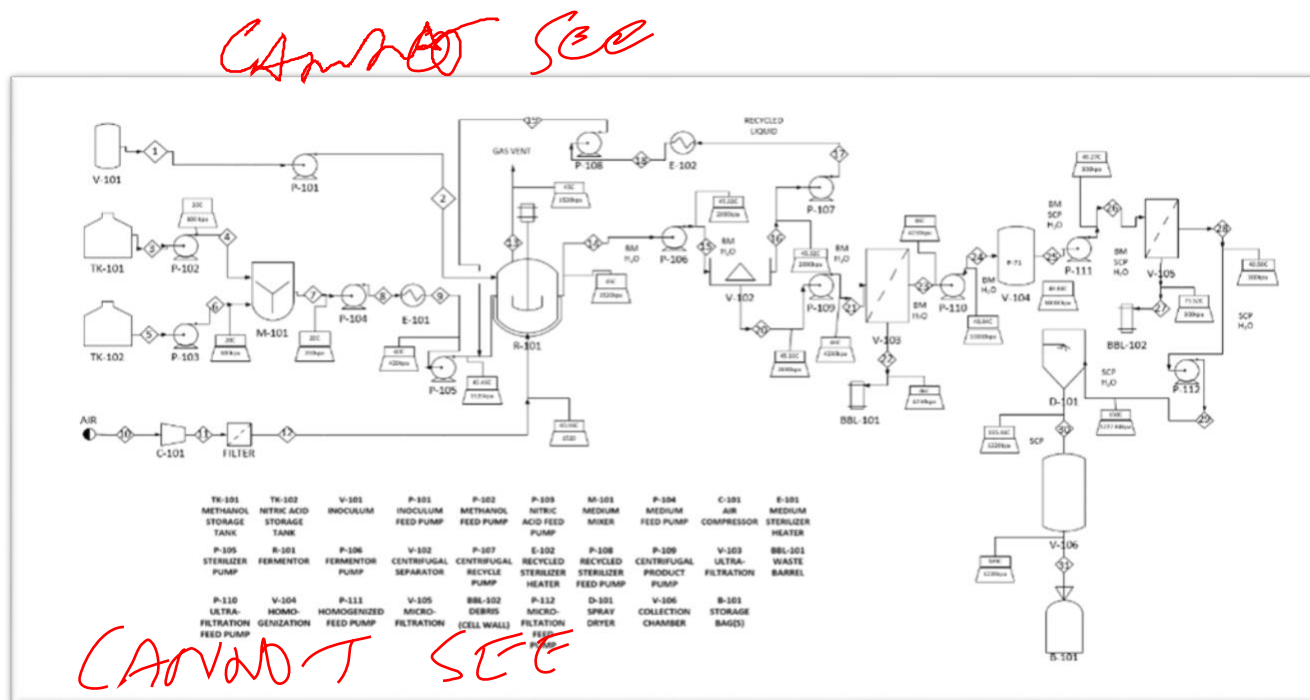


Figure 5. Process Flow Diagram for the Production of Single Cell Protein

For our process, we needed a medium that would contain our minerals such as magnesium, and phosphorus which are some of the essential minerals needed in protein. With our raw materials methanol and nitric acid, our oxygen, and inoculum all going into our batch fermenter, this is where the actual process begins. After being mixed, it is then sent to a centrifugal separator where the biomass is separated. The recycled liquid is ~~then recycled back to the fermenter to be used again in the process but will go through a sterilizer first before going back into the fermenter.~~ After separation, the biomass is then sent to an ultrafilter where it is then filtered more into our desired product, some of the biomass, and more water is given off as waste. Biomass is then sent to a

homogenizer; this is where the biomass is then lysed, and we get our SCP. Exiting the homogenizer, biomass, SCP, and water is pumped to a microfilter where the biomass and SCP are further filtered, and we are now left with our SCP. Unused biomass, SCP, and water are also given off from the microfiltration system as waste which can be used as fertilizer. Our SCP is then pumped to a spray dryer, where SCP is dried at 150°C. After it is dried, we have our desired product.

5.2.1 Raw material preparation

The raw materials that will be utilized in the production of single-cell protein require a source of carbon, nitrogen, and oxygen along with nutrients such as magnesium, phosphorus, and additional minerals required for production. Our choice of carbon source for production is methanol, as it is the main driving force for production when reacted with the bacteria *Methylococcus capsulatus* due to its high productivity. Typically, in the industry, most companies producing single-cell protein prefer using simple sugars such as glucose as their carbon source for production. However, for our process, methanol has proven to be even more successful in protein production using bacteria without any harmful outcomes and trials based on research. Our source of nitrogen will be an azeotropic mixture of Nitric acid and our Methanol will be sourced from Lab Alley in Austin, Texas.

5.2.2 Reaction and reactor operation

The process to produce Biomass from our bioreactors was carried out at a temperature of 45°C (113°F). Since our reaction is exothermic, a vast amount of heat will be released from the bioreactor, which will then be quenched by cooling water to maintain the quality of the effluent leaving the bioreactor for further purification and separation purposes to attain our desired product of SCP. For our process, we will use a Fed-Batch reactor instead of a continuous process.

The many reasons for using a fed-batch process focus on its multi-use capabilities when dealing with biological processes as well as quality control and waste reduction. Because our process requires a pre-prepared inoculation of bacterial cells before it is used within the reaction, it has the potential of causing contamination which would degrade the quality of our desired product or flooding within the vessel if too much feedstock is fed into the reactor, which would result in the cells being washed out. Batch processes mitigate this issue by allowing for scheduling of cleaning time periodically to maintain the quality of our product. The pressure of the reactor was around 2.5 bar (36.3 psia) with an increased air pressure of 10 bars (145 psia). The reactor is maintained at these conditions to improve cell-mass yield and specific growth rate of the Biomass produced. In the production of single-cell protein, there is no alternative catalysis involved in making our product, however, a metabolic catalytic reaction occurs within the reactor when the carbon, nitrogen, and oxygen source are introduced to the medium along with the inoculated cells. The fed-batch reactor is very efficient for microbial processes such as the production of SCP and has low operating costs. Stainless steel would serve as the ideal material component to build the reactor to avoid corrosion.

5.2.3 Separations

There are 4 main vessels for the separation processes occurring in the process. The first, V-102, represents the centrifugal separator. This equipment handles the concentrated biomass and water generated from the bioreactor. The concentrated biomass with some water is sent to V-103. V-103 represents our ultrafiltration unit with the primary function of further concentrating our biomass and eliminating more water from the process. This process occurs similarly to reverse osmosis, using hydrostatic pressure to force water through a semi-permeable membrane to retain solutes and suspended solutes of high molecular weight. V-104 is our homogenization unit that is

operated at high pressure to lyse the suspended solids of biomass to extract our desired product, SCP. V-105, Microfiltration separates the cell debris left from the biomass from our SCP product. The latter is then sent to D-101, our spray dryer to get the SCP in its final form before packaging.

5.2.4 Product to storage

Following the final processing step, SCP is sent from the spray dryer and divided into storage bags located in a safe, humidity-controlled building. The product is stored in this manner because any moisture higher than 10% can cause spoilage to the product. If this occurs, we would be unable to transport that batch of SCP to our clients.

6. Material & Energy Balances

The overall material balances for this process were done to determine the flow rates of all the feed components. We did this to ensure that we had the right amount of feed to produce our target flow rate. This also allowed us to know how much waste our process will be producing. The material balances were also done around each unit in our process including the fermenter, centrifuge, ultra and microfiltration, homogenizer, and spray dryer.

6.1.1 Basis of calculation

By analyzing the market, and looking into other plants that produce SCP, the annual growth rate indicates that the need for SCP will increase. Our goal was to produce 150,000 metric tons of SCP per year. The plant will be operating at 93% in a year which translates to a production run time of 8,160 hours (about 11 months) or 340 days during the year. The time that is set aside will be for maintenance and if any downturns may encounter. Based on how much SCP the plant needs to produce in an hour, the required feed was calculated, and the material balance was done around each unit.

6.1.2 Material Balance around each unit

Bioreactor

In the bioreactor, the feed streams from our inoculum, sparged oxygen and medium mixer which has our nitric acid, methanol, and minerals are combined. An illustration is displayed in Figure 6 below.

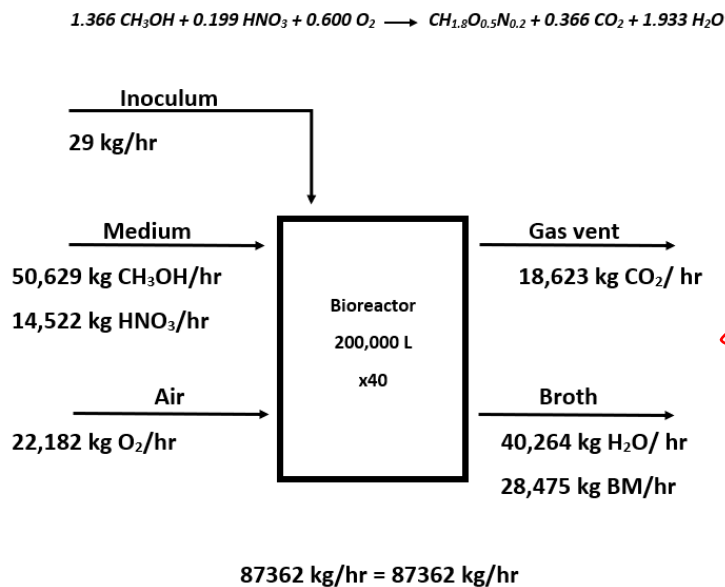


Figure 6. Bioreactor Material Balance

Centrifuge

The combined raw materials create a broth which contains biomass and water, that is then fed into a centrifuge to be separated. The flow rate of

6.1.3 Assumptions and use of heuristics

6.1.3 Overall material balance with process streams

6.2 Energy Balances

7. Discussion

8. Conclusions & recommendations

9. References

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BELOW AVERAGE
PROJECT REPORT

Plant Design of Production of Urea using Natural Gas

Prairie View A&M University

Roy G.Perry College of Engineering

Department of Chemical Engineering



Submitted By: Cherish Vaughn, Shumpert Kirksey, Meredith Meyer, Garred Essissima

Submitted To: Dr. L.L. Martin

Date: December 6, 2021

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Letter of Transmittal

December 8, 2021

Roy G. Perry College of Engineering-Chemical Engineering Department

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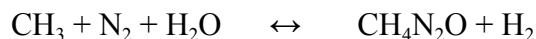
TO: Prof. L.L. Martin

FROM: Meredith Meyer, Cherish Vaughn, Garred Essissima, Shumpert Kirksey

RE: Simulation Case Study for the Design of a Urea Plant

In response to demand for Urea, a local manufacturing company is considering the addition of a urea plant. This company has asked our team to come up with preliminary designs for this addition. The sales department has estimated that they can sell 100,000 tons of urea per year looking at a price of \$.60/lb.

Urea will be made from natural gas, air, and water, via a synthesis reaction:



The natural gas, air and water are used to create ammonia and carbon dioxide using the Haber process. Ammonia is a highly corrosive chemical in the gaseous form, but this process uses the liquid form produced by the catalytically reacting hydrogen from natural gas and nitrogen. The reaction is accelerated with the use of an iron catalyst. We can expect near equilibrium conversions of ammonia and gaseous carbon dioxide to urea with a minimum temperature of 435K.

Please have your team do the preliminary energy and material balances for a urea plant, including the sizing of all heat exchangers. The sizing on reactors is not critical at the time being. The reactor temperature should not exceed 500K. The molar NH_3/CO_2 ratio in the reactors should be between 1.5:1 and 3.5:1. We have been informed that energy costs must be minimized, so please make every effort to make this an energy-efficient process. The members of Martin Team 7 are available to answer any questions regarding this report.

Best regards,

Cherish Vaughn, Meredith Meyer, Garred Essissima, Shumpert Kirksey

Make this shorter.
It should not provide details, only the major points.

Acknowledgements

We would like to express our deepest appreciation to individuals who assisted our team in completing Senior Design & Professional I. Thank you to our senior design professors, Dr. Lealon Martin and Dr. Emmanuel Dada for their constant and consistent support throughout this semester.

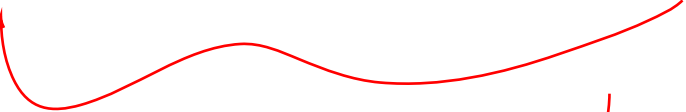
We would also like to thank the Prairie View A&M University Department Of Chemical Engineering Alumni and Industrial Advisory Council for their advice, future consideration, and encouragement given to us to help improve our project.

Project Summary

The objective of this project is to design a profitable urea plant using natural gas. A project's success and completion is dependent on several factors and criteria. A market analysis and knowledge of the urea production in the United States is essential to design a plan with an appropriate capacity to satisfy product demand.

Following the determination of the plant capacity, the production must be chosen by the economic indicator which determines if the process is feasible and efficient. The most sustainable production method will be selected. Material and energy calculations are conducted around each unit and the entire process.

Next, the selected production route and the calculated values are used to simulate the process through HYSYS Aspen. The simulation gives a visual presentation of the process feasibility in steady state conditions. The overall goal for the project was creating a practical urea plant after considering factors such as raw materials availability, economic feasibility and plant safety.


clean-up language.

1. Project Scope

1.1 Project Statement

Due to the increase in demand of urea globally, the fertilizer market, and wide ranges of applications, our team decided to develop a urea plant design using steam methane reforming (SMR) to produce synthetic ammonia. Synthetic ammonia will react with carbon dioxide to create urea. In our overall process, ninety eight percent of synthetic ammonia is produced by catalytic steam reformers. Hydrogen is the lightest element on the periodic table and the most abundant substance in the universe. Natural gas is a feedstock primarily because it decreases air pollutants and greenhouse gas emission. Hydrogen is a clean energy source which only generates water and heat as co-products. Our plant will operate at a production capacity of 100,000 tons of urea and this will be produced three hundred and fifty days a year.

Our product will be sold to fertilizer makers or directly used as ammonia nitrate and monoammonia or diammonia phosphates which are raw materials in polymeric resins, explosives, and nitric acid (1). Natural gas is reduced to carbon and hydrogen which is purified by nitrogen to make synthetic ammonia. The chemicals that are produced as by-products in the steam reforming process include hydrogen sulfide (found in natural gas), carbon monoxide and water. Our team will research how to provide proper handling, safety, and storage which will be explained further in the report. We decided to locate our plant in Louisiana due to natural gas pipelines and fresh water access.

1.2 Client Identification and Recognition Of Need

The demand for urea is projected to continue to increase to 800 million tons by 2021, the agriculture market plays an important role in (Good 2021). Our team plans to meet 5% percent of this demand , therefore our production capacity was estimated to be 100,000 tons of urea. The global market for granular urea is expected to reach 2600 tons due to the large production in India and China. The United States imports more urea than produce due to the weather conditions in Louisiana. Our customer base is the agriculture industry and targeted consumers are National Fertilizers, Neuchem and Yara.

We are focusing on selling our product to the companies stated above as the development of urea increases. Our determination and communication of urea plant production has on the environment and the agriculture industry provides a profitable selling point in the Louisiana area.

1.3 Project Goals and Objectives

The goal of this project is to design a urea plant that produces 100,000 metric tons.

Objective / Deliverables

1. Create a process flow diagram (PFD) of the plant
2. Provide a detailed process description with safety considerations for chemicals used
3. Perform material and energy balances of overall process and around each unit of major equipment
4. Obtain a converged simplified Aspen HYSYS simulation of the process.
5. Present a final presentation and complete a final report detailing our project progress.

Good. You have customers.
Focus this around design activities. For example you determined plant capacity

1.4 Contemporary Issues and Impact of Project on Society

1.4.1 Contemporary Issues Relevant to Project

Urea is a synthetic nitrogen fertilizer that helps grow fresh produce to feed a large portion of the world's population. Its production requires a complex reaction between ammonia and carbon dioxide. Approximately eighty percent of all ammonia globally is used to produce urea. The Haber-Bosch process, the process that produces ammonia, requires high temperature and pressure. The production of urea consumes a great amount of energy. It also discharges the most carbon dioxide of all industrial chemical reactions due to its fossil fuel feedstock of natural gas. (Patel 2020)

1.4.2 Potential Impact of Project on Society

Nitrogen fertilizers are essential for agriculture and necessary for food production around the world. When crops grow, they remove nutrients from the soil. The limiting nutrient in soil is nitrogen, and N-fertilizers are important because they help replenish the lost nutrients. Without them, food production would only be able to support an estimated 50% of the world's population. N-fertilizers, such as urea, provide food security for the globe. (Driver, et al. 2019)

1.5 Project Constraints

For this project, there were numerous challenges. Information on process operating parameters is scarce regarding urea production. From literature review, it was difficult to obtain temperatures and pressures for equipment that were consistent. The operating parameters varied by equipment size and feed flow rate. Another constraint was that our reactor could not exceed 500K.

2. Project Planning and Task Identification

2.1 Task Identification

To complete semester project, we divided our project into phases three which are shown below:

1. Phase 1- Lecture Search and Process Selection
2. Phase 2- Project Design & PFD
3. Phase 3 - Report

2.2 Timelines

Each phase has a subset task with assigned deadlines.

1.Phase 1- Lecture Search and Process Selection (9/11/21-10/2/2021: 21days)

A) Complete preliminary in depth research on the product

- i) Research process methods and alternatives process to gain understanding over project

B) Create an problem statement & design brief

- i) Introduce the project and its purpose, constraints/limitations & design parameters

C) Provide an economic indicator & pick the final process

- i) Evaluate the best production routes and pick the most profitable design

D) Identify the client & demand of the product

- i) Determine the demand of our chemical plant & find plant capacity

2. Phase 2 -Process Design (10/9/2021-11/19/21: 41 days)

A) Design a block flow diagram (BFD) of the production of process

- i) Provide an simple drawing of the process to understand each major equipment
- ii) Identify inputs, outputs and recycle streams

B) Design a process Flow Diagram (PFD) of the production of process

- i) Determine process layout for flow streams and equipment.

C) Perform material and energy calculations for the complete process

- i) Determine how much material is coming and leaving the system
- ii) Energy balance determines the temperature and heat coming out of major equipments

D) Determine process safety considerations

- i) Ensure proper safety, storage, and handling of chemical used in our process

3. Phase -Reporting (11-19/21-12/6/21: 18 days)

A) Homework assignments

- i) Test knowledge on concepts taught in class

B) Final end of semester presentation

- i) Showcase understanding of process

C) Final Report

- i) Detail summary of the overview of project and accomplishments

2.3 Gantt Chart

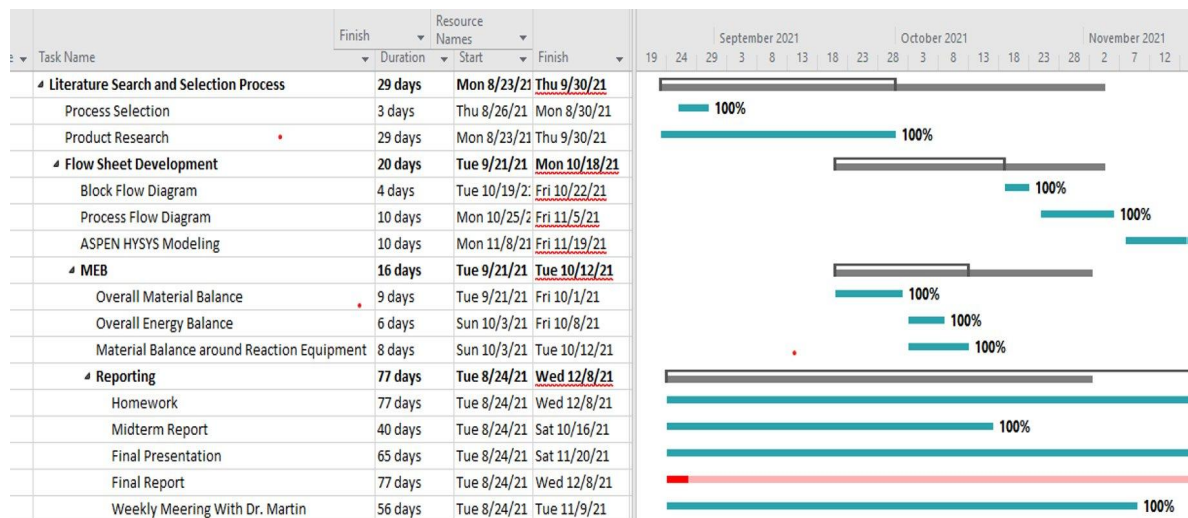


Figure 1: Gantt Chart (Semester I)

3. Overview of Manufacturing Urea using natural gas

Citation missing.

Urea is a low cost fertilizer with the highest nitrogen concentration. Urea production is a two step process, where ammonia and carbon dioxide are reacted to form ammonia carbamate

which is dehydrated to form urea. The urea solution is evaporated into a priller to form pure granules. Ammonia can be produced from many fossil fuels (natural gas and fuel gas) or even renewable resources(eg, biomass and biomass gasification).Natural gas is synthesized in the ammonia/ urea production which requires maximum H₂ production. The most common synthesis gas production is steam reforming, partial oxidation, and autothermal reforming. In the overall process we pick steam reforming due lower energy consumption and cost. All techniques has offer valuable results in product urea, however production via steam reforming is widely favored in the chemical industry,

3.1 Routes of Production

Producing urea from natural gas is a complex process. The first portion of the process produces hydrogen. Hydrogen can be produced by steam reformation, partial oxidation, and autothermal reformation. All the processes utilize natural gas as the primary feedstock, but they differ in secondary feedstock. Steam reformation uses steam as the secondary feed. Partial oxidation uses oxygen as the secondary feed. Autothermal reformation uses both steam and oxygen as secondary feed stocks. The next step in the process is ammonia production. Ammonia can be produced using the Haber-Bosch process, indirect electrochemical synthesis processes, and membrane reactors. The last step in the process is urea production. Technologies for urea production include Kansai Mitsubishi Carbon Dioxide Recovery Process (KM CDR Process ®), Stamicarbon process, and Snamprogetti process.

3.2 Physical and Chemical Properties

Urea appears to be light brown or yellow odorless and crystallized solid. Hydrogen is nontoxic, nonmetallic, nontonic, tasteless, odorless, colorless and highly combustible gas that can be found almost anywhere in the world in the form of chemical compounds. Tables 2 and 3 will show the chemical and physical properties of urea. Hydrogen gas is the byproduct of the production of ammonia and will be properly handled.

Table 1: Physical Properties of Urea

Color	White crystals or pellets
Phase	Melting point of 407°K
Odor	Odorless

Taste	Cooling, saline taste
Density	1.32 g/cm ³
Solubility	Soluble in water ethanol and ammonia

Table 2: Chemical Properties of Urea

Chemical Formula	NH ₂ CONH ₂
Oxidation	Decomposition of urea by strong oxidants When heated to decomposition it emits toxic fumes of nitrogen oxides
Reactivity	Oxalic acid and urea react at high temperatures to form toxic and flammable ammonia and carbon monoxide gases, and inert CO ₂ gas.
Flammability	non flammable
Combustion	Urea decomposes to ammonia and isocyanic acid, the latter leading to biuret, cyanuric acid and ammeline formation

3.3 Handling, Storage and Safety

When operating at a chemical plant, it is very important to have a deep understanding of how chemical species within the process should be handled in order to operate safely and efficiently.

3.3.1 Handling

When handling urea provide a well ventilated area and do not smoke and eat when handling the product. In the steam reformation process hydrogen will be handled, do not smoke where hydrogen is generated or being used. Remove all possible sources of flame and sparks. Hydrogen should be generated and used in well ventilated areas. Precautions must be taken to remove all positives or fire explosives (Hydrogen Data Sheet).

Crossin)
units!!

3.3.2 Storage

Urea can be stored at ambient temperatures and stable at normal conditions. Hydrogen can be stored as either gas or liquid. Storage as gas typically requires high pressure tanks 5,000-10,000 psia tank pressure. Storage of hydrogen as liquid requires cryogenic temperatures because the boiling point of hydrogen at atmospheric pressure is -252.8°C. (Hydrogen Storage).

In the SMR process H₂ gas needs to be properly handled and stored properly to carry out a safe process. Table 4 shows a list of major by-products that are carried in the process.

Table 3: Handling and Storage for Major Chemicals in Urea

Species	Phase	Handling	Storage
H ₂	Gas	Keep away from heat, sparks, and open flame. Use only spark-proof tools explosion-proof equipment	Store with adequate ventilation. Store where temperature will not exceed 125°F
CO ₂	Gas	Avoid breathing gas Do not get in eyes, on skin, or on clothing. Ventilate space before entry. Verify sufficient oxygen concentration	Store away from directed sunlight in a dry, cool, and well ventilated area away from incompatible material and ignition sources
CO	Gas	Do not get contact with eyes or skin. Use only in adequate ventilation Do not breathe gas and only use non-sparking tool	Store away from directed sunlight in a dry, cool and well ventilated area, away from incompatible material and ignition sources

Table 4: Safety Hydrogen Gas Hazardous,First Aid & Prevention

Hazard Statements	Fire/Accidental Release Measures	Prevention Controls	First Aid
● Extremely flammable gas. ● Contains gas under pressure may explode if heated ● May displace oxygen and cause rapid suffocation ● Burns with invisible flame	● If involved in fire, shut of completely ● Fight fire from protected location ● Wear respirator when ventilation is not available ● Keep necessary PPE when entering	● Engineering controls keep the gas, vapor or dust concentrations below any lower explosive limits ● Emissions from ventilation should be checked or work process equipment should be checked to ensure they meet requirements of environmental protection legislation.	● Eye Contact- Immediately flush with plenty of water ● Inhalation- If too dangerous to give mouth-to-mouth resuscitation. Get medical attention ● Skin contact- To avoid risk of static discharge and gas ignition soak contaminated clothing with water

3.3.4 EPA , OSHA Regulations and Environmental Impact

During the steam methane reformation process, large amounts of CO₂ are co-produced and small amounts of hydrogen emissions escape the plant which increases global warming. OSHA states that atmosphere with greater than 10% of lower flammability is immediately dangerous to health and life and entry is not allowed (OSHA, 2016). In the urea process, ammonia gas and carbon dioxide are flared out into the environment.

Due to hydrogen being lighter than air which makes it difficult to recognize. Hydrogen as low minimum ignition energy, it can ignite with any small ignition source. OSHA recommends hydrogen storage tanks to be permanently labeled. OSHA also states the venting piping must be designed so that “moisture cannot collect or freeze in a manner which would interface with propeller operation of the device” (OSHA Part 1910). Urea is

As environmentally stable, hydrogen will be stored in ventailed areas. Any effect on animals would be related to an oxygen deficient environment.

3.4 Uses

Urea product is primarily used in the fertilizing industry which has wide ranges of applications. Some of the applications include feedstock, glue and commercial products. Urea fertilizer has a high nitrogen concentration which promotes faster growth to plant life .

3.5 Product Specifications

Our urea product is analysed for its concentration and granule size. Our urea product is checked for; moisture, biuret, formaldehyde, and pH. We make these checks to make sure our product meets customer standards.

Table 3: Urea Specification Table 3

Components	Concentration
Nitrogen	46% Minimum by weight
Biuret	1% by weight
Moisture content	0.3 Maximum by weight
Sizing	2-4mm by weight
pH	3.6 to 7.2

How is this determined?

4.Process Selection

4.1 Market Analysis and Trends

In recent forecasts, the market for urea is to have an upward trend, especially in the agriculture sector. The trend is driven by an increased demand in nitrogen fertilizers, population increase, feedstock availability for urea production, and low prices. From 2020-2026, the urea market is expected to have an increasing compound annual growth rate of 2.2%. The mass equivalent of this CAGR is approximately a 233 million ton increase in urea demand.

4.2 Reaction Routes to Producing Product

4.3 Process Screening by Comparing the Process Economy of the Reaction Routes

Table 4: Theoretical Profit Indicator

	CH ₄	+ N ₂	+ H ₂ O	= H ₂	NH ₂ CONH ₂
	1	1	11	1	1
MW	16	28	18	2	60
lb	16	28	18	2	60
/lburea	.27	.46	.3	.03	1
\$/lb	.08	0	0	1.08	.59

Gross Profit:

Selling hydrogen: $.59 + .03(1.08) - .27(.08) = .60$ \$/lb of Urea

Without selling hydrogen: $.59 + .27(.08) = .56$ \$/lb of Urea

4.4 Process Selection

Due to scarcity of information for alternative urea production methods, a conventional method of urea production was chosen. The conventional method used for each process is:

- Hydrogen – Steam Reformation
- Ammonia Synthesis – Haber-Bosch process
- Urea Synthesis – Stamicarbon process

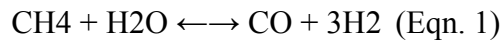
These methods were used in the creation of Figure 5 and Figure 6.

5. Process Description

5.1 Process Chemistry

For the production of urea from natural gas, methane undergoes steam reformation to produce hydrogen (H₂) and carbon monoxide (CO) (Eqn. 1). The carbon monoxide is then reacted with steam to produce more H₂ and carbon dioxide (CO₂), which is sent to the urea synthesis portion (Eqn. 2). CO₂ is removed, and the remaining H₂ is reacted with nitrogen (N₂) taken from the atmosphere to produce ammonia (NH₃) using the

Haber-Bosch process. The NH_3 and redirected CO_2 react to form ammonium carbamate ($\text{H}_2\text{NCOONH}_4$) (Eqn. 4). The ammonium carbamate then forms urea (NH_2CONH_2) and water (H_2O) (Eqn. 5).



Fix equation.

Write a better overview description

5.2 Process (Block) Flow Diagram & Process Description

The figure below represents the block flow diagram (BFD) of our plant process for the production of urea via steam methane reforming. There are six main sections in the production of ammonia which are the steam reforming section where high temperature steam reacts with natural gas, the high temperature water-gas shift (WGS) reaction that improves the yield of our hydrogen product, the CO_2 remover (carbon capture) and ammonia synthesis reactor process that separates our final product (ammonia). Figure 6 will show how carbon dioxide reacts with ammonia to create liquid urea (ammonia carbamate) which is dehydrated to produce liquid urea. The urea solution is evaporated and separated to produce granules urea.

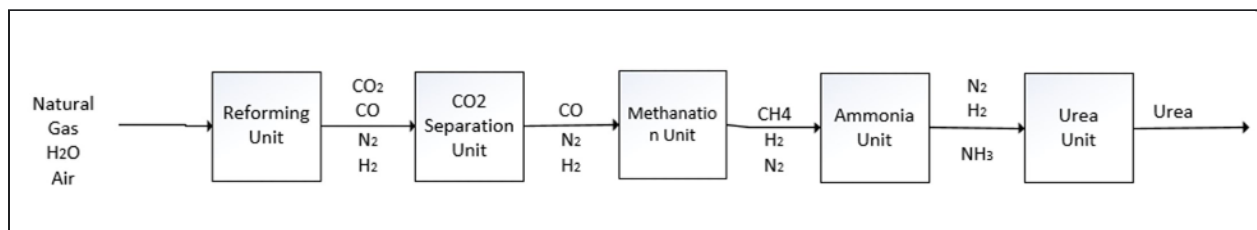


Figure 5: Block Flow Diagram

Figure 5 & 6 shows our process flow diagram (PFD) which gives a detailed layout of our production process including the selection equipment for our unit operations.

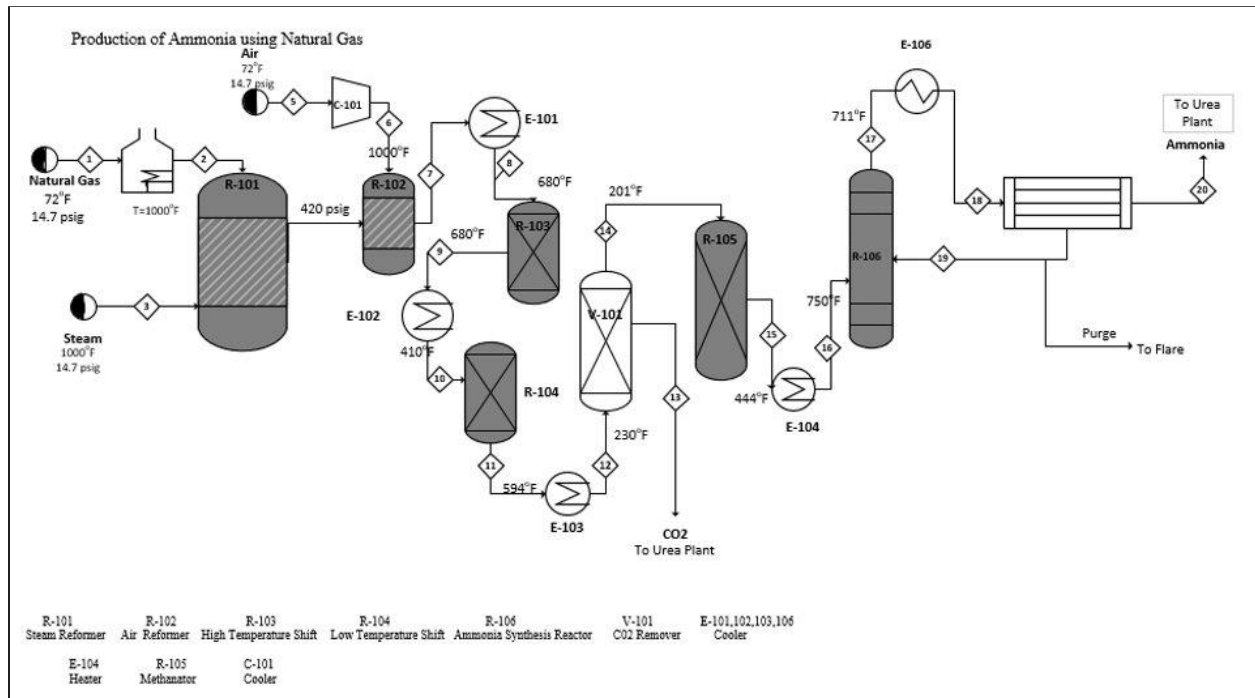


Figure 6: Production of Ammonia using Natural Gas (PFD)

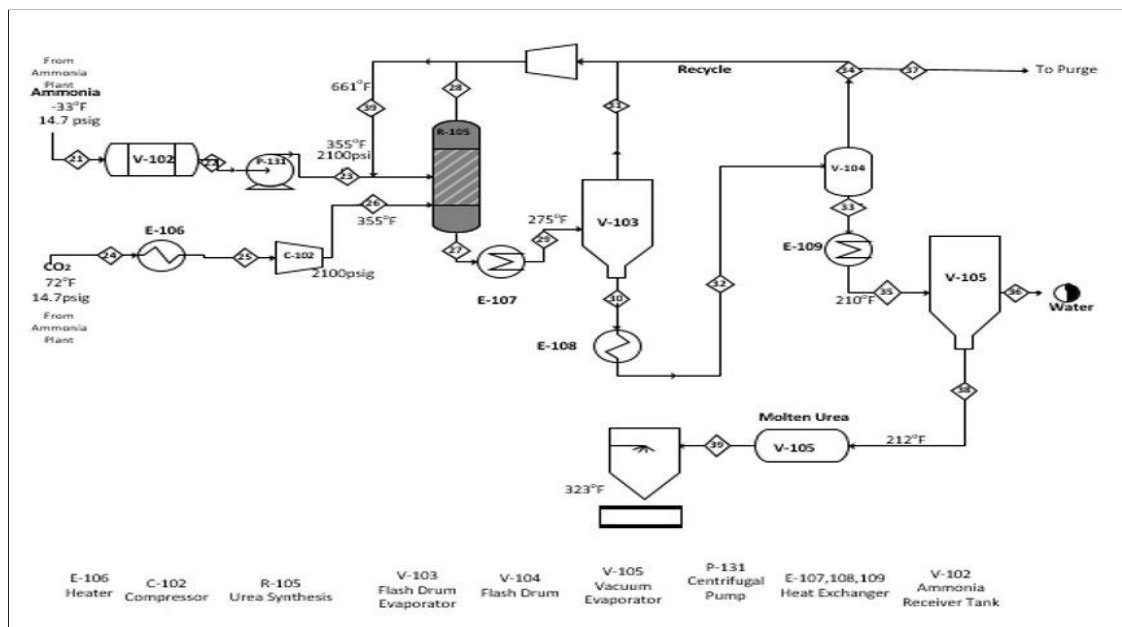


Figure 7: Production of Urea (PFD)

Reference the unit names in the text.

5.2.1 Raw Material Preparation

The two raw materials involved in the production of urea are natural gas whose main component is methane, and superheated steam. During the raw material preparation sour gas is passed through a desulfurization unit to remove hydrogen sulfide from natural gas. In the urea process we have carbon dioxide compressed with ammonia being pumped into the urea synthesis reactor. In both raw material preparations they operate at high temperatures and with iron based catalysts. The figure below shows the inlet temperature of steam reformation and urea process.

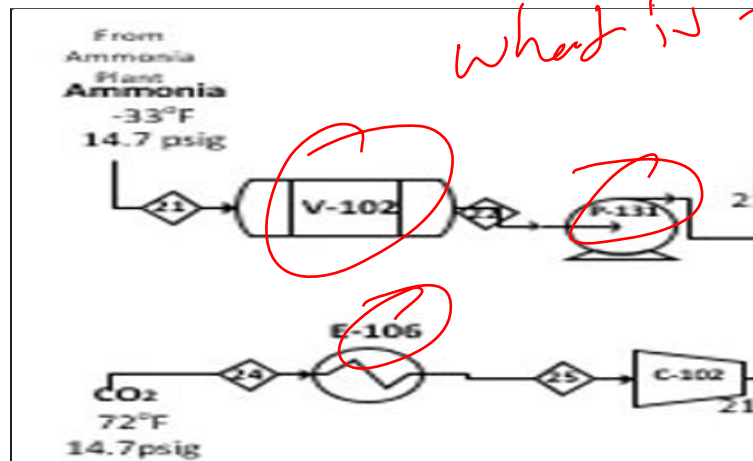


Figure 8: Process Flow Diagram for Raw Material Preparation

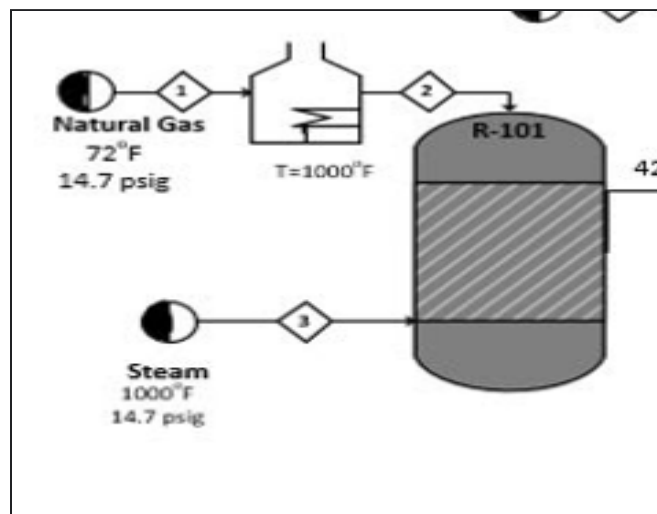


Figure 9: Process Flow Diagram for Raw Material Preparation

5.5.2 Reaction and Reactor Operation

The three major reactions in the plan design occur at urea synthesis, ammonia synthesis and methane reformer reactor. We have a total of five reactors in the overall process

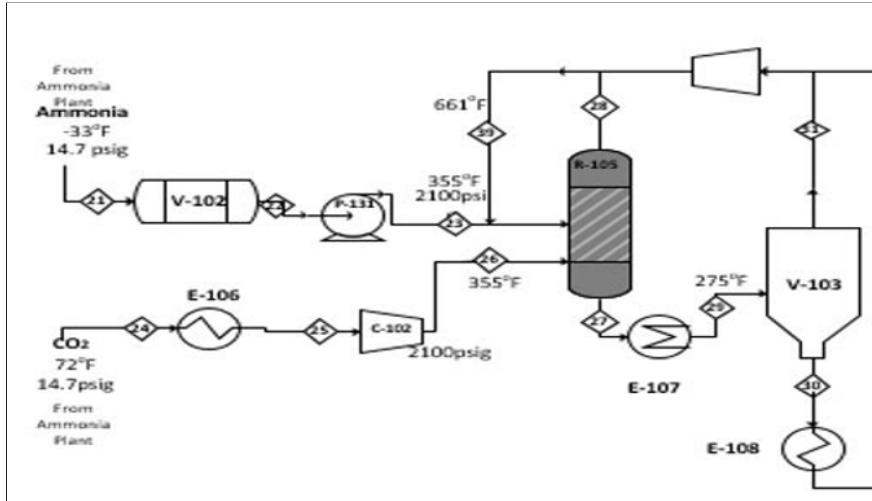


Figure 10: Process Flow Diagram for the Urea Synthesis Reactor and Vacuum Evaporator

Ammonia is inserted into a compressor and pump and CO₂ goes into a heat exchanger and reacts with urea synthesis with zinc oxide. The temperature is heated up to react in the reactor at 661°F. Then urea liquid undergoes a vacuum evaporator to separate the urea liquids and waste products which are flared and recycled back to the raw materials. This process dehydrates the liquid urea to its purity. Which produces 96.8 % pure urea which is prilled to granules.

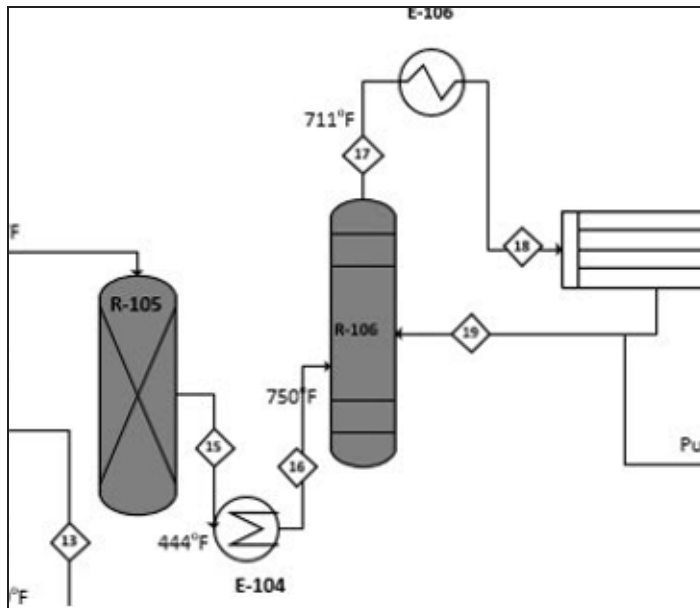


Figure 11: Process Flow Diagram for the Ammonia Synthesis Reactor

The figure above shows an ammonia synthesis reactor, which has a temperature of 750°F. Ammonia synthesis reactions with nitrogen and hydrogen. The by-products of this reactor is hydrogen which will be sold in the market with urea .

5.2.3 Separations

The separation stage goal is to isolate the off gases (NH_3 and CO_2), so it can be recycled back in the process. A flash drum separator removes all off gases and any poisons from the reaction. Biuret is impurity in urea fertilizer caused by a side reaction, which has a huge effect on plant growth. Figure 11 shows a diagram showing the separator.

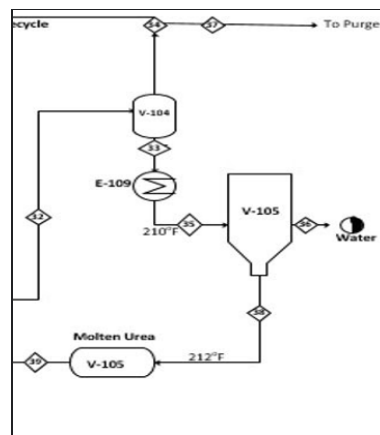


Figure 12: Process flow diagram for Separation Operations

5.2.4 Production to Storage

The final step in our plant process of urea is inserting the hot liquid urea in a prill tower. Air is sucked out the bottom heated and blown to the shaft of the tower. As the fertilizer falls down the shaft it dries and solidifies to form granules which are directed by conveyor belts to be packaged and shipped.

Where are your material
balances
and energy
around each unit??

Not bad - Need to include
missing information.

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ASSIGNMENTS FOR OUTCOME 2

Ability to apply engineering design to produce solutions that meet specified needs with consideration of public health, safety, and welfare, as well as global, cultural, social, environmental, and economic factors.

**CHEMICAL ENGINEERING DEPARTMENT
OUTCOMES SPECIFIC ASSIGNMENT COVER SHEET
SENIOR DESIGN & PROFESSIONALISM II
SPRING 2022**

Instructor: Dr. Emmanuel A. Dada

Title of Assignment

Final Project Report

Outcome Measured Using this Assignment

Outcome 2

An ability to apply engineering design to produce solutions that meet specified needs with consideration of public health, safety, and welfare, as well as global, cultural, social, environmental, and economic factor.

Check the engineering design characteristics related to this assignment

X	Involves identifying the specific needs to be met by defining/understanding the problem and developing plans for the project to satisfy the need
X	Involves conducting a review of the literature and performing preliminary design by generating alternative ideas/solutions and applying creativity
X	Involves performing detailed engineering design leading to specification and fabrication/selection of components for system being designed.
X	Involves consideration of one or more of the following (Please check those involved in this assignment.)
	Public health
X	Safety and welfare
X	Global factors
	Cultural factors
	Social factors
X	Environmental factors
X	Economic factors

Brief justification of why this assignment is suitable for this outcome

Information provided is a portion of the final project report that demonstrates students ability to communicate through formal technical report writing, and the rubric used to score this outcome for one of the groups

End of Semester Project Report Format

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1. Letter of Transmittal

The letter of transmittal captures the main points in in the EXECUTIVE SUMMARY.

(i) It clearly spells out why the report has been prepared.

(ii) Essential results, conclusions and recommendations are presented

See your College of Engineering Senior Design Manual for an example.

2. The EXECUTIVE SUMMARY

Your Executive Summary is a carefully distilled form of your complete design report and should have the following components:.

- (a) It should clearly state the need for the design and its objectives
- (b) It should clearly summarize what was done and main findings (process and production capacity, plant location and plant design and capital cost estimates, the capital investment , return on investment including, discounted cash flow internal rate of return, payback period etc)
- (c) How the final results were obtained
- (d) Clearly presented conclusions and recommendations.

Design Constraints and Design Basis

External constraints:

- 1. Physical laws
- 2. Standards and codes
- 3. Economic
- 4. Government and safety regulations
- 5. Resources

Internal constraints:

- 1. Choice of process
- 2. Process conditions
- 3. Materials and equipment
- 4. Time (for completion of design)
- 5. Personnel

Setting the Design Basis

- 1. Production rate
- 2. Purity specifications of the main product
- 3. The system of units to be used
- 4. The national, local, or company design codes that must be followed
- 5. Details of raw materials that are available

6. Information on potential sites where the plant might be located, including climate data, seismic conditions, and infrastructure availability
7. Information on the conditions, availability, and price of utility services such as fuel gas, steam, cooling water, process air, process water, and electricity that will be needed to run the process

The grading rubrics for evaluation of the Senior Design II projects CHEG 4248 (a continuation of the the fall 2021 Senior Design I CHEG 4247) are presented below. The students are to be evaluated as outlined in the rubrics with emphasis on the following:

-
- Justification of plant location and capacity
 - Provide a process description and Process Flow Diagram (PFD) for the plant showing the major items of equipment, and indicating the materials of construction and the operating temperatures and pressures
 - Material and energy balances with summary table for the process with streams information showing a mass balance for each major equipment
 - A complete HYSYS/ASPEN simulation report of the process
 - Chemical engineering design of major equipment such as (i) reactor(s), (ii) absorption column(s) and (iii) distillation columns
 - Estimates of the Major Equipment Capital Cost (Capex)
 - Estimates of Operating Cost (Opex)
 - Preparation of a net present value and investor's rate of return analysis for the investment over a 15-year life, assuming the company's current capital hurdle rate is 15%.
 - Preparation of a project milestone schedule
 - Preparation of a P&ID for a section of the process showing the control scheme to ensure safe operation of the unit, and carrying out a HAZOP analysis of the section of the process selected
 - Preparation of a safety report indicating the safety measures required for the plant bearing in mind any toxic and flammable materials handled

In addition, the names of the presenters for each design project have been included in the rubrics to enable each presenter to be evaluated as well.

References:

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**DEPARTMENT OF CHEMICAL ENGINEERING
SENIOR DESIGN & PROFESSIONALISM II CHEG 4248
COURSE ASSESSMENT GRADING & OUTCOME
ASSESSMENT SHEET FOR SPRING 2022 SEMESTER**

ABET Student Learning Outcome 2: An ability to apply engineering design to produce solutions that meet specified needs with consideration of public health, safety, and welfare, as well as global, cultural, social, environmental, and economic factor.

Assignments that test competency in this area will include problems testing students' understanding of the design process involving *devising a system, component, or process to meet desired needs and specifications within constraints, through an iterative, creative, decision-making process in which the basic sciences, mathematics, and engineering sciences are applied to convert resources into solutions.*

Name: _____

Title of Assignment: _____ Due Date _____

Competency Area	Points Assigned	Points Received
1. Ability to Define/Understand the Problem and then Plan the Project	60	
(i) Identify the customer and the needs.	8	
(ii) Identify and list the design objectives.	8	
(i) Identify the design constraints.	4	
(ii) Define the design strategy and methodology.	4	
(iii) Identify and break down work into tasks and subtasks and identify the personnel and deliverables for each.	20	
(iv) Develop a Gantt chart and critical path analysis for managing the project.	8	
(v) Establish major milestones for tracking progress and define performance metrics to measure success	8	
2. Ability to Conduct a Review of the Literature	80	
(i) Identify the types of information needed for a complete understanding of all aspects of the project (Based on task described in the project planning).	20	
(ii) Gather information on relevant fundamentals, theory / concept (demonstrate technical competence) and relate them to the design.	40	
(iii) Provide the sources in a list of references properly cited in the literature review section and relevant sections of the report.	20	
3. Ability to perform preliminary design by generation of ideas and applying creativity through generation of ideas and evaluation of candidate solutions	60	
(i) Perform process design and analysis with design constraints; Sorting/screening of process technology alternatives based on availability and cost of raw materials, reaction selectivity and yield, thermodynamic barriers to separating undesired components, and safety and operability	40	
(ii) Evaluate candidate solutions to arrive at feasible designs	20	
4. Ability to Perform Preliminary and Detailed Design	200	
(i) Prepare a process flow diagram (PFD) and present a detailed description of the process indicating the functions of the major equipment components and controls, stream connectivity, safety, and other	20	

technical matters of importance		
(ii) Carry out a HYSYS/ASPEN simulation of the process showing a converged HYSYS/ASPEN model of the process. State assumptions/parameters used in modeling major equipment	20	
(ii) Prepare a chemical engineering design of (i) reactor(s), (ii) absorption column(s) and (ii) product distillation units, stating the materials of construction and the operating temperatures and pressures	60	
(iii) Prepare mechanical engineering design of the reactor(s) and distillation columns with appropriate dimensioned sketches	20	
(iii) Identify applicable codes and standards for the chemical and mechanical engineering designs. Indicate assumptions made and their justification, and support calculations should be in consistent units; either English Units or SI. Indicate possible sources of error	20	
(iv) Economic Evaluation: Estimate capital costs including engineering, materials, installation, interest, return on investment, taxes and contingency. Total unit conversion cost of product, a sensitivity study on the price of the raw material, and the economic methods used should be included	30	
(v) Prepare a control scheme to ensure safe operation of the plant and carry out Safety Reviews; Hazards, operability and inherent safe (including the use of Safety Data Sheets submitted in the Appendix) or HAZOP analysis	30	
Total	400	

INSERT SAMPLE STUDENT FINAL PROJECT REPORT

THE PRODUCTION OF DIMETHYL ETHER

Taylon Owens

Amiya Rogers

Cinthia Sahin

Laura Ukpede

87%

Senior Design Report

Spring 2022

Department of Chemical Engineering

Prairie View A&M University

Faculty Advisor: Dr. Emanuel Dada, Prairie View A&M University

May 3, 2022

Letter of Transmittal

May 3, 2022

Department of Chemical Engineering
Prairie View A&M University
100 University Dr,
Prairie View, TX 77446

Dear Dr. Dada,

As it pertains to our senior design problem statement, we have successfully completed our analysis of the production of dimethyl ether (DME) comes through the dehydration of methanol. We conclude that this method is a more efficient way to produce dimethyl ether versus the other alternatives that were evaluated. The project has the goal of producing 50,000 metric tons per year from a plant that will be based in Plaquemine, Louisiana. This is achieved by sourcing methanol at a relatively subsidized price and using efficient processes to produce DME at a purity level of over 90%. The high quality of DME produced, and the incorporation of a recycling stream and wastewater treatment for other uses means that the process has been determined to not only be economically viable, but also environmentally sustainable.

The report presented here thus expounds on the processes that were undertaken to complete the project objectives in coherence with the realized problem statement. In this regard, the report defines the project's scope and then details how it was planned and the delegation of tasks. The report also contains a literature review section which expounds on previous work that has been done in the production of DME, and how this work presented relevant resources and reference points for the completion of the project. Other sections of the report include process selection and description, the relevant energy and material balances for the chosen process, a discussion of how the process was completed, and finally recommendations for the production of DME in the future.

Four team members were involved in carrying out various tasks to complete the project's objectives. These members are Taylon Owens, Amiya Rogers, Cinthia Sahin and Laura Ukpede. Throughout the course of the project, ~~the~~ team leader, Taylon Owens, assigned specific roles to team members and coordinated each member's efforts to ensure that deliverables were completed within the stipulated timeframe. The estimated overall profit were \$23MM with a 22% return on investment. Consequently, all the project's goals were realized within the given time of eleven (11) weeks. The processes undertaken to accomplish this are thus elaborated in the succeeding report.

OLC

Taylon Owens

Amiya Rogers

Cinthia Sahin

Laura Ukpede

Abstract

The Production of 50,000 metric ton dimethyl ether (DME) was designed by using the dehydration method of methanol. Methanol is fed into a recycle stream and is fed into a reactor where dehydration occurs and produces DME and water. Once this is done, the existing stream is fed into a distillation column that produces DME as product in the distillate and a mixture of methanol and water in the bottoms. The bottoms stream is fed to another distillation column where the remaining methanol is recycled back into the feed and the bottoms stream is disposed of as wastewater. Within this design process one main assumption is considered. The design process assumed to be at 90% conversion.

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1. Project Scope

1.1 Problem Statement

The purpose of this project is to design a system that produces dimethyl ether (DME) at the required 99.9% purity.

1.2 Client Identification and Recognition of Need

For our process we decided that it would be best to get our methanol from the gulf coast which will cost us \$359.00 per metric ton. The reasoning behind this, is because methanol purchased from the gulf coast is relatively cheaper and the gulf coast is transportation hub which would make transporting our product (DME) easier. Once we purchase the methanol, we plan to use to produce 50,000 metric ton of DME per year through the process of methanol dehydration. Once the DME is produced, we plan to sell to Ford, FPT, Powertrain, and China at \$900.00 per metric ton.

1.3 Project Goals and Objectives

For this project we decided it would be best to list out important tasks that would progress our process along. We first started with understanding our process which led us to figuring out parameters regarding major equipment there after we shifted our focus to our process design where we devolved our process flow diagram and overall material balance. Lastly we wrapped up our project by creating a cost analysis followed by safety consideration. Each of the following major tasks were split into phases and sub tasks.

1.4 Contemporary issues and impact of project on society

The production of dimethyl ether is a relatively eco-friendly process being that global warming potentials are low compared to chlorofluorocarbons which are traditionally coolants. However high exposure can lead to headaches, dizziness, light headedness, and even loss of consciousness. Also, it is highly flammable and can cause fires. With this being said, the process of Methanol Dehydration was the best option for our team.

2. Project Planning and Task Identification

2.1 Task Identification

The following is the list of tasks that was delegated to our process. HYSYS/ASPEN simulation of process, chemical engineering design, economic evaluation, safety and hazop analysis, overall report, visual & oral presentation.

2.2 Timelines

In order to ensure all tasks were accomplished, it was important to identify major tasks and subtasks. This allowed for maximum productivity and ensured project completion. The use of a Gantt chart provided a visual reference of what needed to be completed and by when. Table 1 and Figure 1 detail the organization of the project over the course of the semester.

Table 1: Overview of Project Completion

Task	Time period
HYSYS/ASPEN Simulation	Feb. 18-25
Chemical Engineering Design	Feb. 28-March.28
Economic Evaluation	March. 30-April 13
Safety and Hazop Analysis	March. 30-April 13
Finish report	April. 9-16

Above is the identification of the major tasks needed to complete the project and the dates by which each should be completed.

PROJECT TITLE:		PRODUCTION OF DIMETHYL ETHER (DME)																																																				
Project start		2/18/2022																																																				
Display Week		0																																																				
TASKS AND SUB-TASKS			OWNER	START DATE	END DATE	DURATION																																																
HYSYS/ASPEN Simulation of Process																																																						
Incldae Small Equipment			All	18-Feb-22	25-Feb-22	1 week																																																
Verify Recycle Stream			All	18-Feb-22	25-Feb-22	1 week																																																
Converge			All	18-Feb-22	25-Feb-22	1 week																																																
Chemical Engineering Design																																																						
Design of Major Equipment			All	28-Feb-22	28-Mar-22	4 weeks																																																
Detailed Unit P&ID (Reactor)			Taylor & Amiya	28-Feb-22	28-Mar-22	4 weeks																																																
Listing Equipment and Specification			Laura & Cinthia	28-Feb-22	28-Mar-22	4 weeks																																																
Economic Evaluation																																																						
Cost of Major Equipment Using CAPCOST Software			Cinthia and Laura	30-Mar-22	13-Apr-22	2 weeks																																																
Fixed Capital Costs			Taylor	30-Mar-22	13-Apr-22	2 weeks																																																
Utilities			Taylor	30-Mar-22	13-Apr-22	2 weeks																																																
Fixed Capital Investments			Taylor	30-Mar-22	13-Apr-22	2 weeks																																																
Manufacturing Production costs Peters and Timmerhaus			Amiya	30-Mar-22	13-Apr-22	2 weeks																																																
Complete Economic Analysis/ Cash Flow Diagram			All	30-Mar-22	13-Apr-22	2 weeks																																																
Safety and HAZOP Analysis																																																						
Methanol Safety-Hazards			Laura	30-Mar-22	13-Apr-22	2 weeks																																																
Reactor & Catalyst Safety-Hazards			Taylor	30-Mar-22	13-Apr-22	2 weeks																																																
DME Safety-Hazards			Amiya	30-Mar-22	13-Apr-22	2 weeks																																																
Specific Unit Breakdown (Distillation)			Cinthia	30-Mar-22	13-Apr-22	2 weeks																																																
Startup/Shutdown HAZOP			Amiya	30-Mar-22	13-Apr-22	2 weeks																																																
Finish Report																																																						
Complete Rough Draft			All	9-Apr-22	16-Apr-22	1 week																																																
Complete Final Draft			All	9-Apr-22	16-Apr-22	1 week																																																
Visual & Oral Presentation																																																						
Complete Presentation			All	9-Apr-22	16-Apr-22	1 week																																																
Presentation Practice			All	9-Apr-22	16-Apr-22	1 week																																																

Above is the Gantt chart that details the major tasks and subtasks. As shown, the anticipated completion date and duration for each task is listed.

This section of the report gives an overview of the manufacturing processes pertinent to DME. The section also examines DME's production routes, its physical and chemical properties, as well as safety aspects including handling and storage.

3.1. Overview of Manufacture of DME

Dimethyl ether (DME) is an organic compound that is well-known as a propellant and coolant. It can be used as an alternative fuel for diesel engines, due to its relatively low carbon footprint and high-performance characteristics. In normal conditions, DME presents as a colorless gas and liquifies at about 75 psi ("Alternative Fuels Data Center: Dimethyl Ether", n.d.). Other applications of DME include; as a solvent, an aerosol and a refrigerant.

The production of DME encompasses various sources including; biomass, fossil fuels and methanol. In the U.S., the idealized source for the production of DME is natural gas. The most common means of production for DME encompasses synthesis from syngas generated from fossil fuels.

The molecular formula for DME is thus presented as CH_3OCH_3 , which can consequently be simplified to $\text{C}_2\text{H}_6\text{O}$.

3.2. Production Routes

There are two distinctive routes for the production of DME entailing, the indirect route and the direct route. The indirect route involves the dehydration of methanol which is readily available to produce DME. On the other hand, the direct route involves the production of syngas from a variety of sources, which can then be converted to methanol and then to DME. These production routes are examined in details in the following sections.

3.2.1. Indirect Synthesis Route

The indirect synthesis of DME takes a more traditional approach whereby, methanol is obtained from a variety of sources, purified and then converted to DME (Azizi et al., 2014). As

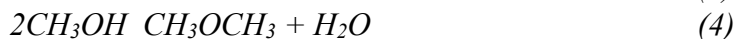
stated above, this production route fundamentally involves the dehydration of methanol resulting in the production of DME, and water as a by-product. This process is given by the following reaction.



According to Azizi et al., (2014), the most preferred method of methanol dehydration to produce DME involves a solid-acid catalyst and involves either the Langmuir-Hinshelwood or Eley-Rideal kinetic models. In both these models, water and DME act as reaction inhibitors at temperatures of above 300°C and therefore, this production route is favored at lower temperatures (Azizi et al., 2014).

3.2.2. Direct Synthesis Route

Recent research and technology have developed means of synthesizing DME directly from syngas using a single reactor. This process encompasses the formation of methanol, a water-gas shift, and methanol dehydration (Falco, 2021). This series of process is presented as follows includes; methanol formation, water-gas shift, methanol dehydration, and the overall reaction.



In the reactions above, both the formation of methanol and the water-gas shift occur within the overall process of converting syngas to DME. The formation of methanol is crucial in the synthesis of DME, whereas water-gas shift produces CO₂ which can then be recycled and use in reforming methane, and consequently syngas. The recycling of CO₂ with methane to produce syngas is given by the following reaction (Azize et al., 2014).



The direct synthesis of DME from syngas is a highly exothermic reaction and measures should be put in place to regulate temperature and prevent run-away. This production although being relatively more efficient, involves a complicated process and is thus more costly and resource intensive.

A summary of the process routes considered for this project is presented in the following table.

Table 2: Characteristics of Each Alternative

ALTERNATIVE	PROCESS	PROS	CONS
1	Methanol Dehydration	- Consumes less time and cost of equipment -Catalyst deactivation occurs at relatively high temp (400C). -Relatively simpler process flow	-Requires more downstream separation technologies -Sourcing of methanol may present challenges. -Marginally lower DME yield
2	Indirect Synthesis from biogas feedstock	-Marginally higher yield of DME -The risk of water build up in the process is alleviated -Energy Efficiency is maximized	-Sourcing of biogas feedstock presents a challenge. -Process requires more equipment. -Relatively Costly and time-consuming
3	Direct Synthesis from Natural Gas Feed Stock	-Higher yield of DME in comparison to methanol dehydration. -No risk of water build-up	-Exothermic reaction may lead to runaway reaction. -Catalyst deactivation at temp above 300C -Relatively more costs and time-consuming.

3.3. Physical and Chemical Properties

At atmospheric pressure and room temperature, DME presents as an odorless, colorless gas. Under severe or prolonged exposure to heat, any DME containers rupture violently ("Dimethyl ether", n.d.). DME has several other physical properties, some of which are summarized in the following table ("Fundamental Aspects of Dimethyl Ether", n.d.).

Table 3: DME Properties

Property	Value
Molecular weight	46.07
Boiling point	248.3 K
Freezing point	131.7 K
Critical pressure	52.5 atm
Critical Temperature	402.0 K
Heat of melting	25.6 cal/g
Heat of vaporization	111.6 cal/g
Specific Heat @ 248 K	0.535 cal/kg
Density at 1 atm and 25C	1.91855 g/L

As a chemical compound, DME is considered relatively stable with reactions or decomposition occurring at severe conditions. In this regard, the decomposition rate of DME is estimated at 1% per year when subjected to a temperature of 493K.

Another chemical property that defines DME is that is a powerful solvent with high solubility for both polar and non-polar substances. In this regard, 1 volume of water takes up 37 volumes of DME. It is also soluble I ether, ethyl alcohol, acetone and chloroform ("Dimethyl ether", n.d.).

3.4. Handling, Safety and Storage

There are various hazard identifiers used to define DME. In the US, the National Fire Protection Association's codes and standards, NFPA 704, categorizes the gas at a flammability of 4 (NFPA, 2021). This means that the gas is extremely flammable with an ability to vaporize completely at ambient environmental conditions (NOAA Office of Response and Restoration, n.d.). The gas' hazard identification information is presented in the following table.

Table 4: DME Identifiers

Category	Designation
DME CAS no.	115-10-06
NFPA Flammability no.	4
NFPA Health no.	2
NFPA stability no.	1

Exposure to the gas has several health effects including frostbites when exposed to the skin, pain and redness when exposed to the eyes, and sore throat, drowsiness, loss of consciousness, and headaches when inhaled ("ICSC 0454 -DIMETHYL ETHER", n.d.). The following table summarizes the health hazards related to exposure to DME.

Table 5: DME Health Hazards

Exposure	Symptom
Inhalation	Headaches, sore throat, drowsiness and loss of consciousness
Skin	Frostbites
Eyes	Blurry vision, pain and redness

The following sections describe the various safety and handling procedures pertinent to DME.

3.4.1. Handling and Storage

Based on the hazardous nature of DME, there are various recommended protocols on how to handle and store the gas. The handling of DME encompasses a variety of personal precautions

such as the wearing and usage of protective gear as well as an intricate understanding of emergency procedures pertinent to the gas. These precautions include; the wearing of self-contained breathing apparatus when in contaminated areas, constant monitoring of oxygen levels and supply within production of contaminated areas ("Safety Data Sheet -DME", 2018), and only allowing trained personnel to respond to uncontrolled leakages. An additional precaution is the use of Personal Protective Equipment PPE of a grade B minimum encompassing; fire-retardant clothing, mechanical resistant gloves and self-contained breathing apparatus ("ICSC 0454 -DIMETHYL ETHER", n.d.). Finally, the lower explosive limit (LEL) should be 10% for the combustible gas ("Safety Data Sheet -DME", 2018).

There are also a variety of measures that should be adopted to handle and store the equipment used in the process of manufacturing and using DME. The most important measures in this regard include, constant inspection of gas cylinders to ensure no damage, not tampering with pressure relief devices in valves and cylinders ("Safety Data Sheet -DME", 2018), and storing gas containers in a cool, well-ventilated and dry area away from direct sources of heat. Additionally, the temperature in the storage area should be limited to a maximum of 52°C (or 125°F), the gas containers for DME should be stored in an upright, well-fastened position, and there should be segregation of full and empty containers. Finally, the cylinders containing DME should be kept at least 20 ft from any heat source.

3.4.2. Safety

As an alternative fuel source, DME exhibits a better safety proposition than other synthetic fuels, because it is a circular hydrogen carrier, meaning it utilizes hydrogen to store energy in a vector form (Styring et al., 2021). DME is synthesized using different methods and

from varying sources, which means that each of its synthesis processes have different safety ratings.

Generally, the synthesis of DME using direct synthesis has lower risk potential, than using indirect synthesis because of the additional processes involved in the latter (De Falco, n.d.). In this regard, the direct synthesis of DME bypasses the synthesis of methanol. Indirect synthesis of DME on the other hand, involves the synthesis of methanol from shale/natural gas. Because methanol is categorized as a category 2 flammable liquid and category 3 toxic substance (De Falco, n.d.), safety precautions have to be put in place when using the indirect method for the synthesis of DME.

The safety risks associated with indirect synthesis include risk of fires and exposure to toxins if in contact with the reactants over prolonged periods of time. In this regard, 200 ppm is the permissible exposure limit (PEL) dictated by the Occupational Safety and Health Administration (Yang et al., 2015).

Another safety consideration in the production of DME using indirect synthesis from methanol, is the incorporation of a floating head storage tank (Yang et al., 2012). This tank alleviates the safety concerns associated with the flammability and volatility of methanol and other raw materials.

3.5. Uses of DME

DME has a variety of uses. The most prominent of these include as a refrigerant (R-E170), as a solvent, as a propellant in industrial aerosol products, and finally, for purposes including transportation fuel, domestic use, and power generation.

4. Process Selection

4.1 Market Analysis and Trends

In order to determine our plant capacity, an analysis had to first be conducted to determine how much DME is currently being produced and compare it with the future demand of DME. The current capacity for DME is about 3 million metric tons while the demand is expected to grow by 530,000 tons by 2025 (Fleisch et. al 2012). It is important to note that specific demand data could not be found so we predicted the future demand using previous years' growth as an indicator. After finding the current production, competitors were researched to see how much they were producing. Plant capacities were found ranging from 20,000 metric tons per year (MTPY) to 100,000 MTPY. From these numbers it was deemed that 50,000 MTPY was a reasonable capacity for the plant design. From this capacity, the material balance was able to be calculated, which will be discussed later in this report.

4.2 Reaction Routes to Producing Product

After conducting a literature review, the proposed alternatives were narrowed to: Methanol Dehydration to form DME (alternative 1), DME production using biogas feedstock (alternative 2), and indirect DME production using a natural gas feedstock (alternative 3). These three were specifically chosen due to representing the present and future possibilities of DME while taking into account availability of research to complete the design.

4.3 Process Screening Using Gross Profit Analysis

One of the main goals for the design was to design a system that is profitable. In order to make sure the selected alternative was profitable, a theoretical economic indicator analysis, shown in equation 1, had to be completed to ensure profitability.

$$\text{Products} * \text{Price} - \text{Reactants} * \text{Price} \quad (6)$$

If the difference came out to be negative then the calculated alternative would not be profitable, but rather cause debt. If the difference was positive then the given alternative would be profitable, thus being a good choice to start a design around.

4.4 Process Comparison and Selection

For the process comparison and selection, each alternative was compared on the basis of economics, impact on the environment, potential location, and safety. Each team member rated the category on a scale of 1-5 based on the literature review and discussed aspects of each alternative. The following chart shows how each alternative scored in each category.

Table 6: Process Comparison and Selection

Considerations:	Alternative 1	Alternative 2	Alternative 3	Weight, %
Economics	18	10	12	40
Environment	13	16	20	25
Location	14	13	9	25
Safety	13	13	16	10
Total	<u>15.25</u>	12.5	13.65	100

As shown in Table 6, the alternative with the highest score was methanol dehydration to form DME. The chemical formula can be seen below and was used to conduct the theoretical economic indicator analysis.

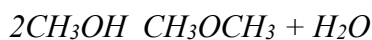


Table 7: Theoretical Economic Indicator for Methanol Dehydration to form DME

	A	B	C
mol	2	1	1
Molecular Weight kg/mol	.03204	.04607	.01802

kg	.06408	.04607	.01802
kg/kg DME	1.39	1	.391
cents/kg	\$0.36	\$0.71	0

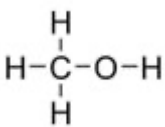
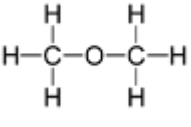
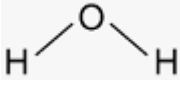
Shown in Table 7 is the preliminary economic analysis that was conducted to ensure that the chosen alternative would be profitable. A represents methanol, B is DME, and C is water. After utilizing equation 6 the theoretical indicator was found to be \$0.21cents/kg DME or \$210/MT DME.

5. Process Description

5.1 Process Chemistry

The irreversible chemical equation for methanol dehydration, equation 1, shows that for every two moles of methanol, one mole of DME and water is produced. The chemical conditions for each component used in the process is show in Table 8.

Table 8: Chemical Conditions for Components

Conditions	Components		
	<i>Methanol</i>	<i>Dimethyl Ether</i>	<i>Water</i>
<i>Molecular Weight</i>	32.04 g/mol	46.07 g/mol	18.02 g/mol
<i>Chemical Formula</i>	CH ₃ OH	CH ₃ OCH ₃	H ₂ O
<i>Chemical Structure</i>			
<i>Boiling Point</i>	64.70°C	-24°C	100°C
<i>Melting Point</i>	-94.60°C	-141°C	0°C
<i>Flash Point</i>	9.7°C	-41.1°C	-
<i>Density</i>	0.79 g/cm ³	1.97 g/cm ³	1 g/cm ³

The mole balance and rate law equations are shown in Table 9. F is defined as flow rate, while W, represents catalyst weight. The rate law equations also show the relationship between

the reactants and products. Methanol dehydration is favored at lower temperatures because it is an exothermic reaction. Therefore, a tubular packed bed reactor is used due to its low operating cost, high conversion per unit mass of catalyst, and ideal for catalytic processes with low temperatures. Maintaining a low temperature is critical to reduce the formation of by-products such as ethylene, carbon monoxide, hydrogen, and coke.

Table 9: Kinetic Rate Equations

Species	Mole Balance Equation	Initial Flow Rate	Rate Laws
<i>Methanol</i>	$dF_{\text{CH}_3\text{OH}}/dW = r'_{\text{CH}_3\text{OH}}$	$F_{\text{CH}_3\text{OH}}(0) = 274$ kmol/hr	$r'_{\text{CH}_3\text{OH}} = -k_1 C_{\text{CH}_3\text{OH}}^2$
<i>Dimethyl Ether</i>	$dF_{\text{CH}_3\text{OCH}_3}/dW = r'_{\text{CH}_3\text{OCH}_3}$	$F_{\text{CH}_3\text{OCH}_3}(0) = 0$	$r'_{\text{CH}_3\text{OCH}_3} = -2r_{\text{CH}_3\text{OH}}$
<i>Water</i>	$dF_{\text{H}_2\text{O}}/dW = r'_{\text{H}_2\text{O}}$	$F_{\text{H}_2\text{O}}(0) = 0$	$r'_{\text{H}_2\text{O}} = -2r_{\text{CH}_3\text{OH}}$

5.2 Process Flow Diagram and Process Description

The dimethyl ether process receives pure liquid methanol from a pipeline, it is then pumped into a mixer and mixes with the recycled liquid methanol. This methanol mixer is then pumped into a vaporizer where it will change phases from liquid to vapor. This vapor methanol mixer continues into a heater that heats up the combined vapor stream to the desired reactor inlet temperature. The effluent from the furnace is fed to the catalytic packed bed reactor. In the reactor, the methanol is being dehydrated by a gamma alumina catalyst and converted into DME and Water. The reactor operates at 90% conversion and the tubes are packed with $\gamma\text{-Al}_2\text{O}_3$. The product from the reactor is then cooled and sent to the first distillation column where the DME separation occurs. The overhead product is the desired DME product which is stored in a tank

between a 7 through 14 bar and up to 52°C. The bottoms products are, now in the liquid phase, methanol and water which are sent to a second distillation column for further separation. The second distillation overhead product is methanol which will be recycled back into the system and the bottoms product is wastewater which will be sent to SNF Holding Company Plaquemine treatment facility. Wastewater treatment will reduce pollutants in water and negative health effects on life species.

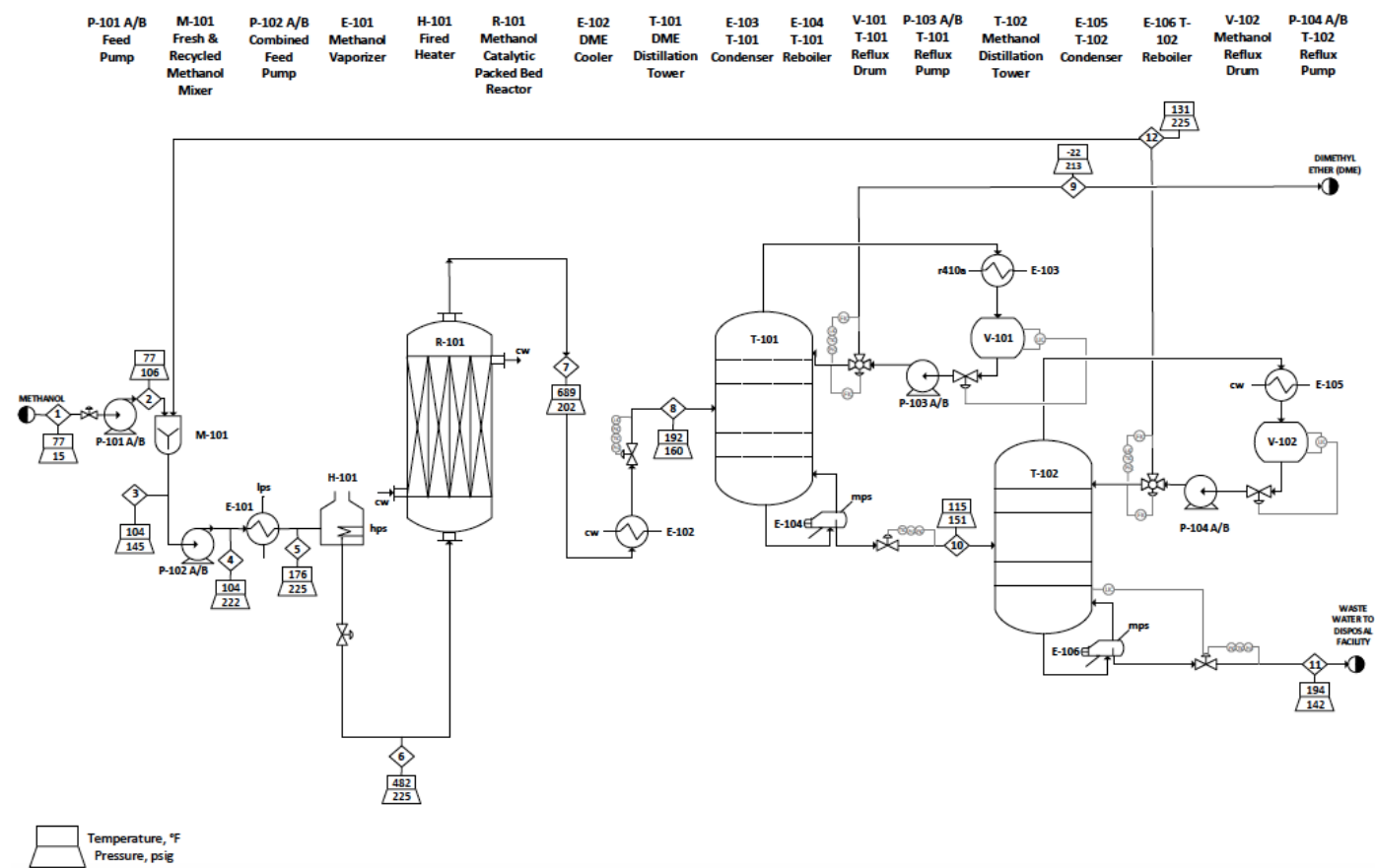


Figure 2: Production of Dimethyl Ether Process Flow Diagram

6. Material and Energy Balances

6.1 Material Balances

As previously mentioned, the basis of calculation was determined to be 50,000 MTPY of DME.

From this number, the overall material balance was able to be calculated using the stoichiometric ratio of the reaction. The capacity was first taken from a yearly time period to 152 MTPD. This number was then converted into a mass flow rate and then to a molar flow rate. After applying the stoichiometric ratio, the wastewater flow rate and feed flow rate were calculated. In order to complete the individual unit balances, assumptions about the molar compositions were made (Diemer et. al 2010).

Block Flow Diagram Material Balance

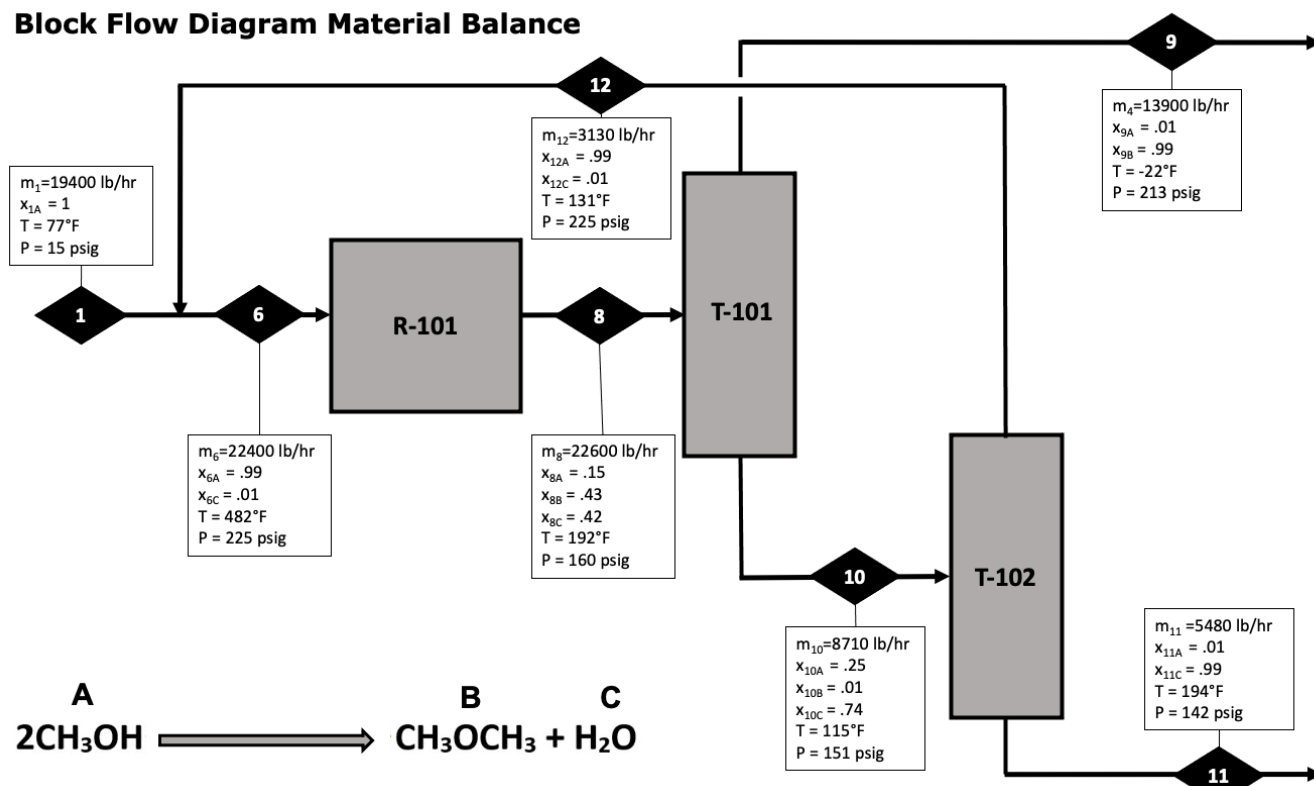


Figure 3: Material Balance for Design

Figure 3 shows the total material balance for each process stream. Using the assumed molar compositions and the degree of freedom (DOF) analysis, the individual stream flowrates were able to be calculated.

6.2 Energy Balances

In order to complete the energy balance around the reactor, temperature, flowrates, and specific heat capacities were needed, as shown in Equation 7. The temperature for the reactor was determined based off the literature review and the specific heat capacity was calculated at ambient temperature. Since the streams were mixed, the molar compositions were used to determine the specific heat capacity for each component in the stream. The individual heat capacities were then added to get the total heat capacity for the stream.

$$\sum mC_pT_2 = \sum mC_pT_3 \quad (7)$$

In order to calculate the total energy balance, the process was simulated in ASPEN. Using the degree of freedom (DOF) analysis, the ASPEN simulation was simulated vessel by vessel. First, the reactor was converged by defining the temperatures and pressures for each stream and only defining the molar composition and molar flow for the input streams. After checking to see if the output values matched the calculated values in Figure 3, a separator was added to the simulation. Since the input stream for the first distillation column was calculated by Aspen, the composition and molar flow rate for the bottoms stream was only defined. Once the simulation ran again, it was proved that the molar flow rate and compositions Aspen calculated for the first overhead stream also matched the calculations in Figure 3. Lastly, the same steps were followed for the last distillation column until a fully converged simulation which molar flows and compositions for each stream matched the material balance that is shown in Figure 3. The recycle stream is split into two streams to make it easier to converge and more accurate. Each stream converged

and the simulated energy balance for the reactor was compared with the calculated energy balance to check accuracy. Since all values were within a 5% error, the simulation was deemed correct and the total energy balance can be seen in Figure 3. The simulated ASPEN is shown in Figure 3 and the energy balance values can be seen in Table 10.

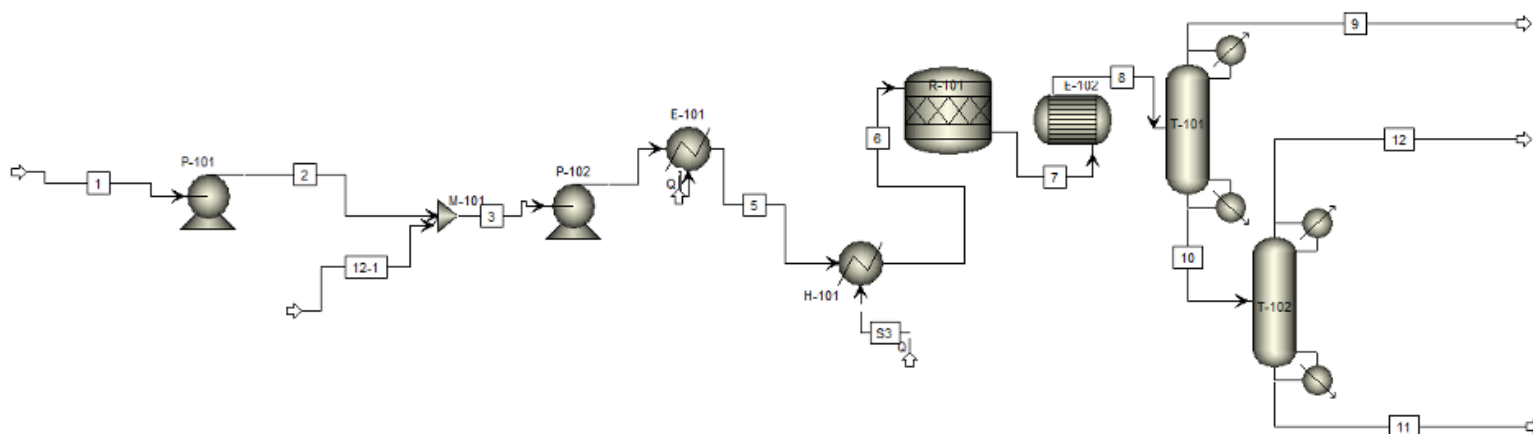


Figure 4: Simulated and Converged ASPEN Plus Diagram

Table 10. Energy Balance Calculations

Methanol Dehydration R-101	
Temperature	689°F
R-101 Duty	-1.36×10^7 BTU/hr
E-101 Duty	9.67×10^6 BTU/hr
H-101 Duty	5.40×10^6 BTU/hr
E-102 Duty	-1.14×10^7 BTU/hr

DME Distillation T-101	
Temperature	86°F/114.8°F
E-103 Duty	-3.39×10^6 BTU/hr
E-104 Duty	2.36×10^6 BTU/hr

Methanol Distillation T-102	
Temperature	158°F/194°F
E-105 Duty	-1.18×10^7 BTU/hr
E-106 Duty	1.14×10^7 BTU/hr

7. Utilities

To carry out the production of DME, power, steam, cooling water, wastewater disposal, and refrigerants were all considered. Table 11 summarizes the necessary utility requirements for each piece of major equipment.

Table 11. Summary of Utilities

Power kWh/y	
P-101 A/B	56900
P-102 A/B	75800
P-103 A/B	41100
P-104 A/B	7900
Steam kg/y	
E-101 (lps)	193000
H-101 (hps)	50000
E-104 (mps)	10000
E-106 (mps)	49000
Cooling Water m ³ /y	
R-101	104000
E-102	149000
E-105	29100
Wastewater Disposal m ³ /y	
T-102	19900
Refrigerant r140a GJ/y	
E-103	432

8. Equipment List and Description

8.1 P-101

This pump is responsible for increasing and regulating the initial pressure of methanol before it is delivered the system. The pump increases the pressure of fresh methanol from 1 bar to 7.3 bar, before it is fed to the vaporizer.

8.2 P-102

This pump is responsible for increasing and regulating the pressure of the combined stream of methanol after it leaves the mixer. The pump increases the pressure of fresh methanol from 10.0 bar to 15.2 bar, before it is fed to the vaporizer.

8.3 E-101

This is a vaporizer that takes methanol from a liquid to a gaseous state. It is made of carbon steel and has a cross-sectional area of 1.02 m². The vaporizer has a heat transfer area of 56.3 m² and a duty of 1.02×10^7 kJ/hr.

8.4 H-101

The third component in the process flow is a furnace that is responsible for heating methanol to the idealized temperature of 250°C before it is fed to the reactor. The furnace is constructed using carbon steel to withstand high temperature. It has a maximum pressure rating of 45 bar and a duty of 5.7×10^6 kJ/hr.

8.5 R-101

This is a catalytic packed bed reactor. There are 34 tubes each comprised of 733.03 kg of γ -Al₂O₃ catalyst and as the methanol passes through the tubes it is dehydrated to form DME and water. Each tube has a diameter of .03m while the reactor has a diameter of 1.33 meters and an overall height of 4.48 meters. The construction of the tower section of the reactor comprises mild carbon steel (A516 grade), whereas the tubing is made of stainless steel (grade 316). This reaction is exothermic and if the temperature gets too high, the process will begin to form byproducts and

the catalyst will deactivate. To prevent this, cooling water is passed through the shell side of the reactor to maintain the desired temperature. Its maximum pressure rating is 15 bar.

8.6 E-102

This is a shell and tube heat exchanger made of carbon steel. It acts as a cooler lowering the temperature of the mixture leaving the reactor. The heat exchanger cools DME/water/methanol mixture from 365°C to 89°C before it is fed to the first distillation column which is responsible for separating DME from the mixture. The maximum pressure rating of the heat exchanger is 14 bar. It comprises a floating-head shell and tube design with the main construction material being carbon steel.

8.7 T-101

This is a tray-type distillation column with 22 valve trays, a reboiler and a condenser. The average tray spacing is .61m, and the column is responsible for the separation of DME from a water/methanol mixture. It is predominantly made of carbon steel, with an overall height of 16m and a diameter of 12m. The feed for the column contains DME, water and methanol. The distillate on the other hand comprises of DME whereas water and methanol mixture is collected at the bottom. The maximum pressure rating for the column is 15 bar.

8.8 T-102

This is a tray-type distillation column with 15 valve trays, a reboiler and a condenser. The average spacing between the trays is .8m. The column is responsible for the separation of methanol that goes into the recycling stream from waste water. It is predominantly made of carbon steel,

with an overall height of 20m and a diameter of 13m. The feed for the column contains traces of DME, water and methanol. The distillate on the other hand comprises of methanol whereas water is collected at the bottom. The maximum pressure rating for the column is 15 bar.

9. Specification Sheets

9.1 P-101A/B Specifications

Pump				
Identification:	Item:	Pump		
	Item No:	P-101	Date	2/23/2022
	No. Required	2		
	C _{TPI} (\$)			
Function:	Pump liquid methanol from 1 bar to 15.2 bar			
Operation	Continuous			
	Inlet	Outlet		
Materials Handled				
Mass Flow(kg/hr)	8778	8778		
Mole flow (kgmol/hr)	274	274		
Component Flow (kgmol/hr):				
Dimethyl Ether	0	0		
Methanol	274	274		
Water	0	0		
Temperature (C)	25	25		
Pressure (bar):	1	15.5		
Vapor Fraction:	0.0	0		
Design Data:				
Power (kW)	7.2	Material:	Carbon Steel – A36	
Efficiency (%)	60	Type:	Centrifugal	
ΔP	6.3			
Utilities:				

Comments:	
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9.2 P-102A/B Specifications

Pump				
Identification:	Item:	Pump		
	Item No:	P-102	Date	2/23/2022
	No. Required	2		
	C _{TPI} (\$)			
Function:	Pump liquid methanol from 10 bar to 15.2 bar			
Operation	Continuous			
	Inlet	Outlet		
Materials Handled				
Mass Flow(kg/hr)	10,200	10,200		
Mole flow (kgmol/hr)	318	318		
Component Flow (kgmol/hr):				
Dimethyl Ether	0	0		
Methanol	315	315		
Water	3.18	3.18		
Temperature (C)	40	40		
Pressure (bar):	10	15.2		
Vapor Fraction:	0.0	0		
Design Data:				
Power (kW)	9.6	Material:	Carbon Steel – A36	
Efficiency (%)	60	Type:	Centrifugal	
ΔP	5.2			
Utilities:				
Comments:				

9.2 E-101 Specifications

Vaporizer

Identification:	Item:	Vaporizer		
	Item No:	M-101	Date	3/24/2022
	No. Required	1	By:	C.Sahin
	C _{TPI} (\$)			
Function:	Vaporization of liquid methanol			
Operation	Continuous			
	In	Out		
Materials Handled				
Mass Flow(kg/hr)	10,200	10,200		
Mole flow (kgmol/hr)	318	318		
Component Flow (kgmol/hr):				
Dimethyl Ether	0.0	0.0		
Methanol	315	315		
Water	3.18	3.18		
Temperature (C)	40	80		
Pressure (bar):	15.2	15.5		
Vapor Fraction:	0.0	1.0		
Design Data:				
Cross-sectional area	1.02 m ²	Material:	Carbon Steel	
Diameter	1.14 m			
Duty (Q) kJ/hr	1.02 * 10 ⁷			
Heat transfer area	56.3 m ²			
Maximum Pressure rating	15 bar			
Utilities:	Low Pressure Steam 4.5 bar = 24160 kg/hr			
Comments:				

9.3 H-101 Specifications

Electric Furnace				
Identification:	Item:	Electric Furnace		
	Item No:		Date	3/24/2022
	No. Required	1	By:	C.Sahin
	C _{TPI} (\$)			
Function:	Heat stream to 250°C			

Operation	Continuous			
	In	Out		
Materials Handled				
Mass Flow(kg/hr)	10,200	10,200		
Mole flow (kgmol/hr)	318	318		
Component Flow (Kmol/hr):				
Dimethyl Ether	0	0		
Methanol	315	315		
Water	3.18	3.18		
Temperature (C)	80	250		
Pressure (bar):	15.5	15.5		
Vapor Fraction:	1	1		
Design Data:				
Superheated Temperature (C)	400	Material:	Carbon Steel	
Duty (Q) kJ/hr	$5.7 * 10^6$			
Maximum Pressure rating	45 bar			
Utilities:	hps = 6255 kg/hr			
Comments:				

9.4 R-101 Specifications

Reactor				
Identification:	Item:	Catalytic Packed Bed Reactor		
	Item No:	R-101	Date	3/24/2022
	No. Required	1	By:	C.Sahin
	C _{TPI} (\$)			
Function:	Dehydration of methanol to produce DME and water			
Operation	Continuous			
	In	Out		
Materials Handled				
Mass Flow(kg/hr)	10,200	10,200		
Mole flow (kgmol/hr)	318	318		
Component Flow (Kmol/hr):				
Dimethyl Ether	0	136.92		
Methanol	315.25	47.76		

Water	3.18	133.74		
Temperature (C)	250	365		
Pressure (bar):	15.5	13.9		
Vapor Fraction:	1.0	1.0		
Design Data:				
Diameter (m)	1.33	Material:	Carbon Steel	
Overall height (m)	4.48			
Number of Tubes	34	Area (m ²)	12.41	
Maximum Pressure rating	15 bar			
Combined Tube Volume m ³	19			
Utilities:	CW	12951.38 kg/hr		
Comments:	Temperature maintained by cooling water Catalyst in tubes is γ -Al ₂ O ₃ Total catalyst weight is 24923 kg			

9.5 E-102 Specifications

Reactor Effluent Cooler				
Identification:	Item:	Shell and Tube Heat Exchanger		
	Item No:	E-102	Date	3/24/2022
	No. Required	1	By:	C.Sahin
	C _{TPI} (\$)			
Function:	To cool the DME stream coming from the reactor to 89°C			
Operation	Continuous			
	Hot in	Hot out		
Materials Handled				
Mass Flow(kg/hr)	10,200	10,200		
Mole flow (kgmol/hr)	318	318		
Component Flow (Kmol/hr):				
Dimethyl Ether	136.92	136.92		
Methanol	47.76	47.76		
Water	133.74	133.74		
Temperature (C)	365	89		

Pressure (bar):	13.9	10.4		
Vapor Fraction:	1.0	1.0		
Design Data:				
Q (kJ/h)	1.2×10^7	Material:	Carbon Steel	
A (m ²)	101.8			
Maximum Pressure rating	14 bar			
Utilities:	cw	18566.41 kg/h	T _{in} = 30°C T _{out} = 45°C	
Comments:	Process stream in shell (DME/methanol/water)			

9.6 T-101 Specifications

1 st Distillation Column				
Identification:	Item:	DME Separator		
	Item No:	T-101	Date	3/24/2022
	No. Required	1	By:	C.Sahin
	C _{TPI} (\$)			
Function:	Separate DME from methanol/water			
Operation	Continuous			
	Feed	Liquid Distillate	Liquid Bottoms	
Materials Handled	Methanol/DME/Water	Methanol/DME	Methanol/Water	
Mass Flow(kg/hr)	10245.83	6292.36	3952.83	
Mole flow (kgmol/hr)	318.43	137	181.4	
Component Flow (kgmol/hr):				
Dimethyl Ether	136.92	135.63	1.81	
Methanol	47.76	1.37	45.35	
Water	133.74	0.00	134.24	
Temperature (C)	89	-30	46	
Pressure (bar):	11	14.7	10.4	
Vapor Fraction:	1	0.0	0.0	

Design Data:					
Reflux ratio	1.7	Material:	Carbon Steel		
Number of actual trays	22				
Tray Spacing (m)	1				
Total tower height (m)	16				
Column diameter (m)	.8				
Maximum Pressure rating	15 bar				
Associated Component					
Condenser (E-103)	refrigerant : 432 GJ/y	A = 100.6 m ²	Q = 3.58x10 ⁶ kJ/hr	Fixed head, carbon steel	Max pressure = 10bar
Reboiler (E-104)	mps: 1256 kg/hr	A = 22m ²	Q = 2.49x10 ⁶ kJ/hr	Floating head, carbon steel	Max pressure = 11bar
Reflux Drum (V-101)	L = 2.89m	D = 1.14m	Carbon Steel	Max pressure = 10.3 bar	
Reflux Pump (P-103 A/B)	Power = 5.2 kW	Efficiency = 40%	ΔP = 4.6bar	Centrifugal/Carbon Steel	
Utilities:					
Comments:					

9.7 T-102 Specifications

2 nd Distillation Column				
Identification:	Item:	Methanol Separator		
	Item No:	T-102	Date	3/24/2022
	No. Required	1	By:	C.Sahin
	C _{TPI} (\$)			
Function:	Separate methanol from water			
Operation	Continuous			
	Feed	Liquid Distillate	Liquid Bottoms	
Materials Handled				
Mass Flow(kg/hr)	3952.83	1417.3	2485.26	
Mole flow (kgmol/hr)	181.4	44.43	137	

--- (Contd)

Component Flow (kgmol/hr):					
Dimethyl Ether	1.81	0.00	0.00		
Methanol	45.35	43.99	1.37		
Water	134.24	.44	135.63		
Temperature (C)	46	55	90		
Pressure (bar):	10.4	15.5	9.8		
Vapor Fraction:	0.0	1.0	0.0		
Design Data:					
Reflux ratio	4.472	Material:	Carbon Steel		
Number of actual trays	15				
Tray spacing (m)	1				
Total tower height (m)	20				
Column diameter (m)	1.16				
Maximum Pressure rating	15 bar				
Associated Components					
Condenser (E-105)	cw: 294250 kg/hr	A = 22.7 m ²	Q = 1.24x10 ⁷ kJ/hr	Floating head, carbon steel	Max pressure = 7 bar
Reboiler (E-106)	mps: 6130 kg/hr	A = 83.0 m ²	Q = 1.20x10 ⁷ kJ/hr	Floating head, carbon steel	Max pressure = 11 bar
Reflux Drum (V-102)	L= 2.53m	D = .85m	Carbon steel	Max pressure 7.3 bar	
Reflux Pump (P-104 A/B)	Power = 1.0 kW	Efficiency = 40%	ΔP = 4.1bar	Centrifugal/Carbon Steel	
Utilities:					
Comments:					

10. Equipment Costs and Capital Investment

To determine the various equipment costs, a modified version of CAPCOST software was applied on Microsoft Excel. In this regard, the software used properties such as vessel sizing and construction material to determine the estimated costs of various equipment throughout the process flow. The Chemical Engineering Plant Cost Index (CEPCI) was then used to adjust the realized estimates for inflation to the current year. Using CAPCOST, the purchased equipment costs and bare module costs were realized and summarized in Table 11 as shown below.

Table 12. Summary of Equipment Costs Using CAPCOST

			<u>Unit Number</u>	100				
			<u>CEPCI</u>	710				
User Added Equipment								
Evaporators	Type	Area (square meters)	Pressure (barg)	MOC	Volume (cubic meters)		Purchased Equipment Cost	Bare Module Cost
K-101	Vessel with Internal Coil		20	Carbon Steel	16.6		\$65,100	\$284,000
Exchangers	Exchanger Type	Shell Pressure (barg)	Tube Pressure (barg)		MOC	Area (square meters)	Purchased Equipment Cost	Bare Module Cost
E-101	Floating Head	85	16.7		Stainless Steel / Carbon Steel	118	\$34,300	\$194,000
E-102	Fixed, Sheet, or U-Tube	13.7	12		Stainless Steel / Carbon Steel	101	\$42,200	\$201,000
E-103	Floating Head	13.4	13.2		Stainless Steel / Carbon Steel	22	\$32,700	\$155,000
E-104	Floating Head	18.6	8.4		Stainless Steel / Carbon Steel	22.7	\$32,800	\$158,000
E-105	Floating Head	8.88	13.2		Stainless Steel / Carbon Steel	83	\$42,100	\$199,000
E-106	Fixed, Sheet, or U-Tube	12.4	16.6		Stainless Steel / Carbon Steel	12.4	\$27,600	\$133,000

Fired Heaters	Type	Heat Duty (MJ/h)	Steam Superheat (°C)	MOC	Pressure (barg)		Purchased Equipment Cost	Bare Module Cost
H-101	Process Heater	5070		Carbon Steel	54		\$868,000	\$1,990,000
Pumps (with drives)	Pump Type	Power (kilowatts)	# Spares	MOC	Discharge Pressure (barg)		Purchased Equipment Cost	Bare Module Cost
P-101	Centrifugal	7.2	1	Carbon Steel	31		\$12,640	\$65,000
P-102	Centrifugal	9.6	1	Carbon Steel	15.2		\$9,810	\$42,700
P-103	Centrifugal	5.2	1	Carbon Steel	11.2		\$11,480	\$46,800
P-104	Centrifugal	1	1	Carbon Steel	8.8		\$8,760	\$34,900
Towers	Tower Description	Height (meters)	Diameter (meters)	Tower MOC	Demister MOC	Pressure (barg)	Purchased Equipment Cost	Bare Module Cost
T-101	22 Stainless Steel Valve Trays	16	0.8	Carbon Steel		18	\$82,600	\$220,000
T-102	10 Stainless Steel Valve Trays	20	1.16	Carbon Steel		18	\$73,600	\$309,000
Vessels	Orientation	Length/Height (meters)	Diameter (meters)	MOC	Demister MOC	Pressure (barg)	Purchased Equipment Cost	Bare Module Cost
V-101	Vertical	2.89	1.14	Carbon Steel		12.4	\$9,640	\$55,700
V-102	Vertical	2.53	0.85	Carbon Steel		8.8	\$6,650	\$30,500
						Total Purchased		\$1,359,980

----- Contd.

						Equipment Cost		
						Total Adjusted 10%		\$1,495,978
Catalyst		Weight (Kg)	Unit Cost	Units	Cost			Total Cost
γ -Al ₂ O ₃		24523	207.4	24523				\$5,086,070.20
Project Estimate								Total
Project Estimate								\$6,582,048.20

The realized costs were then adjusted using a 10-percent margin of error to accommodate any additional equipment that may have been overlooked. From the table above the final project estimate was determined to be \$6,583,797.20.

11. ASPEN Simulation of Process

As shown in Figure 4, the process was simulated using ASPEN Plus. In order to ensure that the system converged, a step-by-step design was implemented. What this means is that each piece of equipment was individually placed and converged before moving to the next piece of equipment. By having each piece of equipment converge, the overall design was able to converge once all equipment was simulated.

12. Economic Evaluation

An overview of the economic analysis can be seen in Table 13 below.

Table 13. Economic Summary

Economic Evaluation	
Total Capital Investment, 10^6	\$10.2
Annual Total Production Costs, 10^6	\$34
Annual Sales, 10^6	\$37
Payback Period, yrs	4.2
Return on Investment, %/year	22
Discounted Cash Flow Rate of Return, %/yr	13
Net Present Value, 10^6	\$8
Salvage Value, 10^6	\$1
Cumulative profit, 10^6	\$23

Figure 5 shows the cash flow diagram for the system. It is important to note that the values represented already take into account the total production costs. As seen, in year 13, profit turns back negative. This is due to an assumed 2% inflation rate for total production costs coupled with the depreciation of equipment.

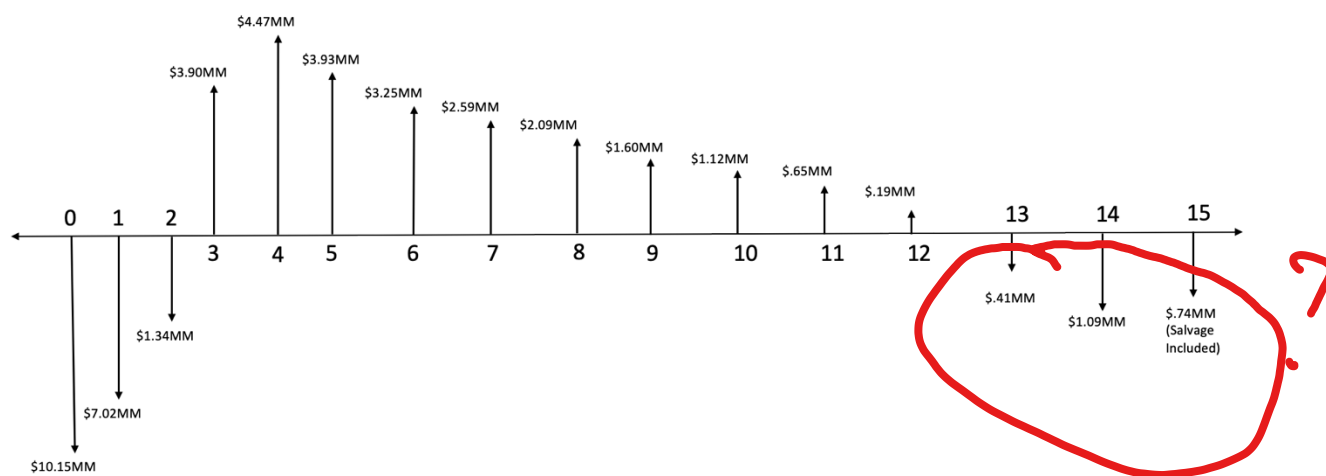


Figure 5. Cash Flow Diagram

13. Safety and HAZOP Analysis

Safety plays a crucial role in the success of the project. A hazard and operability (HAZOP) analysis presents a means of assessing how various components within the plant may deviate from their normal operations and pose safety and health risks to personnel, and how to mitigate these deviations. For this project, a HAZOP analysis was conducted for the second distillation column, the methanol tower, which is responsible for the separation of methanol for recycling from water/methanol mixture.

The methanol tower is a distillation column comprising of a feed line, a distillate line and a bottom line. It is a crucial component in the proposed plant for the synthesis of DME from methanol to be established in Plaquemine, Louisiana.

The general Guidelines for Safety Guidelines in Accordance with Rules and Regulations of Plaquemine, Louisiana are as follows (Ayres, 2016):

I. Pre Line Opening Job Preparations –

- The shutting down and energy isolation of all process systems prior to any line opening involving process piping, equipment or vessels (4.1.1).
- The draining and/or depressurization of all process piping, equipment or vessels to ensure clearance of hazardous materials (4.1.2).
- Ensuring temperatures for the process piping, equipment or vessels have sufficiently cooled to allow for safe work (4.1.3).

II. Line Opening Job Planning –

- The barricading of affected areas with a minimum of 10 ft radius as a precautionary area (4.2.1.1)
- The issuance of permits strictly by authorized personnel (4.2.2.1)

With the above guidelines the project involved a maximum exposure of 200 ppm from methanol. In addition, the general guidelines adopted by the City of Plaquemine where the proposed plant is expected to be established, the HAZOP analysis for the second distillation which constitutes the methanol tower can be conducted as follows.

I. T-102 Feed Line – Entry of reactants (methanol/water mixture) into the distillation column.

No.	Parameter	Guideword	Deviation	What if?	Possible Causes	Consequence	Safeguards	Action
1	Pressure	More	Pressure increase in the feed line	There is pressure build up in the feed line leading into the tower	- Blockage in the system	- Failure of feed line tube - Risk of expansion of column and bursting	Installation of quick-pressure relief valves at strategic locations before and after the column.	- Installation of a secondary pressure relief device. - Checking maintenance schedule and procedures
		Less	Pressure decreases in feed line	There are sudden pressure losses in the streams leading to the column	- Leakages in the system	- Insufficient reactant material entering the column	Pressure alarms at the feed, distillate and bottom streams	- Installation of pressure gauge - Checking maintenance schedule and procedures
3	Flow	Reverse	Backflow from T-102	The contents of the tower flow back to the feed line	- Clogging and blockages within the tower	- Pressure and temperature increase in the column	- Check valve to prevent backflow	- determining the best utilization of energy from recycle stream while preventing backflow- Following the stipulated maintenance schedule and procedures
4	Temperature	More	Increase in feed temperature	There is sudden increase in temperature at the feed of T-102	- Clogging of inlet into tower	Subsequent increase in pressure, risk of explosion and ineffectiveness of the tower	- Temperature alarms at feed entry point. - Panel alarms to warn of high pressure or temperature	- Installation of a temp gauge - Checking maintenance schedule and procedures

II. T-102 Distillate Line – Transportation of recycled methanol from the distillation column back to the mixer.

No.	Parameter	Guideword	Deviation	What if?	Possible Causes	Consequence	Safeguards	Action
1	Pressure	More	Pressure increase in the distillate line	There is pressure build up in the distillate line transporting recycled methanol to the mixer	-Blockage in the mixer or further up the distillation line	- Failure of distillate line tube - Risk of expansion of mixer and bursting. - Failure of mixer	Installation of quick-pressure relief valves at strategic locations before the mixer.	- Installation of a secondary pressure relief device. - Checking maintenance schedule and procedures
		Less	Pressure decreases in feed line	There are sudden pressure losses in the stream leading to the mixer	- Leakages in the distillate line	- Inefficiencies within the tower leading to less methanol distillate	Pressure alarms at the exit of the column where the distillate line begins.	- Installation of pressure gauge - Checking maintenance schedule and procedures
3	Flow	Reverse	Backflow to T-102	The contents of the distillate line flow back to the tower	- Clogging and blockages within the line	- Pressure and temperature increase in the column	- Check valve to prevent backflow	- determining the best utilization of energy from recycle stream while preventing backflow- Following the stipulated maintenance schedule and procedures
4	Temperature	More	Increase in distillate line temperature	There is sudden increase in temperature at distillate line transporting recycled methanol	- Clogging of inlet into the mixer	Subsequent increase in pressure, risk of explosion and ineffectiveness of the tower	- Temperature alarms at mixer entry point. - Panel alarms to warn of high pressure or temperature	-Installation of a temp gauge - Checking maintenance schedule and procedures

III. T-103 Bottom Line – Transportation of wastewater from the distillation column to treatment plant.

No.	Parameter	Guideword	Deviation	What if?	Possible Causes	Consequence	Safeguards	Action
1	Pressure	More	Pressure increase in the bottom line	There is pressure build up in the bottom-line transporting wastewater to treatment plant	-Blockages within bottom line	- Failure of bottom-line tube - Risk of expansion and bursting of the line.	Installation of quick-pressure relief valves at strategic locations within the line.	- Installation of a secondary pressure relief device. - Checking maintenance schedule and procedures
		Less	Pressure decreases in bottom line	There are sudden pressure losses in the stream within the bottom line leading away from the tower	- Leakages in the bottom line	- Inefficiencies within the tower causing decreased flow of wastewater from the tower	Pressure alarms at the exit point from the tower joining the bottom line	- Installation of pressure gauge - Checking maintenance schedule and procedures
3	Flow	Reverse	Backflow to T-102	The contents of the bottom line flow back to the tower	- Clogging and blockages within the line	- Pressure and temperature increase in the column	- Check valve to prevent backflow	- determining the best utilization of energy from recycle stream while preventing backflow- Following the stipulated maintenance schedule and procedures
4	Temperature	More	Increase in bottom line temperature	There is sudden increase in temperature at bottom line transporting wastewater to the treatment plant	- Clogging of the line at various points	Subsequent increase in pressure, risk of explosion and ineffectiveness of the tower	- Temperature alarms at exit point of the tower to the bottom line. - Panel alarms to warn of high pressure or temperature	-Installation of a temp gauge - Checking maintenance schedule and procedures

14. Discussion

Over the course of completing the design, there were assumptions made for the molar compositions of the process streams and for the heat exchanger duties. These values were obtained through literature reviews. As mentioned, the energy balance was assumed to be correct from ASPEN Plus due to similar results being obtained for the reactor energy balance. The economic analysis was assumed to be over a 15 year life span, and a 2% inflation rate was assumed. It is also important to note that for calculation purposes, 8,000 on stream hours was used. Moreover, the median salary for an operator in Plaquemine is \$59,029 (Glassdoor 2022). As a result, we generously set our operator salary at \$70,000 per year and determined that we need three operators per shift and three shifts per day.

not

clear

15. Conclusion and Recommendations

Overall, 50,000 MTPY of DME is being produced at 99.9% purity. This system would be in operation for 329 days out of the year (90% utilization). It is recommended to not produce more than that due to the still emerging market for DME. It has not yet been discovered how to solely rely on DME for transportation fuel, so the market is currently limited. The selected process of methanol dehydration allows for pure methanol to be imported via pipeline and reacted to form DME. Specifically for this design, it is recommended to salvage after year 12 to prevent the negative losses in years 13-15. However, with the present salvage at year 15, the overall profit is \$23MM with a 22% return on investment. As a result of this, it is recommended to continue with the design of this plant. Further analysis on E-102 is also recommended due to the drastic drop in temperature. There may be an additional opportunity for energy savings by recovering the lost heat.

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17. Appendix

Direct Costs	
Purchased equipment, E'	1.496
Delivery, fraction of E'	0.150
Subtotal: delivered equipment	1.646
Purchased equipment installation	0.773
Instrumentation&Controls(installed)	0.592
Piping (installed)	1.119
Electrical systems (installed)	0.181
Buildings (including services)	0.296
Yard improvements	0.165
Service facilities (installed)	1.152
Total direct costs	5.924
Indirect Costs	
Engineering and supervision	0.543
Construction expenses	0.675
Legal expenses	0.066
Contractor's fee	0.362
Contingency	0.724
Total indirect costs	2.370
Fixed capital investment (FCI)	8.294
Working capital (WC)	1.465
Total capital investment (TCI)	9.758

Figure 6. Direct and Indirect Costs