DESIGN OF POLYURETHANE PLANT FROM POLYOLS AND ISOCYANATES

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CERTIFICATE

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DEDICATION

This work is dedicated to our families for their constant support, our teachers for their insightful guidance, and our friends for their continuous encouragement.

ACKNOWLEDGEMENT

We would like to begin by expressing our profound gratitude to **Allah Almighty** for His boundless mercy and blessings. It is through His guidance and support that we have been able to successfully complete this project.

Our heartfelt appreciation goes to our supervisor, **Dr. Nouman Ahmed**, for his continuous support and invaluable guidance throughout this project. Dr. Nouman's insights and availability have been significant in our project, and we are deeply thankful for his commitment.

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Furthermore, we extend our sincere thanks to our parents for their constant prayers, faith, and encouragement. Their support has been a pillar of strength for us throughout this journey.

Lastly, we would like to acknowledge the help and encouragement from our friends and seniors, whose motivation and assistance have been invaluable in overcoming the challenges we faced during this project.

Authors

ABSTRACT

Polyurethane is a versatile polymer widely used as foam in furniture and automotive seating, insulation, coatings, adhesives and as elastomers. It is preferred over other polymers due to its exceptional properties such as resilience, flexibility, and resistance to abrasion and chemicals. The annual worldwide production of polyurethane is around 26 million metric tons, and it is primarily produced by the polyaddition reaction of polyols and isocyanates. Triethylamine is used as a catalyst to enhance reactivity between polyols and isocyanates and to allow the reaction to take place at room temperature. Water is used as a blowing agent during the preparation of polyurethanes to provide foams.

Despite the large number of applications and huge market for polyurethanes, certain issues such as sustainability concerns and toxicity are associated with polyurethanes. Isocyanates, which are the key component in the production of polyurethane, are highly toxic compounds that pose several health and safety concerns.

Moreover, the conventional phosgenation route for isocyanate production requires phosgene as a raw material which is a highly toxic compound and have significant adverse effects on the environment such as water pollution, climate change, and ozone depletion. This process involves reaction of phosgene and toluene diamine at elevated temperature (~300°C) producing toluene diisocyanate and hydrogen chloride.

To address these issues, the objective is to come up with a more suitable and environmentally friendly alternative method for toluene diisocyanate synthesis. One such method is to use a phosgene free process for toluene diisocyanate production which involves oxy-carbonylation reaction of toluene diamine, oxygen, and carbon monoxide, producing carbamate which then decompose thermally to produce toluene diisocyanates. This continuous process is carried out in two packed bed reactors for effective utilization of reactants. This continuous production and utilization of toluene diisocyanate reduces storage and handling problems.

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CHAPTER 1

INTRODUCTION

1.1 Problem Statement:

Design of Phosgene Free Route for Polyurethane production from Polyols and Isocyanates.

We are designing an economically feasible and environmentally friendly process design for producing TDI in high yield from toluene diamine (TDA), which is then used to form polyurethane. Our goal is to create a design that recycles most unreacted starting materials as well as dispose of any waste material in an economical and eco-friendly manner. We also want to minimize the plant's utility requirements to increase its sustainability.

1.2 Problem Identification:

The phosgene-free method of producing TDI by reacting TDA, oxygen, and carbon monoxide in 2,2,2-trifluoroethanol (TFE) offers a safer and environmentally friendly alternative. To enhance TDI production yield and reduce costs, two major reactor system options have been proposed.

1.2.1 Option 1:

The use of a single 3-loop pass reactor system. This setup aims to significantly enhance the overall TDI production yield from 64% (as reported by Fernandez et al.) to an impressive 97.2%. The key advantage of this option is the substantial yield improvement, which is expected to be maintained once the operation reaches a steady state. However, the complexity of this reactor system is notable. It comprises several components, including a holding vessel, a packed bed reactor, a cooler, and a pump.

The intricacy arises from the need to optimize the size and operation of each component to ensure efficient TDI production. One challenge is the uncertainty associated with the effectiveness of the actual reactions taking place within the reactor. This uncertainty stems from the limited availability of reaction kinetics data for this specific process. Without precise data on reaction rates and mechanisms, optimizing the volumetric flow rate passing through the reactor becomes challenging. Additionally, the increased complexity of the reactor system in Option 1 also translates to higher electricity consumption, primarily due to the greater work required by the pump to maintain the desired flow rates and pressures.

1.2.2 Option 2:

This option presents a more straightforward approach by utilizing two smaller individual packed-bed reactors. These reactors are designed to handle the reaction between TDA, oxygen, and carbon monoxide in 2,2,2-trifluoroethanol (TFE) efficiently. The focus of Option 2 is to maximize the utilization of TDA, and any intermediate products obtained from the first reactor. Despite the potential for a slightly lower overall yield compared to Option 1, the simplicity and feasibility of installing two smaller reactors make Option 2 a more practical and cost-effective choice. This option reduces the complexity of the reactor system assembly, minimizing the uncertainties associated with reaction kinetics and offering operational flexibility while still aiming for significant yield improvements.

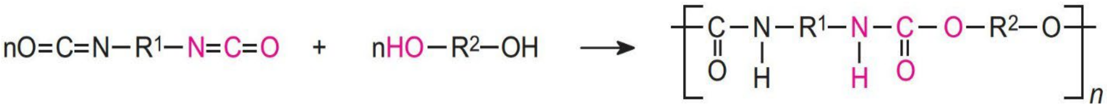
We opted design of option 2 by considering that installing two smaller reactors is more feasible than building one considerably bigger reactor.

CHAPTER 2

LITERATURE REVIEW

2.1 Introduction:

Reaction polymers are a group of related polymer compounds that include polyurethane. Two chemicals are used to create all polyurethanes: polyols (hydroxyl groups) ($R'–(OH)n\geq2$) and isocyanate groups ($R–(N=C=O)\ n\geq2$). The following reaction can be used to illustrate the overall manufacturing of PU polymer: -



$$nO{=}C{=}N{-}R^1{-}N{=}C{=}O \quad + \quad nHO{-}R^2{-}OH \longrightarrow \left[\underset{\underset{O}{\|}}{C} - \underset{\underset{H}{|}}{N} - R^1 - \underset{\underset{H}{|}}{N} - \underset{\underset{O}{\|}}{C} - O - R^2 - O \right]_n$$

2.2 Properties of Polyurethane:

The selection of isocyanates and polyols throughout the synthesis process has a major impact on the characteristics of polyurethane (PU) polymers. Which of the following polyurethane's characteristics—soft and elastic, firm and tough, stretchy, or hard—is determined by these antecedents. These properties are explained below.

2.2.1 Soft and Elastic Polymers:

Long, flexible polyols are used to create these kinds of PUs. Because of its long chains' great elasticity and flexibility, the polymer is appropriate for uses requiring a pliable, soft substance.

2.2.2 Firm and Inflexible Polymers:

Polyols with a high degree of cross-linking are employed to create firm and durable polymers. The process of forming chemical links between distinct polymer chains to build a three-dimensional network is known as cross-linking. This network limits the user's mobility.

2.2.3 Stretchy Polymers:

Long chains with little to no cross-linking should make up the precursors of polymers that need to be stretchy but not necessarily soft. The material is extensible because of its long chains and low cross-linking, which makes it perfect for elastomer applications where the material may stretch without breaking.

2.2.4 Hard Polymers:

These are composed of highly cross-linked, shorter polyol chains. Short chains are less flexible, and a dense network is created by extensive cross-linking, making the material strong and rigid and appropriate for applications that demand great strength and little deformation.

2.2.5 Foam Production:

Long-chain polyols and moderate cross-linking are combined to create polyurethane foams. The lengthy chains give the foam its cellular structure and contribute to its compressibility and toughness.

In conclusion, the length of the polyol chains and the degree of cross-linking during synthesis are used to modify the mechanical properties and uses of PU polymers. Because of its adaptability, PUs can be found in a variety of products, such as stiff plastics, durable coatings, soft foams, and elastic fibers.

2.3 Applications of Polyurethane:

Because of its many characteristics, including resilience to abrasion and chemicals, flexibility, and durability, polyurethane (PU) is a versatile polymer that finds use in a wide range of applications. The following list of major uses for polyurethane is followed by an explanation of each:

2.3.1 Foams:

Flexible foams: Used as cushions in automobile seats, mattresses, and furniture. Because of their softness and comfort, these foams are perfect for products like car seats, pillows, and beds.

Rigid foams: utilized as insulation in refrigerators, appliances, and structures. Because of their superior thermal insulation qualities, they are useful for regulating temperature and saving energy.

2.3.2 Coatings:

Protective Coatings: Surfaces covered with protective coatings are shielded from weathering, corrosion, and abrasion. Polyurethane coatings are often applied to industrial equipment, floors, bridges, and ships to increase their longevity and durability.

Automotive coatings: Applied to automotive surfaces to provide a glossy appearance and defense against environmental deterioration, UV rays, and scratches. These coatings support the preservation of cars' structural integrity and visual appeal.

2.3.3 Adhesives and Sealants:

Construction Adhesives: Utilized in building and construction for bonding various materials such as wood, metal, and concrete. These adhesives provide strong, durable bonds and can withstand environmental stresses.

Sealants: Used for sealing joints and gaps in buildings, vehicles, and other structures. Polyurethane sealants offer flexibility and resistance to water, chemicals, and weathering, making them suitable for various sealing applications.

2.3.4 Elastomers:

Automotive Parts: Used in gaskets, bushings, and other parts that need to be flexible and long-lasting. Car parts operate better and endure longer because to polyurethane elastomers' superior resistance to deterioration.

Industrial Applications: Applied to conveyor systems, machinery, wheels, and rollers. These elastomers are perfect for industrial settings because of their great load-bearing capability and abrasion resistance.

2.3.5 Textiles and Apparel:

Synthetic fibers: Found in flexible textiles like spandex. Since they are comfortable and elastic, polyurethane fibers are widely used in sportswear, swimming, and other flexible clothing items.

Coated Fabrics: Found in outdoor gear, upholstery, and waterproof/weather-resistant apparel. These textiles combine the protective qualities of polyurethane coatings with the suppleness of textiles.

2.3.6 Footwear:

Due to their durability and cushioning properties, shoe insoles and soles are produced. Since polyurethane soles are lightweight and wear-resistant, they offer support and comfort.

2.3.7 Electronics:

Encapsulation and Potting Compounds: Used to shield electrical parts from mechanical harm, moisture, and dust. These substances improve the resilience and insulation of electronic equipment.

2.3.8 Medical Applications:

Implants and Devices: Found in some implants, some medical devices, and wound dressings. Biocompatible polyurethane materials can be developed to possess qualities - like flexibility and durability - that are necessary for medical applications.

Orthopedic braces and supports: Used in products that need to be strong and flexible, these items give patients comfort and support.

2.3 Chemistry of Polyurethane:

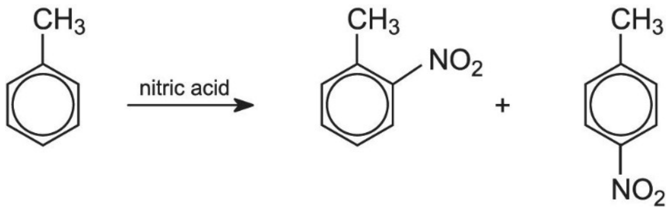
Understanding the synthesis of isocyanates and polyols, the precursors of polyurethanes, is crucial to understanding the chemistry and manufacturing of polyurethanes. Since they usually serve as examples of the more general ideas involved in synthesizing these precursors, the discussion will concentrate on the most often utilized compounds. Polyurethanes are often created via the interaction of isocyanates with polyols, as was previously explained. This section will be broken up into three sections to give a thorough rundown:

2.3.1 Synthesis of Isocyanate:

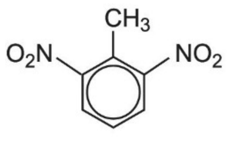
Isocyanates, which are key precursors for polyurethane polymers, come in various forms, including aromatic and aliphatic types. Nevertheless, two specific isocyanates dominate industrial polyurethane production, accounting for about 95% of usage. These are toluene diisocyanate (TDI) and methylene diphenyl diisocyanate (MDI), represented by the following chemical structures:

2.3.1.1 Toluene diisocyanates (TDI):

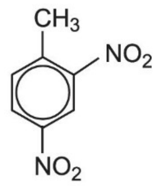
The raw material used in synthesizing TDI is toluene. When toluene reacts with nitric acid, it produces two nitro-toluene isomers: -



And as these products further nitrated, they gan more nitrite group producing dinitro-toluene (DNT) where the isomer yield at 80% 2,4-DNT and 20% 2,6-DNT.

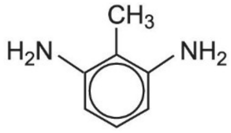


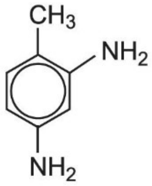
2,6-DNT



2,4-DNT

These two DNT isomer are then reduced, using metal catalysts to obtain amines that are commercially known as toluene diamines (DTA): -





The process can be carried out in a liquid phase with chlorobenzene as solvent at low temperature of 77^0C. The other method is carried out in gas phase mixed with carbonyl chloride at temperature of 327^0C.

2.3.1.2 Applications of Toluene diisocyanates (TDI):

TDI serves as an intermediate in creating polyurethanes and polycarbonates, both of which have numerous valuable properties. Polycarbonates are extensively utilized in the production of CD and DVD discs, while polyurethanes are employed in making foams, elastomers, and rigid polymers. The report outlines a chemical process that produces nearly 100% pure TDI without the use of phosgene, a common component in traditional methods.

2.3.1.3 Phosgene Compound:

Phosgene is a colorless, volatile liquid or gas produced by passing purified carbon monoxide and chlorine gas over a bed of porous activated carbon. It is a valuable reagent and building block in industrial organic synthesis, but it is also highly toxic. Industrial leaks of phosgene have resulted in numerous casualties. Historically, phosgene was used as a chemical weapon in World War I. At 70°F (room temperature), phosgene is a toxic gas that can appear colorless or as a white to pale yellow cloud. Its odor is not always detectable to those exposed.

Though not as infamous as mustard gas, phosgene is a deadly poison that has caused more fatalities. During World War I, phosgene was responsible for about 85% of the 100,000 deaths caused by chemical weapons. It reacts violently and decomposes into toxic compounds when it encounters moisture, producing chlorine, carbon monoxide, and carbon tetrachloride. Exposure to phosgene can occur through skin or eye contact, inhalation, or consumption of contaminated water or food. Inhalation is particularly dangerous as phosgene reacts with water in the lungs, releasing HCl and causing severe respiratory damage. It can also harm the skin, eyes, nose, and throat.

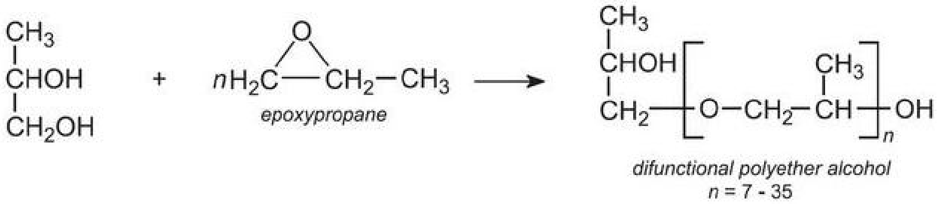
2.3.2 Synthesis of Polyol:

Polyols, which are organic compounds containing two or more hydroxyl groups, are essential in the production of polyurethane (PU) polymers. Among the various types of polyols available, hydroxyl-terminated polyether's and hydroxyl-terminated polyesters are the most used, accounting for approximately 90% of PU manufacturing.

The selection of polyols is critical as factors such as the number of hydroxyl groups, chain length, size, and the flexibility of the polyol structure play a significant role. These factors determine the degree of cross-linking between molecules in PU polymers, which in turn profoundly influences the final properties of the polymers.

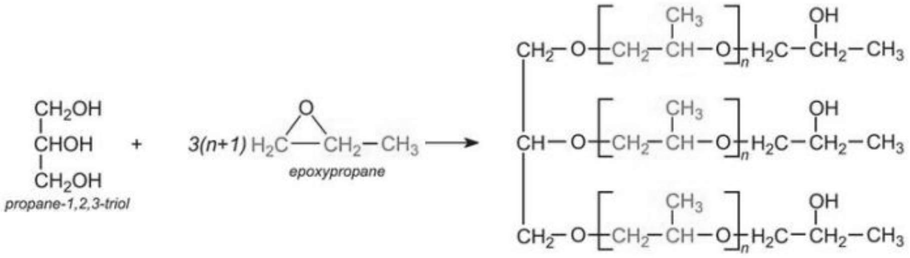
2.3.2.1 Hydroxyl-terminated polyether:

These polyols are synthesized from propane-1,2-diol and epoxypropane (propylene oxide) where this reaction is followed by hydrolysis: -



2.3.2.2 Hydroxyl-terminated polyester:

These polyols are synthesized similarly by hydrolysis from reacting propane-1,2,3-triol and epoxypropane as showing: -



2.3.3 Synthesis of Polyurethane:

In the synthesis of polyurethane (PU) using a common catalyst, consider a straightforward precursor scenario involving a diol as the polyol and MDI (methyl diphenyl diisocyanate) as the isocyanate, catalyzed by 1,4-diazabicyclo [2.2.2] octane (DABCO).

2.3.3.1 Role of DABCO Catalyst:

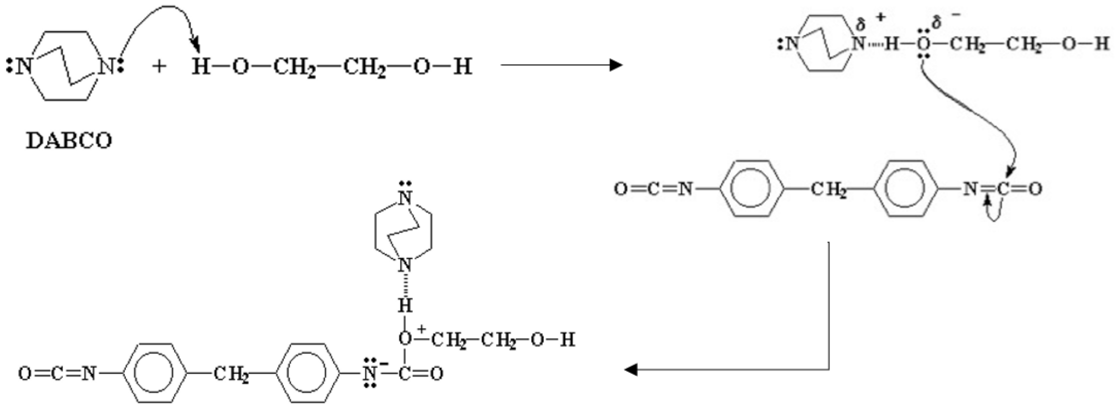
DABCO plays a crucial part in the PU synthesis process. It forms hydrogen bonds with the diol, causing the nitrogen in DABCO to become partially positive and the oxygen in the diol to become partially negative. This interaction sets the stage for subsequent reaction steps.

2.3.3.2 Interaction with MDI:

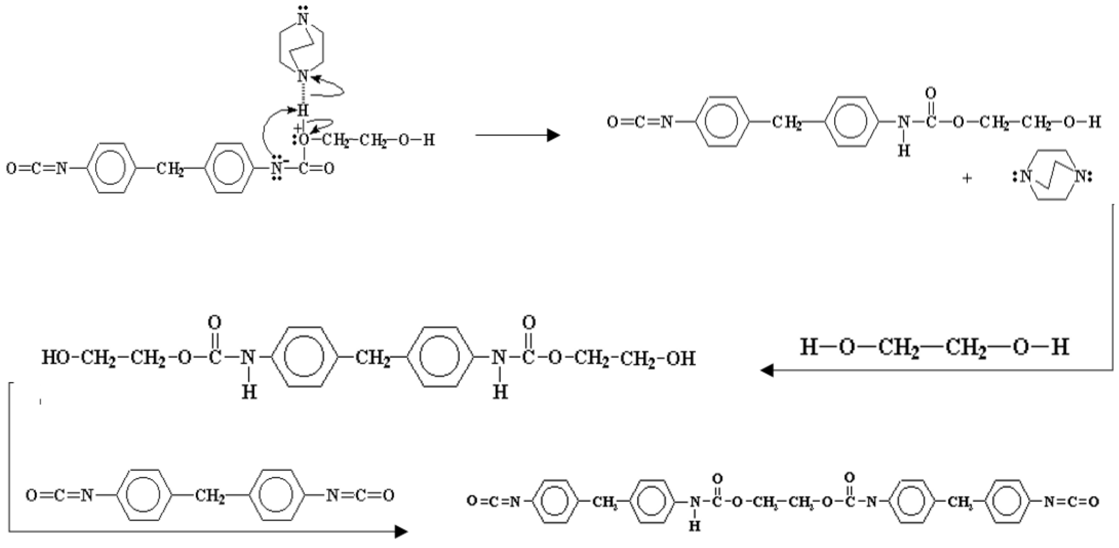
When MDI is introduced, the partially negative oxygen in the diol donates electrons to the carbon in MDI. This results in the oxygen becoming partially positive and the nitrogen in MDI becoming partially negative. This charge distribution facilitates the nucleophilic attack of the nitrogen on the electrophilic carbon in MDI, leading to the formation of a urethane linkage.

2.3.3.3 Polyurethane Formation:

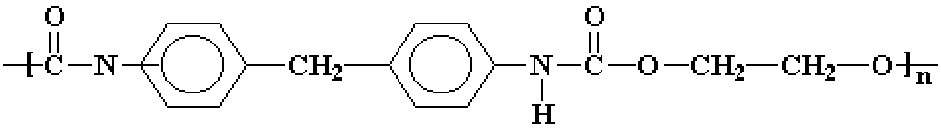
The nucleophilic attack by the nitrogen in MDI on the carbon creates a bond between the isocyanate group (-NCO) of MDI and one of the hydroxyl groups (-OH) of the diol, forming the urethane linkage (-NHCOO-). This process repeats with other hydroxyl groups of the diol and isocyanate groups of MDI, resulting in the formation of a polyurethane polymer chain.



Partially negative nitrogen in MDI pulls hydrogen from the diol where it forms a urethane dimer. The dimer can react with either another diol or MDI to produce a trimer and so on this process goes to produce polyurethane polymer. The isocyanate part is the hard and rough part of the polymer while polyol is responsible to soft flexibly part where this behavior is due to the oxygen atom in the polyol part.



The final product of this sequential process can be presented by the following: -



CHAPTER 3

PROCESS DESCRIPTION

3.1 Process Flow Diagram:

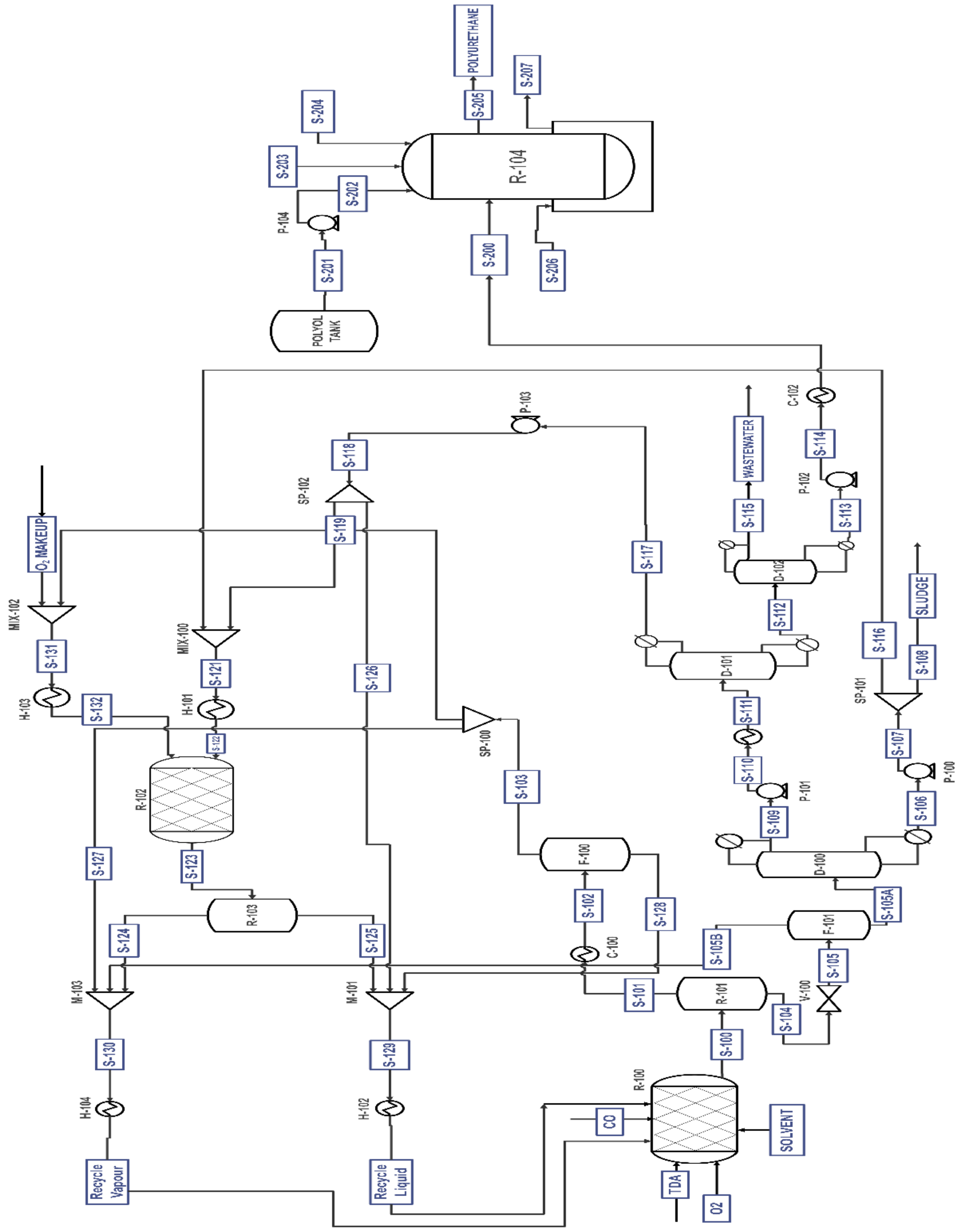


Figure 1 Process Flow Diagram

3.2 Block Flow Diagram:

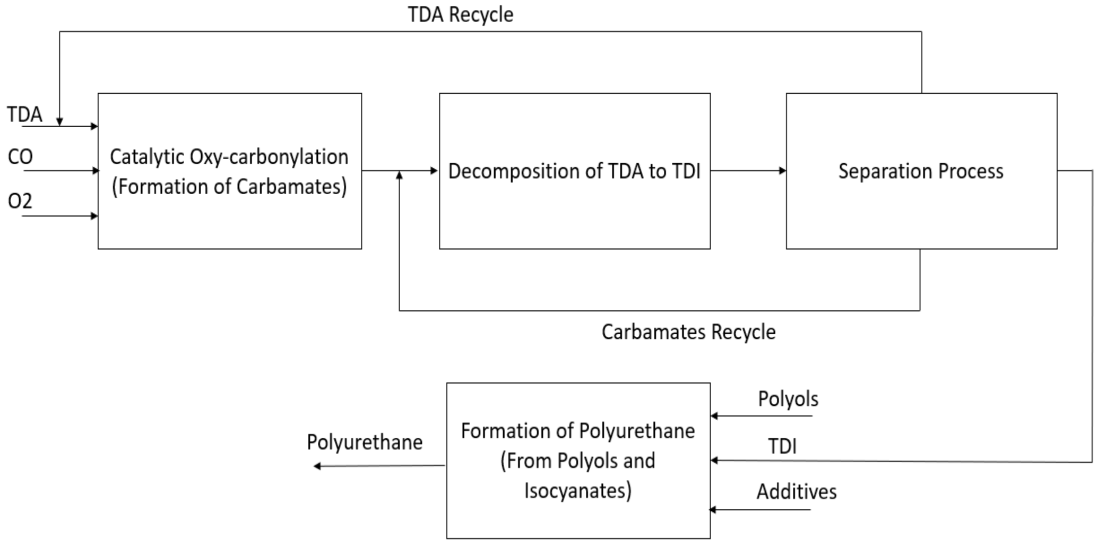


Figure 2 Block Flow Diagram

3.3 Process Description:

The block flow diagram illustrates the flows to and from the key sections of the phosgene-free polyurethane production process. There are two major sections of the process: the reaction section and the separation section. The conversion from TDA to TDI is achieved through the following two-step catalytic reaction.

Reaction 1: $\text{TDA} + 2\text{CO} + \text{O}_2 + 2\text{TFE} \longrightarrow \text{Carbamate} + 2\text{S.I} + 2\text{H}_2\text{O}$

Reaction 2: $\text{Carbamate} + 2\text{S.I} \longrightarrow \text{TDI} + 2\text{TFE}$

These reactions are carried out at temperatures between 120°C and 180°C and pressures of 5 to 100 bar. Two reactors are used in the process to maximize hourly yield. The reactors operate non-adiabatically, with feeds entering at 120°C, the lower end of the optimal temperature range. The temperature increases to 139.3°C in the first reactor and to 137.5°C in the second reactor. The first step involves the oxy-carbonylation of TDA, producing isomeric carbamates. The second step involves the decomposition of carbamates into TDI. Both steps occur within one reactor, facilitated by a Schiff Base-Type Ligand Catalyst using cobalt fixed to a silica bead solid support.

The solvent 2,2,2-trifluoroethanol (TFE) is used as an intermediate, maintaining stoichiometric amounts of O2 and CO in the liquid phase for the reaction while keeping O2 levels below the combustion limit.

The reactor effluent streams containing TDI, H2O, TFE, unreacted TDA, carbamates, CO, and O2 are decompressed and either recycled back through one of the reactors or sent through a series of three low-pressure distillation columns for separation. The separation process operates at low pressure, with a slight pressure drop gradient from 0.83 to 0.62 bar over the three-column distillation chain. A valve decompresses the stream connecting the reaction section to the separation section. In the first column, unused TDA and carbamates are removed as bottoms product and sent to the second reactor. After the next separation step, the solvent and reactant gases are recycled back to the reactor system, while the heavier wastewater and TDI are sent to the third distillation column for separation, yielding pure TDI.

Once pure TDI is obtained, it is combined with ethylene glycol and additives in a reactor. The production of polyurethane from polyols and isocyanates occurs through a polyaddition reaction at 25°C and 120 bar. In the main reaction, toluene di-isocyanates and ethylene glycol react to form a urethane compound. The reaction is as follows.

$$C_9H_6N_2O_2 + 2C_2H_2O_2 \longrightarrow C_{13}H_{10}N_2O_6$$

The isocyanates also react with water to form carbon dioxide and polyurea compounds. The reaction is as follows.

$$C_9H_6N_2O_2 + 2H_2O \longrightarrow 2CO_2 + C_7H_{10}N_2$$

Carbon dioxide acts as a blowing agent in the foam-making process. Due to the high reactivity of isocyanates, a 97% conversion of reactants into polyurethane is achieved. The reaction is highly exothermic, so a cooling jacket is installed around the reactor.

CHAPTER 4

MATERIAL BALANCE

The material balance involves tracking the quantities of Toluene diamine, polyols, and other raw materials entering the system and comparing them with the quantities of polyurethane and byproducts produced. The material balance equations are typically based on the principle of conservation of mass and can be expressed as follows:

Mass In – Mass Out + Generation – Consumption = Accumulation

Units are (kg/hr)

Basis: 1-hour steady state operation on a close system

4.1 Reactor R-100:

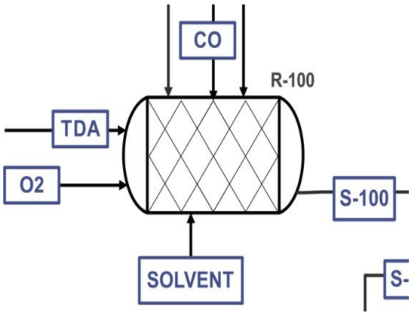


Figure 3 Reactor R-100

The oxy-carbonylation reaction takes place in this reactor. The toluene diamine, oxygen and carbon monoxide are first converted to carbamate which then decompose to form Toluene diisocyanate. The solvent is regenerated in the second step.

Material Balance:

Steady state operation

Mass Out = Mass In + Generation – Consumption

Reactions:

Reaction 1: $TDA + 2CO + O_2 + 2TFE \longrightarrow Carbamate + 2S.I + 2H_2O$

Conversion (TDA to Carbamate) = 82.5%

Reaction 2: $Carbamate + 2S.I \longrightarrow TDI + 2TFE$

Conversion (Carbamate to TDI) = 82%

Extent balance is used to calculate the moles of reactants and products at product side.

Extent = (Moles In – Moles Out) / Stoichiometric coefficient

Table 1 Reactor R-100 Material Balance

Inlet							Outlet
Component	CO	TDA	O2	Solvent	Recycle Vapor	Recycle Liquid	S-100
CO	5805.1	0	0	0	47751.7	1701.2	50335.4
O2	0	0	2778.83	0	576.51	46.49	492.36
TFE	0	0	0	43.2	34240.2	473656.2	506011.6
TDA	0	12683.7	0	0	0.13	340.5	2293.3
TDI	0	0	0	0	5.42	4445.9	19975.7
H2O	0	0	0	0	609.7	1029.5	3939.4
Carbamate	0	0	0	0	132.8	1836.0	4012.6

4.2 Phase Separator R-101:

Material Balance:

Mass In = Mass out 1 + Mass out 2

Table 2 Phase Separator R-101 Material Balance

Components	S-100	S-101	S-104
CO	50335.4	44809.6	5525.8
O2	492.4	415.30	77.1
TFE	506011.6	47217.2	458794
TDA	2293.3	0.8901	2292.4
TDI	19975.7	21.88	19953.8
H2O	3939.4	568.31	3371.1
Carbamate	4012.6	133.4	3879.2
Total	587060.5	93166.6	493893.4

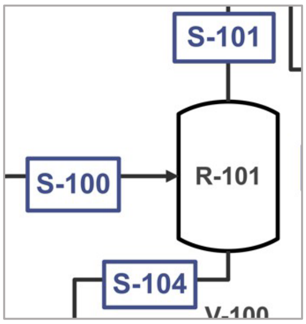


Figure 4 Phase Separator R-101

4.3 Distillation Column D-100:

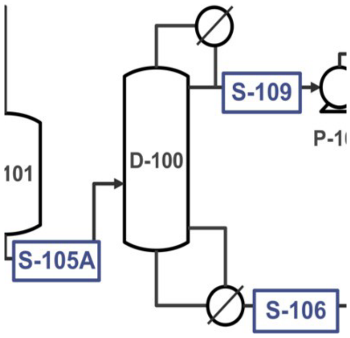


Figure 5 Distillation Column D-100

LKC and HKC are decided based on their relative volatilities.

LKC: Toluene diisocyanate (TDI)

HKC: Toluene diamine (TDA)

Overall Mass Balance:

F = D + W

R = L/D

Reflux ratio = R = 2.4

Table 3 Distillation Column D-100 Material Balance

Components	**S-105 A**	**S-106**	**S-109**
CO	3.1386	0	3.1386
O2	0.369	0	0.369
TFE	436631	0	436631
TDA (**HKC**)	2292.38	2287.79	4.585
TDI (**LKC**)	19952.9	3.99	19948.91
H2O	2868.04	0	2868.04
Carbamate	3804.04	3804.04	0
Total	465551.87	6095.826	459456.04

4.4 Pump P-100:

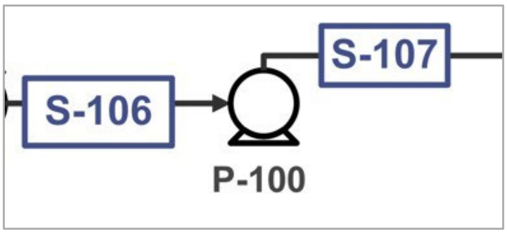


Figure 6 Pump P-100

Mass In = Mass Out

Table 4 Pump P-100 Material Balance

Components	**S-106**	**S-107**
CO	0	0
O2	0	0
TFE	0	0
TDA	2287.79	2287.79
TDI	3.99	3.99
H2O	0	0
Carbamate	3804.04	3804.04
Total	6095.826	6095.826

4.5 Splitter SP-101:

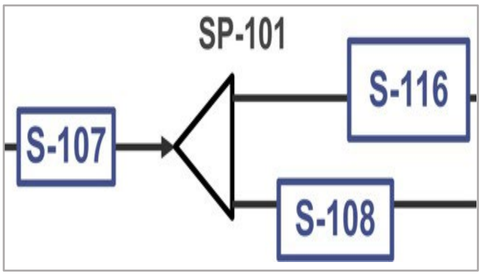


Figure 7 Splitter SP-101

Mass In = Mass out 1 + Mass out 2

Table 5 Splitter SP-101

Components	**S-107**	**S-108**	**S-116**
CO	0	0	0
O2	0	0	0
TFE	0	0	0
TDA	2287.8	22.88	2264.9
TDI	3.99	0.040	3.95
H2O	0	0	0
Carbamate	3804.0	38.04	3766
Total	6095.83	60.96	6034.9

4.6 Heat Exchanger H-100:

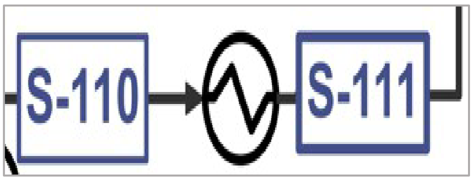


Figure 8 Heat Exchanger H-100

Mass In = Mass Out

Table 6 Heat Exchanger H-100 Material Balance

Components	S-110	S-111
CO	3.14	3.14
O2	0.37	0.37
TFE	436631	436631
TDA	4.59	4.59
TDI	19948.91	19948.91
H2O	2868.04	2868.04
Carbamate	0	0
Total	459456.04	459456.04

4.7 Distillation Column D-101:

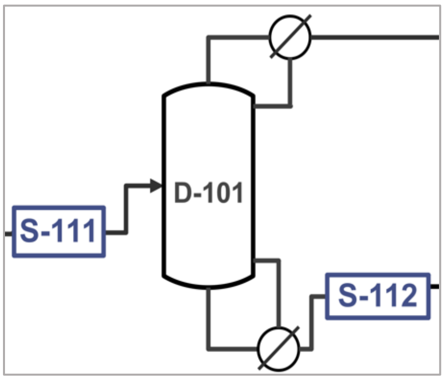


Figure 9 Distillation Column D-101

LKC and HKC are decided based on their relative volatilities.

LKC: Trifluoroethanol (TFE)

HKC: Water (H_2O)

Overall Mass Balance:

F = D + W

R = L/D

Reflux ratio = R = 1.05

Table 7 Distillation Column D-101 Material Balance

Components	S-111	S-112	S-117
CO	3.14	0	3.14
O2	0.37	0	0.37
TFE (**LKC**)	436631	43.7	436587.3
TDA	4.585	4.59	0
TDI	19948.91	19948.91	0
H2O (**HKC**)	2868.04	2867.47	0.57
Carbamate	0	0	0
Total	459456.04	22864.63	436591.4

4.8 Distillation Column D-102:

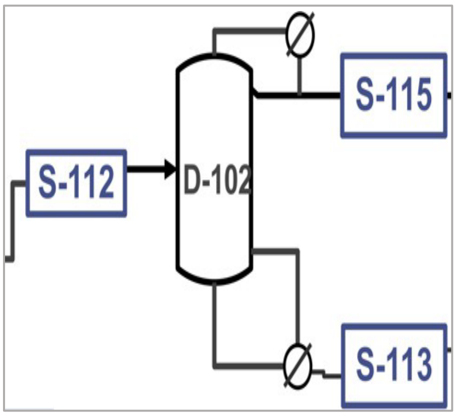


Figure 10 Distillation Column D-102

LKC and HKC are decided based on their relative volatilities.

LKC: Trifluoroethanol (TFE)

HKC: Water (H_2O)

Overall Mass Balance:

F = D + W

R = L/D

Reflux ratio = R = 3.2

Table 8 Distillation Column D-102 Material Balance

Components	S-112	S-115	S-113
CO	0	0	0
O2	0	0	0
TFE	43.7	43.7	0
TDA	4.59	0	4.59
TDI (**HKC**)	19948.9	7.98	19940.9
H2O (**LKC**)	2867.47	2865.75	1.72
Carbamate	0	0	0
Total	22864.63	2917.4	19947.2

4.9 Mixer MIX-102:

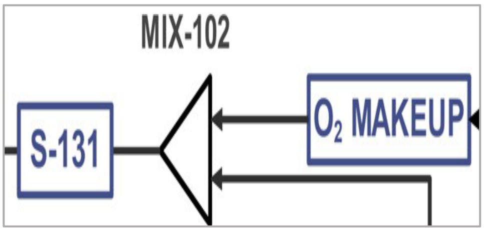


Figure 11 Mixer MIX-102

Mass In 1 + Mass In 2 = Mass Out

Table 9 Mixer MIX-102 Material Balance

Components	S-120	O2 Makeup	S-131
CO	13341	0	13341
O2	122.5	635	757.6
TFE	339.9	0	339.9
TDA	4.66E-07	0	4.66E-07
TDI	0.00028	0	0.00028
H2O	10.41	0	10.41
Carbamate	0.43	0	0.43
Total	13814.3	635	14449.3

4.10 Reactor R-102:

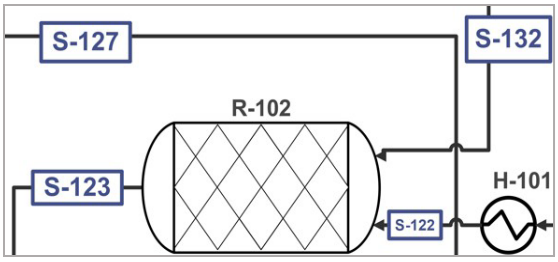


Figure 12 Reactor R-102

Material Balance:

Steady state operation

Mass Out = Mass In + Generation – Consumption

Reactions:

Reaction 1: $TDA + 2CO + O_2 + 2TFE \xrightarrow{\hspace{2cm}} Carbamate + 2S.I + 2H_2O$

Conversion (TDA to Carbamate) = 82.5%

Reaction 2: $Carbamate + 2S.I \xrightarrow{\hspace{2cm}} TDI + 2TFE$

Conversion (Carbamate to TDI) = 82%

Extent balance is used to calculate the moles of reactants and products on the product side.

Extent = (Moles In – Moles Out) / Stoichiometric coefficient

Table 10 Reactor R-102 Material Balance

Components	S-132	S-122	S-123
CO	13341	0.88	12485.38
O2	757.55	0.103	268.124
TFE	339.88	122244.45	125004.38
TDA	4.66E-07	2.26E+03	396.36
TDI	0.00027	3.951	4775.29
H2O	10.41	0.161	561.17
Carbamate	0.433	3766	1250.16
Total	14449.27	128280.47	144740.87

4.11 Reactor R-104:

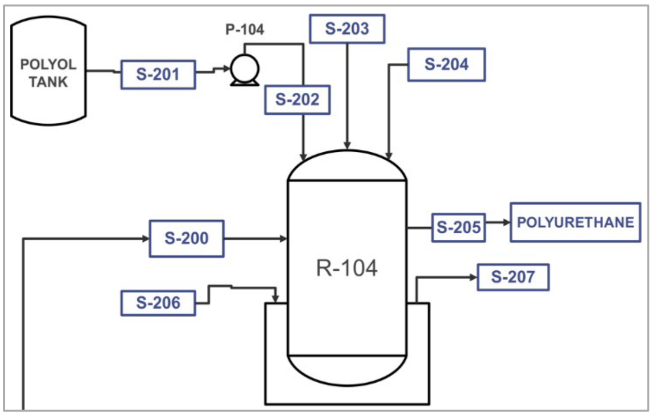


Figure 13 Reactor R-104

Material Balance:

Steady state operation

Mass Out = Mass In + Generation – Consumption

Reactions:

Main Reaction: $C_9H_6N_2O_2 + 2C_2H_2O_2 \longrightarrow C_{13}H_{10}N_2O_6$

Conversion (TDI to Polyurethane) = 97%

Side Reaction: $C_9H_6N_2O_2 + 2H_2O \longrightarrow 2CO_2 + C_7H_{10}N_2$

Conversion (TDI to CO_2) = 70%

We use the extent balance to calculate the moles of reactants and products on the product side.

Extent = (Moles In – Moles Out) / Stoichiometric coefficient

Table 11 Reactor R-104 Material Balance

Components	S-200	S-202	S-203	S-204	S-205
TDI	19941.9	0	0	0	179.48
Ethylene Glycol	0.000	19941.9	0.000	0	6157.07
Water	0.000	0.000	1994.19	0	1907.65
Triethylamine	0.000	0.000	0.000	315.4	315.4
Urethane	0.000	0.000	0.000	0	32202.44
Polyurea Compounds	0.000	0.000	0.000	0	293.29
CO2	0.000	0.000	0.000	0	134.625
Total	19941.9	19941.9	1994.19	315.4	41189.93

CHAPTER 5

ENERGY BALANCE

After finalizing the material balance, Energy balance was performed on the appropriate equipment. Based on the idea of energy conservation, the energy balance equations have the following form:

Total Energy In = Total Energy Out

As energy can neither be created nor destroyed but it can be converted to other forms of energy so all the energy going into the system will be converted to heat or performed work. Energy balance applied on the equipment are:

5.1 Reactor R-100:

Energy Balance:

$\Delta\dot{H} = \xi\Delta\dot{H}_r + \sum H_{out} - \sum H_{in}$

$Q = m(\mathbf{\Delta}H)$

$Q = mCp(\mathbf{\Delta}T)$

Enthalpy of reaction is calculated by heat of formation method where heat of formation is determined through literature and enthalpy balance is applied on the reactor. Enthalpy of reaction is calculated for both reactions.

Table 12 Reactor R-100 Energy Balance

Properties	**Units**	**TDA**	**O2**	**Solvent**	**CO**	**Recycle vapor**	**Recycle liquid**	**S-100**
Pressure	bar	45	45	45	45	45	45	45
Temperature	°C	120	120	120	120	120	120	139.3
Mass Flow	kg/hr	12683.7	2778.83	43.25	5805.12	83316.50	483055.80	587060.46
Hin	kJ/hr	106425438.9						-
Hout	kJ/hr	-						135542285.1
ΔH	kJ/hr	-18954654.34						

5.2 Phase Separator R-101:

Energy Balance:

Enthalpy In = Enthalpy Out

Enthalpy is calculated using relation:

Q = mCp(**Δ**T)

Table 13 Phase Separator R-101 Energy Balance

Properties	**Units**	**S-100**	**S-101**	**S-104**
Pressure	bar	45	45	45
Temperature	°C	139.3	139.3	139.3
Mass Flow	kg/hr	587060.46	93166.58	493893.42
Hin	kJ/hr	135542285.1	-	-
Hout	kJ/hr	-	10887265.97	122439979.4
ΔH	kJ/hr	0		

5.3 Distillation Column D-100:

Enthalpy of feed, distillate and bottoms are calculated using relation:

ΔH = m$Cp(\Delta T)$

Condenser duty is calculated by this relation.

Qc = V * lamda v

Where;

V= (R+1) D

V = 1562150.54

lamda v = 2092.5

Qc = 3268800011 kJ/hr

Boiler Duty is calculated using relation.

Qb= Hd+Hw+Qc-Hf

Qb = 3261843932 kJ/hr

Table 14 Distillation Column D-100 Energy Balance

Properties	**Units**	**S-105 A**	**S-106**	**S-109**
Pressure	bar	0.345	0.34	0.138
Temperature	°C	11.14	40.71	2
Mass Flow	kg/hr	465551.87	6095.83	459456.04
H	kJ/hr	8805300.17	314637.32	1534583.18

5.4 Pump P-100:

Pumps are used to increase the pressure of liquids. Pump duty is calculated using Bernoulli's equation:

$$Q_{pump} = \frac{m}{\eta}\left(\frac{\Delta P}{\rho}\right)$$

η = 75%

Table 15 Pump P-100 Energy Balance

Parameters	Units	S-106	S-107
Temperature	°C	65.41	66.1314
Pressure	kPa	33.7843	4502.28
Density	kg/m^3	1484.13	1483.47
Mass Flow Rate	kg/h	6095.82582	6095.826
Pump Duty	kW	24476.948	

5.5 Pump P-101:

Pumps are used to increase the pressure of liquids. Pump duty is calculated using Bernoulli's equation:

$$Q_{pump} = \frac{m}{\eta}\left(\frac{\Delta P}{\rho}\right)$$

η = 75%

Table 16 Pump P-101 Energy Balance

Parameters	Units	S-109	S-110
Temperature	°C	1.65	1.68
Pressure	kPa	13.7895	82.7371
Density	kg/m^3	1436.54	1436.62
Mass Flow Rate	kg/h	459456.042	459456.042
Pump Duty	kW	29401.67286	

5.6 Heat Exchanger H-100:

Heat exchangers are the devices used to exchange the heat between the two fluids. Energy released by the hot fluid must be equal to the energy absorbed by the cold fluid.

Energy balance:

$\Delta H_{HOT} + \Delta H_{COLD} = 0$

As there is no phase change while releasing or absorbing the energy in the fluids so no latent heat is involved.

Q = $mcp\Delta T$

Table 17 Heat Exchanger H-100 Energy Balance

Properties	units	S-110	S-111
Temperature	°C	1.68	48.89
Pressure	bar	0.83	0.73
Mass flow	kg/h	459456.042	459456.042
Mass heat capacity	kJ/kg K	1.677	1.777
H	kW	-17852665.3	19626722.96
Heater Duty (Q)	kW	1.77E+10	

5.7 Distillation Column D-101:

Enthalpy of feed, distillate and bottoms are calculated using relation:

$\mathbf{\Delta}$H = m$Cp(\mathbf{\Delta}T)$

Condenser duty is calculated by this relation.

Qc = V * lamda v

Where;

V= (R+1) D

V = 895011.55

lamda v = 194.55

Qc = 174124497.1 kJ/hr

Boiler Duty is calculated using relation.

Qb= Hd+Hw+Qc-Hf

Qb = 159519910.8 kJ/hr

Table 18 Distillation Column D-101 Energy Balance

Properties	**Units**	**S-111**	**S-117**	**S-112**
Pressure	bar	0.48	0.34	0.54
Temperature	°C	24.03	2	68.88
Mass Flow	kg/hr	459456.04	436591.42	22864.62
H	kJ/hr	18548424.2	1463454.43	2480383.53

5.8 Distillation Column D-102:

Enthalpy of feed, distillate and bottoms are calculated using relation:

$\mathbf{\Delta}\mathrm{H} = \mathrm{m}Cp(\mathbf{\Delta}T)$

Condenser duty is calculated by this relation.

Qc = V * lamda v

Where;

V= (R+1) D

V = 15381.093

lamda v = 7296.15

Qc = 112222761.7 kJ/hr

Boiler Duty is calculated using relation.

Qb= Hd+Hw+Qc-Hf

Qb = 114091614.5 kJ/hr

Table 19 Distillation Column D-102 Energy Balance

Properties	**Units**	**S-112**	**S-115**	**S-113**
Pressure	bar	0.54	0.345	0.54
Temperature	°C	68.88	13.87	153.03
Mass Flow	kg/hr	22864.62	2917.39	19947.23
H	kJ/hr	2480383.53	188158.43	4145329.48

5.9 Pump P-102:

Pumps are used to increase the pressure of liquids. Pump duty is calculated using Bernoulli's equation:

$$Q_{pump} = \frac{m}{\eta}\left(\frac{\Delta P}{\rho}\right)$$

η = 75%

Table 20 Pump P-102 Energy Balance

Parameters	**Units**	**S-117**	**S-118**
Temperature	°C	1.15	1.2
Pressure	bar	34.4738	4502
Density	kg/m^3	1469.51	1474.82
Mass Flow Rate	kg/h	464396.9	464396.9
Pump Duty	kW	1879051.436	

5.10 Pump P-103:

Pumps are used to increase the pressure of liquids. Pump duty is calculated using Bernoulli's equation:

$$Q_{pump} = \frac{m}{\eta}\left(\frac{\Delta P}{\rho}\right)$$

η = 75%

Table 21 Pump P-103 Energy Balance

Parameters	**Units**	**S-113**	**S-114**
Temperature	°C	168.33	169.10
Pressure	bar	14	1200
Density	kg/m^3	1020.1	1022.69
Mass Flow Rate	kg/h	19947.2351	19947.24
Pump Duty	kW	30882.49675	

5.11 Heat Exchanger C-100:

Heat exchangers are the devices used to exchange the heat between the two fluids. Energy released by the hot fluid must be equal to the energy absorbed by the cold fluid.

Energy balance:

$\Delta H_{HOT} + \Delta H_{COLD} = 0$

As there is no phase change while releasing or absorbing the energy in the fluids so no latent heat is involved.

$Q = mcp\Delta T$

Table 22 Heat Exchanger C-100 Energy Balance

Properties	units	S-101	S-102
Temperature	°C	139.45	37.78
Pressure	bar	45	44.66
Mass flow	kg/h	9.32E+04	9.32E+04
Mass heat capacity	kJ/kg K	1.47	1.45
H	kW	1.57E+07	1.75E+06
Heater Duty (Q)	kW	-3.42E+07	

5.12 Reactor R-102:

Energy Balance:

$\Delta H^{\cdot} = \xi \Delta H^{\cdot}r + \sum Hout - \sum Hin$

$Q = m(\Delta H)$

$Q = mCp(\Delta T)$

Enthalpy of reaction is calculated by heat of formation method where heat of formation is determined through literature and enthalpy balance is applied on the reactor. Enthalpy of reaction is calculated for both reactions.

Table 23 Reactor R-102 Energy Balance

Properties	Units	S-132	S-122	S-123
Pressure	bar	45	45	45
Temperature	°C	120	120	120
Mass Flow	kg/hr	14449.27	128280.47	144740.87
Hin	kJ/hr	1484089.77	24554957.51	-
Hout	kJ/hr	-	-	32694037.05
ΔH	kJ/hr	-722627058.8		

5.13 Pump P-200:

Pumps are used to increase the pressure of liquids. Pump duty is calculated using Bernoulli's equation:

$$Q_{pump} = \frac{m}{\eta}\left(\frac{\Delta P}{\rho}\right)$$

η = 75%

Table 24 Pump P-200 Energy Balance

Parameters	Units	S-201	S-202
Temperature	°C	25	26
Pressure	bar	1	12
Density	kg/m^3	1091.82	1093.17
Mass Flow Rate	kg/h	19941.930	19941.93
Pump Duty	kW	26771.897	

5.14 Reactor R-104:

Energy Balance:

$\Delta H^{\cdot} = \xi \Delta H^{\cdot}r + \sum Hout - \sum Hin$

Q = m(ΔH)

Q = mCp(ΔT)

Enthalpy of reaction is calculated by heat of formation method where heat of formation is determined through literature and enthalpy balance is applied on the reactor. Enthalpy of reaction is calculated for both reactions.

Table 25 Reactor R-104 Energy Balance

Properties	**Units**	**S-200**	**S-202**	**S-203**	**S-204**	**S-205**
Pressure	bar	12	12	12	12	12
Temperature	°C	25	25	25	25	
Mass Flow	kg/hr	19941.93	19941.93	1994.19	315.38	41189.93
Hin	kJ/hr	0				
Hout	kJ/hr	-	-	-	-	781830.93
Hrxn1 (308.15K)	kJ/hr	842604.4				
Hrxn2 (308.15K)	kJ/hr	-2392.472				
ΔH	kJ/hr	94341307.2				

Table 26 Water Jacket R-104 Energy Balance

Water Jacket			
Properties	**units**	**S-206**	**S-207**
Temperature	K	298.15	323.15
Pressure	bar	1	0.9
Mass flow	kg/h	8.86E+05	8.86E+05
Mass heat capacity	kJ/kg K	4.189	4.19
Q	kW	9.28E+07	

CHAPTER 6

EQUIPMENT DESIGN

6.1 Reactor R-100:

A reactor is a device or container designed to facilitate chemical reactions. It plays a crucial role in the process industry by transforming raw materials into valuable products.

6.1.1 Theory of Reactors:

The following are the most used reactor types in industry.

1. Batch Reactors
2. Continuous Stirred Tank Reactor
3. Fluidized Bed Reactor
4. Fixed Bed Reactor

6.1.1.1 Batch Reactor:

In a batch reactor, a specific number of reactants is handled, with the reaction taking place under controlled conditions. After the reaction starts, it continues until it is fully completed, at which point the products are extracted.

6.1.1.2 Continuous Stirred Tank Reactor:

A continuously stirred reactor, which allows for the constant addition and removal of reactants and products, is utilized in industrial applications for steady-state processes and continuous flow operations. It is ideal for reactions requiring thorough mixing, including homogeneous reactions, catalytic reactions, and enzymatic processes.

6.1.1.3 Fluidized Bed Reactor:

Fluidized bed reactors suspend and fluidize solid particles with the flow of gas or liquid, making the particles act like a fluid. This created bed exhibits characteristics of both liquids and solids. FBRs are particularly effective for catalytic reactions due to their improved heat and mass transfer capabilities.

6.1.1.4 Fixed Bed Reactor:

A fixed bed reactor is characterized by solid particles arranged in a stationary configuration, forming a packed bed. These particles remain immobile while reactants flow through them, facilitating the desired chemical reactions.

6.1.2 Selection of Fixed Bed Reactor:

Here are several key factors that led us to choose a fixed bed reactor for our process.

6.1.2.1 Efficient Utilization of Catalyst:

A fixed bed reactor optimizes catalyst usage by offering a large surface area for catalyst-reactant interactions, resulting in higher conversion rates and selectivity.

6.1.2.2 Continuous Operation:

A fixed bed reactor is utilized for continuous and stable operations, making it highly suitable for industrial applications. The feed is introduced into the reactor continuously while the products are simultaneously removed. It is assumed that the concentration of product in the outlet stream is same as the concentration inside the reactor.

6.1.2.3 Scalability:

The size of a fixed bed reactor can be easily adjusted by adding the catalyst, allowing it to be adaptable to various production needs.

6.1.2.4 Life Span of Catalyst:

In a fixed bed reactor, the catalyst particles remain stationary and do not interact with each other. Consequently, this extends the catalyst's lifespan. Additionally, there is no catalyst entrainment in a fixed bed reactor.

6.1.3 Design Calculations:

The design of a fixed bed reactor is crucial for ensuring efficient reaction kinetics, optimal conversion rates, and safe operation. This section provides an overview of key design considerations, and essential components involved in designing a packed bed reactor.

6.1.3.1 Key Design Considerations:

Designing an effective packed bed reactor involves several critical considerations:

6.1.3.1.1 Reactor Dimensions:

Determining the appropriate diameter and length of the reactor to ensure sufficient contact time and catalyst utilization.

6.1.3.1.2 Packing Material:

Selecting the appropriate catalyst or packing material based on the specific reaction requirements and physical properties.

6.1.3.1.3 Flow Distribution:

Ensuring uniform flow distribution to prevent channeling and maximize contact between reactants and the catalyst.

6.1.3.1.4 Heat Management:

Designing for effective heat removal or addition to maintain the desired reaction temperature, which may involve using heat exchangers or cooling jackets.

6.1.3.1.5 Pressure Drop:

Minimizing pressure drops across the packed bed to maintain efficient flow rates and reduce energy consumption.

6.1.3.1.6 Material of Construction:

Choosing materials that can withstand the chemical environment and operating conditions, such as temperature and pressure.

6.1.3.1.7 Safety and Control:

Implementing safety measures and control systems to manage reaction conditions and prevent hazards such as catalyst deactivation or runaway reactions.

6.1.3.2 Design Equation:

$W = \int \frac{F_{A0}\,dX}{-r_a}$

Where,
W = Catalyst Weight
F_{A0} = Initial Molar Flow of Component A
X = Conversion
r_a = Rate of Reaction

6.1.3.3 Reactions:

Reaction 1: $TDA + 2CO + O_2 + 2TFE \longrightarrow Carbamate + 2S.I + 2H_2O$

Conversion (TDA to Carbamate) = 82.5%

Reaction 2: $Carbamate + 2S.I \longrightarrow TDI + 2TFE$

Conversion (Carbamate to TDI) = 82%

6.1.3.4 Reactor Specifications:

Table 27 Reactor R-100 Specifications

Reactor Specifications	
Reactor Type	Packed bed reactor
Temperature (°C)	120
Pressure (bar)	45
Feed flowrate (kg/hr)	587159.013
Catalyst	3,5-di-Tert-butylsalicylidene-1,2-cyclohexadiamino-cobalt
Bulk density of Catalyst (kg/m3)	556.05
Void fraction	0.45

6.1.3.5 Design Procedure:

1. Residence time calculation through Euler's Method for solving ODEs.
2. Volume of reactor = residence time × volumetric flowrate
3. Volume of reactor =πr^2 L
4. L/D = 3
5. Volume of catalyst bed = (1+ E) * Volume of reactor
6. Pressure drop Calculations:

$$\frac{\Delta P}{L} = \frac{150\mu(1-\mathcal{E})2}{Dp2 \times \mathcal{E}3} \times vs + \frac{1.5\, vs2\rho(1-\mathcal{E})}{Dp\mathcal{E}3}$$

6.1.3.6 Calculated Parameters:

Table 28 Reactor R-100 Calculated Parameters

Parameters	Value
Residence time (hr)	0.496
Volume of reactor (m3)	995.23
Length of reactor (m)	22.5
Diameter of reactor (m)	7.5
Volume of catalyst bed (m3)	547.37
Length of catalyst bed (m)	18.4
Diameter of catalyst particle (mm)	0.9
Superficial velocity (m/s)	0.0126
Viscosity of fluid (pa.sec)	0.00028
Pressure drop (bar)	0.486

6.2 Distillation Column D-100:

Distillation is a fundamental separation process widely used in chemical, petrochemical, and pharmaceutical industries to purify and separate liquid mixtures based on differences in their boiling points. A distillation column is a key piece of equipment in this process, facilitating the efficient separation of components in a mixture through successive vaporization and condensation steps.

6.2.1 Purpose and Significance:

The primary purpose of a distillation column is to separate a liquid mixture into its individual components, each with a distinct boiling point. This separation is crucial for producing high-purity products, recycling solvents, and optimizing reaction conditions in various industrial applications. Distillation columns are essential in refining crude oil into gasoline, diesel, and other valuable products, as well as in the production of spirits, pharmaceuticals, and specialty chemicals.

6.2.2 Basic Principle:

Distillation columns operate on the principle of relative volatility, which describes how easily one component of a mixture can be vaporized compared to another. The process involves the following key steps:

Feed Introduction:

The liquid mixture (feed) is introduced into the column at a specific point.

Heat Application:

Heat is applied to the reboiler at the bottom of the column, causing the feed to vaporize.

Vapor-Liquid Equilibrium:

As the vapor rises through the column, it encounters cooler liquid flowing downward, creating multiple vapor-liquid equilibrium stages.

Condensation and Re-boiling:

At each stage, the vapor condenses into liquid, enriching the vapor with the more volatile component and the liquid with the less volatile component.

Product Collection:

The more volatile components are collected as distillate (overhead product) at the top of the column, while the less volatile components are collected as bottoms (residue) at the bottom.

Distillation columns can be designed in various configurations, such as packed columns, tray columns, and multiple-effect distillation systems, to accommodate different separation needs and efficiency requirements.

6.2.3 Design Calculations:

6.2.3.1 Feed Specifications:

Table 29 Table 29 Distillation Column D-100 Feed Specification

Components	**S-111**	**S-112**	**S-117**
CO	3.1386	0	3.1386
O2	0.369	0	0.369
TFE	436631	0	436631
TDA (HK)	2292.38	2287.79	4.585
TDI (LK)	19952.9	3.99	19948.91
H2O	2868.04	0	2868.04
Carbamate	3804.04	3804.04	0
Total	465551.8676	6095.82	459456.0426

6.2.3.2 Design Procedure:

1. Deciding Low Key and Heavy Key Components on the basis of relative volatilities.

   HKC = Toluene diamine (TDA)

   LKC = Toluene diisocyanates (TDI)

2. Calculation of relative volatilities of LKC and HKC using Antoine Equation for k value calculations.

   $\text{Log}(P^S) = A - \frac{B}{C+T}$

   $k_i = P^S / P$

   $\alpha = k_{HK} / k_{LK}$

Table 30 Antoine Equation Parameters

Antoine equation constants			
Component	A	B	C
TDI	6.240	230.27	260.01
TDA	5.79	3021.8	30.878

Table 31 Calculated relative volatilities.

Parameters	
Component	α
TDI	1.5
TDA	1

3. Calculation of Minimum Number of Stages using **Fenske's method**

$$N_m = \frac{\log\left[\frac{x_{LK}}{x_{HK}}\right]_d \log\left[\frac{x_{HK}}{x_{LK}}\right]_b}{\log \alpha_{LK}}$$

4. Draw the graph using feed line equation to find x' and y'.

$$q = \frac{\lambda + H_{fs} - H_f}{\lambda} = 1$$

q = 1 shows feed is at boiling point

$$Y = \frac{-q}{1-q}(x) + \frac{x_f}{1-q}$$

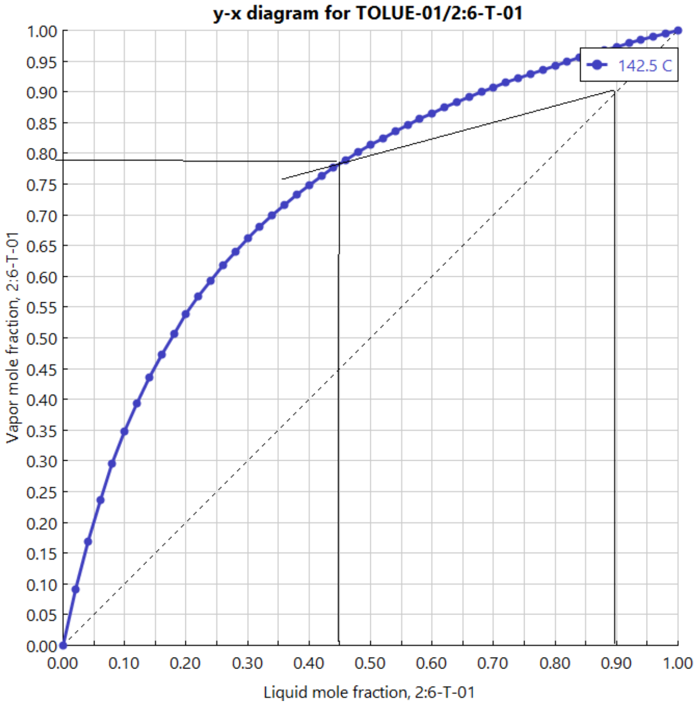


Figure 14 y-x diagram for TDI

5. Calculation of Rm, R, Nm & N using Gilliland Relation:

$$R_m = \frac{x_D - y'}{y' - x'}$$

$$R = R_m\,(1.5)$$

$$X = \frac{R - R_m}{R + 1}$$

$$\mathrm{Y} = \frac{1 - \mathrm{X}^{0.0031}}{1 - 0.99357 * \mathrm{X}^{0.0031}}$$

$$N = \frac{Y + N_m}{1 - Y}$$

6. Calculation of Efficiency using O'Connell correlation

   $E_0 = 51 - 32.5 \log (\mu a\ \alpha a)$

7. Calculation of Actual Number of stages using relation

   $E_0 = \frac{\text{Actual Stages}}{\text{Ideal Stages}}$

8. Calculation of height and diameter of column

$$D_c = \sqrt{\frac{4At}{0.8\,\pi}}$$

   Height of column = (no. of plates) × (plate spacing)

6.2.3.3 Calculated Parameters:

Table 32 Calculated Parameters for D-100

Specification of distillation Column	
No. of Theoretical plates	12.37
No. of Actual plates	38
Type of Plates	Bubble cap tray
Hole size (mm)	4
Reflux Ratio	0.7
Column Diameter (m)	4.09
Column Height (m)	22.8

6.3 Heat Exchanger H-100:

It is a 1-2 shell tube pass exchanger with Cold Water in the tubes and Feed solution in the shell side. We have designed the shell & tube heat exchanger using Kern's Method.

6.3.1 Shell Side Specifications:

Table 33 Shell Side Specifications

Shell Side (Hot Fluid)	
Properties	Lean Solution
Temperature (Inlet) (°C)	412
Temperature (Outlet) (°C)	310
Cp (average) (kJ/kg-°C)	1.25
Density (average) (kg/m3)	49.2599
Viscosity (average)(kg/ms)	0.00001985
Thermal Conductivity (average) (W/m K)	0.033
Mass Flow Rate (Kg/hr)	93165

6.3.2 Tube Side Specifications:

Table 34 Tube Side Specification

Tube Side (Cold Fluid)	
Properties	Water
Temperature (Inlet) (°C)	305
Temperature (Outlet) (°C)	322
Cp (average) (kJ/kg-°C)	6.129
Density (average) (kg/cm3)	700
Mass Flow Rate (kg/hr)	9555.53

6.3.3 Design Procedure:

1. Heat Duty Calculations using the following formula,

$$\boldsymbol{Q} = \boldsymbol{m} \times \boldsymbol{C_p} \times \Delta \boldsymbol{T}$$

2. LMTD Calculations using the following formula,

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

LMTD = (107-12)/ln (107/12) = 43.4°C

3. F_T correction factor Calculations

   R =107/12 = 8.91

   S = (322-305)/ (412-305) = 0.155,

Using these values of R and S, we find the value of the Correction factor from the given graph:

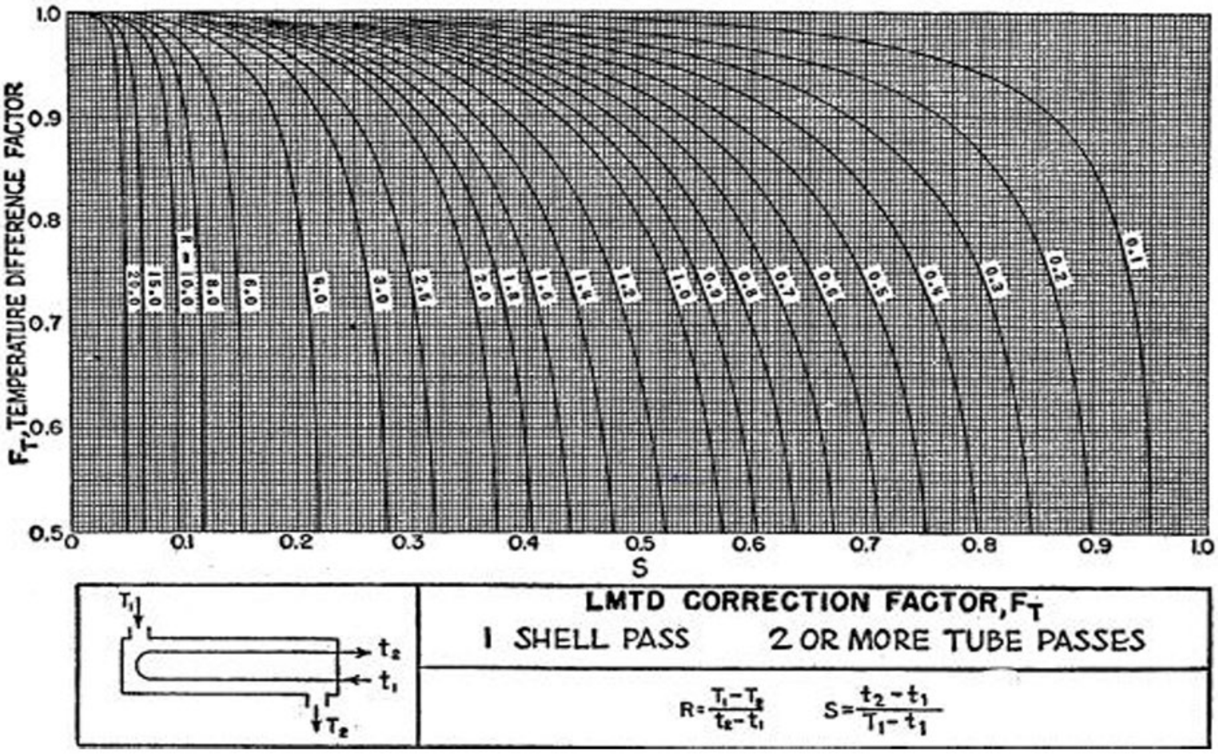


Figure 15 FT Correction Factor Calculation

F_T = 0.97

4. Corrected LMTD

   LMTD = 0.97 * 43.4°C = 42.1

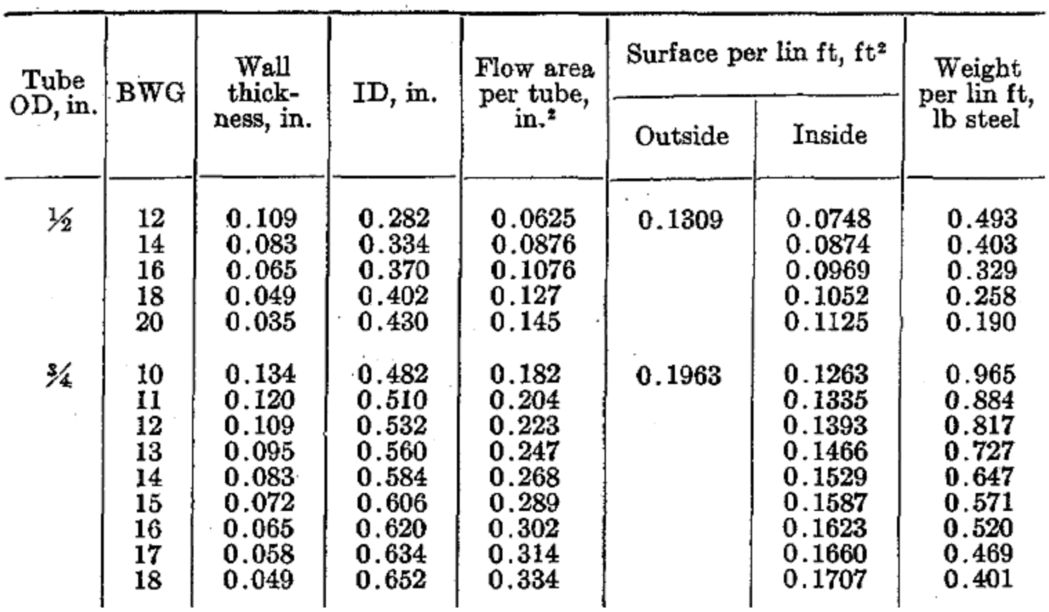
5. Calculation of Heat Transfer Area using formulas,

$$Q = UA \times \Delta T_m$$

$$A = \frac{3255000}{42.1 * 1000} = 77.31\text{m2}$$

6. Size Specifications of Tube

For the tube ID and the flow area the following data table is referred to, using the OD (19mm) and BWG (18) assumed.



Tube OD, in.	BWG	Wall thickness, in.	ID, in.	Flow area per tube, in.²	Surface per lin ft, ft²		Weight per lin ft, lb steel
					Outside	Inside	
½	12	0.109	0.282	0.0625	0.1309	0.0748	0.493
	14	0.083	0.334	0.0876		0.0874	0.403
	16	0.065	0.370	0.1076		0.0969	0.329
	18	0.049	0.402	0.127		0.1052	0.258
	20	0.035	0.430	0.145		0.1125	0.190
¾	10	0.134	0.482	0.182	0.1963	0.1263	0.965
	11	0.120	0.510	0.204		0.1335	0.884
	12	0.109	0.532	0.223		0.1393	0.817
	13	0.095	0.560	0.247		0.1466	0.727
	14	0.083	0.584	0.268		0.1529	0.647
	15	0.072	0.606	0.289		0.1587	0.571
	16	0.065	0.620	0.302		0.1623	0.520
	17	0.058	0.634	0.314		0.1660	0.469
	18	0.049	0.652	0.334		0.1707	0.401

Figure 16 Tube Size Specifications

7. Calculation of Area and number of tubes

For the assumed tube dimensions, the area is calculated as follows:

Area of one tube= π×D×L= π ×0.020×4.88= 0.306 m^2

The number of tubes required for this area would then be,

Number of tubes= (Total Area Required)/(Area of one tube)

Assuming Overall heat transfer coefficient (U) = 1000 W/m^2.K according to the given range available in the literature. Now total area required can be calculated as follows,

Number of tubes= 77.31/0.306=252

8. Tube Pitch and Tube Clearance Calculations

The pitch chosen for this type of heat exchanger is "Triangular Pitch", because of the higher rates of the heat transfer provided by this type of pitch along with the ease of cleaning. The tube pitch is calculated as follows,

$$\boldsymbol{Tube\ pitch\ (p_t)} = 1.25\ \times\ d_o = 1.25\ \times 0.020 = 0.025\ m$$

In addition, the tube clearance would then be calculated using the following formula,

$$\boldsymbol{Tube\ Clearance} = p_t - d_o = 0.025 - 0.020 = 0.005m$$

Table 35 Tube Specification Parameters

Specification Title	**Specification Value**
Number of Passes (N_P)	2
Tube Length (L)	4.88 m
Outer Diameter (d_o)	0.020 m
Inner Diameter (d_i)	0.016 m
BGW	18
Number of Tubes (N_T)	252
Surface area per tube	$0.291m^2$
Tube Pitch (p_t)	0.025 m
Tube Clearance	0.005 m
Flow area per tube	0.000215 m^2

9. Calculation of Shell Dimensions:

The following assumptions have been made for the calculation of shell dimensions,

Table 36 Shell Dimensions

Number of shell passes	1
Baffle Spacing (m)	0.094 (1/5 D_s)
Shell Diameter (m)	0.546
Baffle cut percentage (%)	25
Bundle Diameter (m)	0.456
Bundle Clearance(m)	0.090 (Pull Through Head)

Shell Internal Diameter is calculated as,

$$D_s = Bundle\ Diameter\ (D_b\ ) + Clearance = 0.456 + 0.090$$

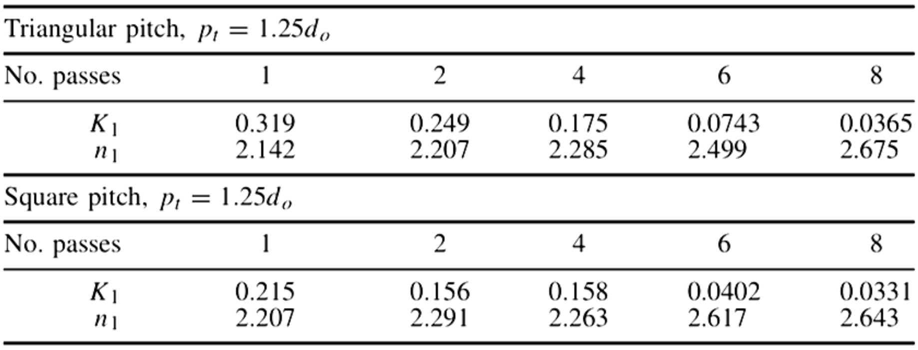
$$= 0.546m$$

$$Bundle\ Dia\ (D_b\ ) = d_o \times \left(\frac{N_T}{K_1}\right)^{\frac{1}{n_1}} = 0.020 \times \left(\frac{248}{0.249}\right)^{\frac{1}{2.207}} = 0.456m$$

Where the values of K_1 and n_1 are considered according to the pitch type,

$$K_1 = 0.249$$

$$n_1 = 2.207$$



Triangular pitch, $p_t = 1.25d_o$					
No. passes	1	2	4	6	8
K_1	0.319	0.249	0.175	0.0743	0.0365
n_1	2.142	2.207	2.285	2.499	2.675
Square pitch, $p_t = 1.25d_o$					
No. passes	1	2	4	6	8
K_1	0.215	0.156	0.158	0.0402	0.0331
n_1	2.207	2.291	2.263	2.617	2.643

Figure 17 Constants for Shell Diameter Calculations

Shell Equivalent Diameter:

For triangular pitch, the shell equivalent diameter is calculated as,

$$D_e = \frac{4 \times \left(\frac{P_t}{2} \times 0.86\, P_t - \frac{\pi d_o^2}{8}\right)}{\frac{\pi d_o}{2}}$$

$$D_e = \frac{4 \times \left(\frac{0.025}{2} \times 0.86 \times 0.025 - \frac{\pi (0.020)^2}{8}\right)}{\frac{\pi (0.020)}{2}} = 0.014\, m$$

10. Calculation of Flow areas for shell and tube side:

Table 37 Flow Areas calculation for Shell and Tube Side

Shell Side	**Tube Side**
$a_s = \frac{Internal\ dia \times (Clearance \times Baffle\ spacing)}{Pitch}$ $a_s = \frac{ID \times C'B}{P_t}$ $a_s = \frac{0.546 \times (0.005 \times 0.090)}{(0.025)}$ $a_s = 0.010\, m^2$	$a_t = \frac{No.of\ tubes \times Flow\ area/tube}{number\ of\ passes}$ $a_t = \frac{N_t \times a_t'}{n}$ $a_t = \frac{252 \times 0.000215}{2}$ $a_t = 0.027\, m^2$

11. Calculation of Mass Velocities for Shell and Tube side:

Table 38 Mass Velocities Calculation for Shell and Tube Side

Shell Side	**Tube Side**
$G_s = \frac{mass\ flowrate\ (W)}{flow\ area\ (a_s)}$ $G_s = \frac{93165}{0.01} = 218.91 \frac{kg}{s.m^2}$	$G_t = \frac{mass\ flowrate\ (w)}{flow\ area\ (a_t)}$ $G_t = \frac{9555.53}{0.027} = 98.31 \frac{kg}{s.m^2}$

12. Calculation of Reynold Number for Shell and Tube side Fluids:

Table 39 Reynold Number Calculations for Shell and Tube side fluid

Shell Side	**Tube Side**
$Re_s = \frac{D_e \times G_s}{\mu_s}$ $\boldsymbol{Re_s} = \frac{0.014 \times 218.16}{0.00001985} = 19750$ *(> 2100 Turbulent Flow)*	$Re_t = \frac{D \times G_t}{\mu_t}$ $\boldsymbol{Re_t} = \frac{0.016 \times 98.31}{0.0000883} = 17813.8165$ *(> 2100 Turbulent Flow)*

13. Calculation of Prandtl Number for Shell and Tube side Fluid:

Table 40 Prandtl Number Calculations for Shell and Tube Side Fluids

Shell Side	**Tube Side**
$\boldsymbol{P_r} = \frac{C_p \times \mu_s}{k_s}$ $\boldsymbol{P_r} = \frac{1250 \times 0.00001985}{0.033}$ $\boldsymbol{P_r} = \mathbf{0.75}$	$\boldsymbol{P_r} = \frac{C_p \times \mu_t}{k_t}$ $\boldsymbol{P_r} = \frac{6129 \times 0.0000883}{0.60}$ $\boldsymbol{P_r} = \mathbf{0.90}$

14. Calculation of Heat Transfer factor for Shell and Tube Side:

The following graph is used for the shell side calculations of heat transfer factor,

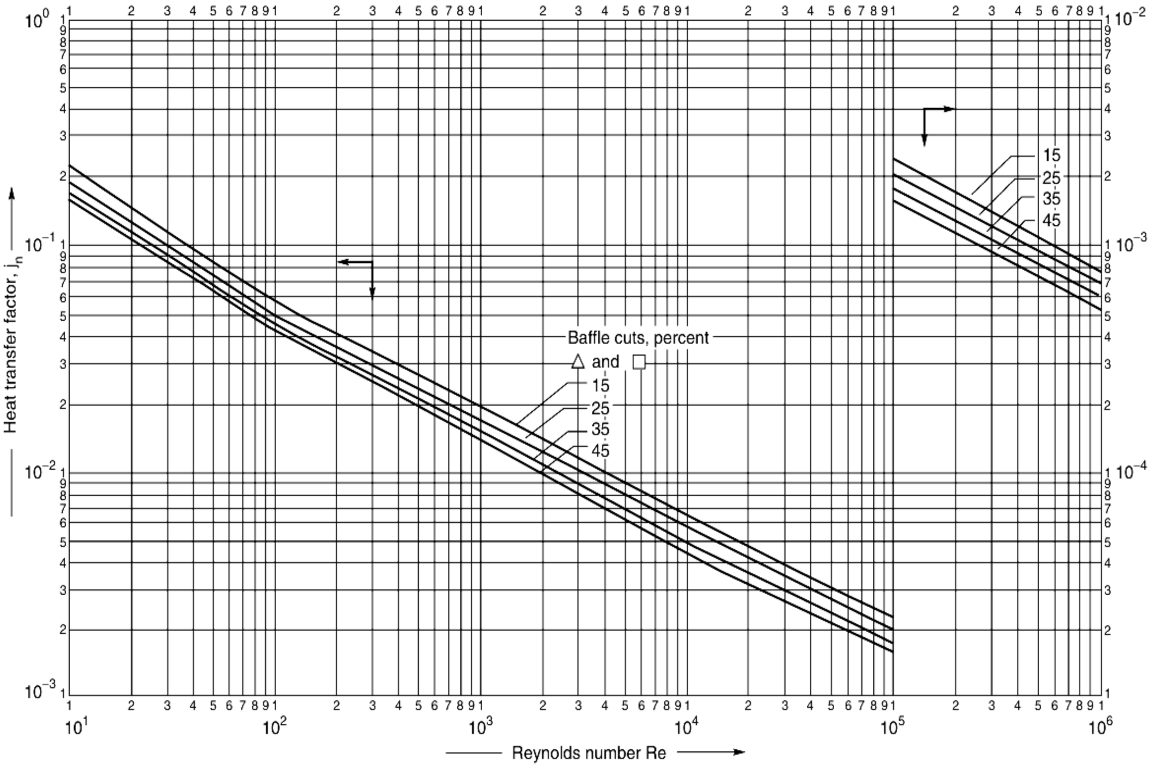


Figure 18 Shell side Heat Transfer Factor

$$j_h = 0.014$$

The following graph is used for the tube side calculations of heat transfer factor:

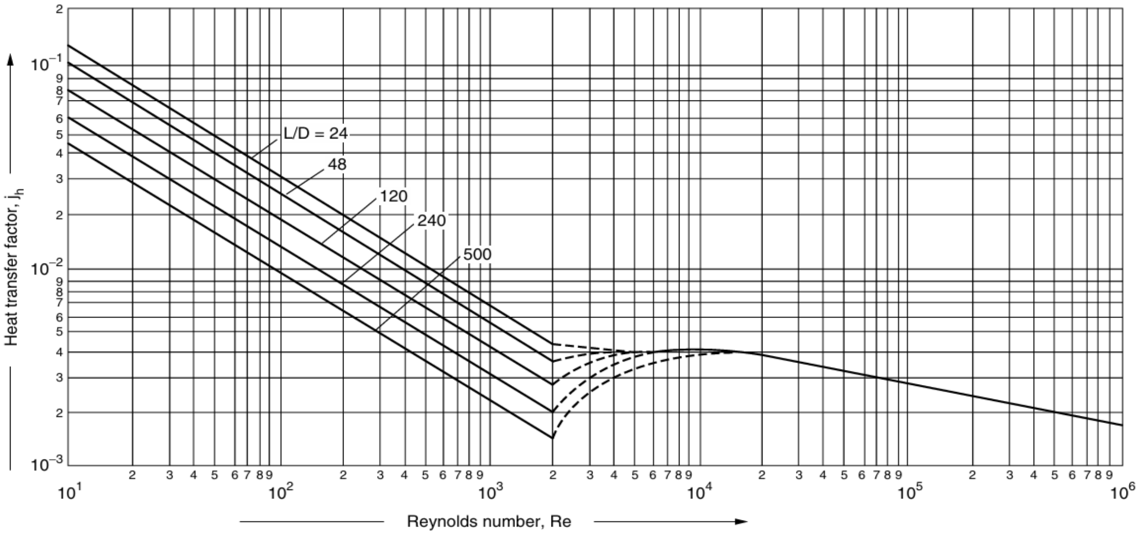


Figure 19 Tube Side Heat Transfer Factor Calculations

$j_h = 0.04$, $\frac{L}{D} = \frac{4.88}{0.016} = 305$

15. Calculation of Film Transfer Coefficient for shell and tube side:

Tube Side Calculations:

$$h_i = (j_h \times Re_t) \times \frac{k}{D} \times (Pr_t)^{0.33} \times \left(\frac{\mu}{\mu_w}\right)^{0.14}$$

$$h_i = (0.04 \times 17813.8165) \times \frac{0.603}{0.016} \times (0.90)^{0.33} \times (1)^{0.14}$$

$$h_i = 25936 W/m^2 °C$$

Shell Side Calculations:

The shell-side heat transfer coefficient can be calculated using the Dittus-Boelter equation:

$Nu = 0.023 \times Re^{0.8} \times Pr^{0.4}$

Where,

Nu = Nusselt Number

Re = Reynold Number

Pr = Prandtl Number

The Reynold number can be calculated as:

$Re = \frac{G \times Dh}{\mu}$

Where,

G = Mass Velocity (kg/m^{2}sec)

Dh = hydraulic diameter (m)

μ = Dynamic viscosity (Pa.sec)

For shell and tube heat exchanger:

$Dh = \frac{4 \times Ac}{P}$

Where,

Ac = Cross-sectional area of the flow (m^2)

P = Wetted Parameter (m)

Nu=0.023× (19750)0.8× (0.75)0.4

Nu = 56

$h_s = \frac{k \times Nu}{Dh}$

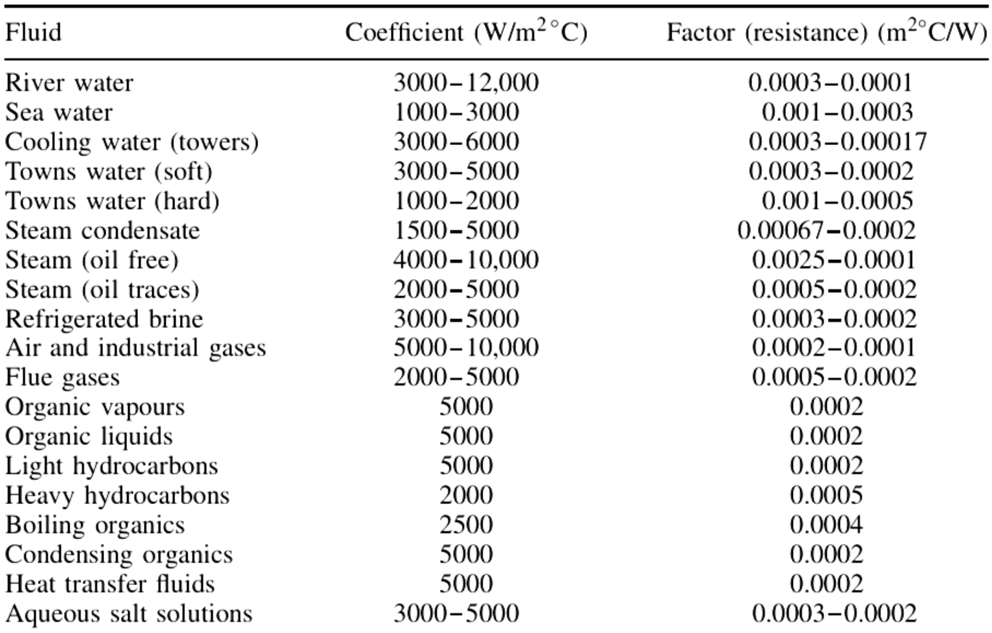
h_s = 0.45*56/0.010

hs ≈ 2520 W/m^2°C

16. Calculation of Design Overall Coefficient:

$$\frac{1}{Uo} = \frac{1}{ho} + \frac{1}{hod} + \frac{do\ln\left(\frac{do}{di}\right)}{2kw} + \frac{do}{di} \times \frac{1}{hid} + \frac{do}{di} \times \frac{1}{hi}$$

Fouling factors for tube and shell side are obtained from the following table,



Fluid	Coefficient (W/m^2°C)	Factor (resistance) (m^2°C/W)
River water	3000–12,000	0.0003–0.0001
Sea water	1000–3000	0.001–0.0003
Cooling water (towers)	3000–6000	0.0003–0.00017
Towns water (soft)	3000–5000	0.0003–0.0002
Towns water (hard)	1000–2000	0.001–0.0005
Steam condensate	1500–5000	0.00067–0.0002
Steam (oil free)	4000–10,000	0.0025–0.0001
Steam (oil traces)	2000–5000	0.0005–0.0002
Refrigerated brine	3000–5000	0.0003–0.0002
Air and industrial gases	5000–10,000	0.0002–0.0001
Flue gases	2000–5000	0.0005–0.0002
Organic vapours	5000	0.0002
Organic liquids	5000	0.0002
Light hydrocarbons	5000	0.0002
Heavy hydrocarbons	2000	0.0005
Boiling organics	2500	0.0004
Condensing organics	5000	0.0002
Heat transfer fluids	5000	0.0002
Aqueous salt solutions	3000–5000	0.0003–0.0002

Figure 20 Fouling Factor Coefficient

$$h_{od} = \frac{5000W}{m^2}°\text{C} \qquad , \qquad h_{id} = 5000W/m^2°\text{C}$$

Conductivity of Carbon Steel is $k_w \ = 54\ W/m^2°\text{C}$

$U_o \ = 1069.17.58\ W/m^2°\text{C}$

17. Pressure Drop Calculations:

Shell side:

For calculating the pressure drop, first we must find the shell side friction factor based on the Reynold's number on the shell side using the following graph,

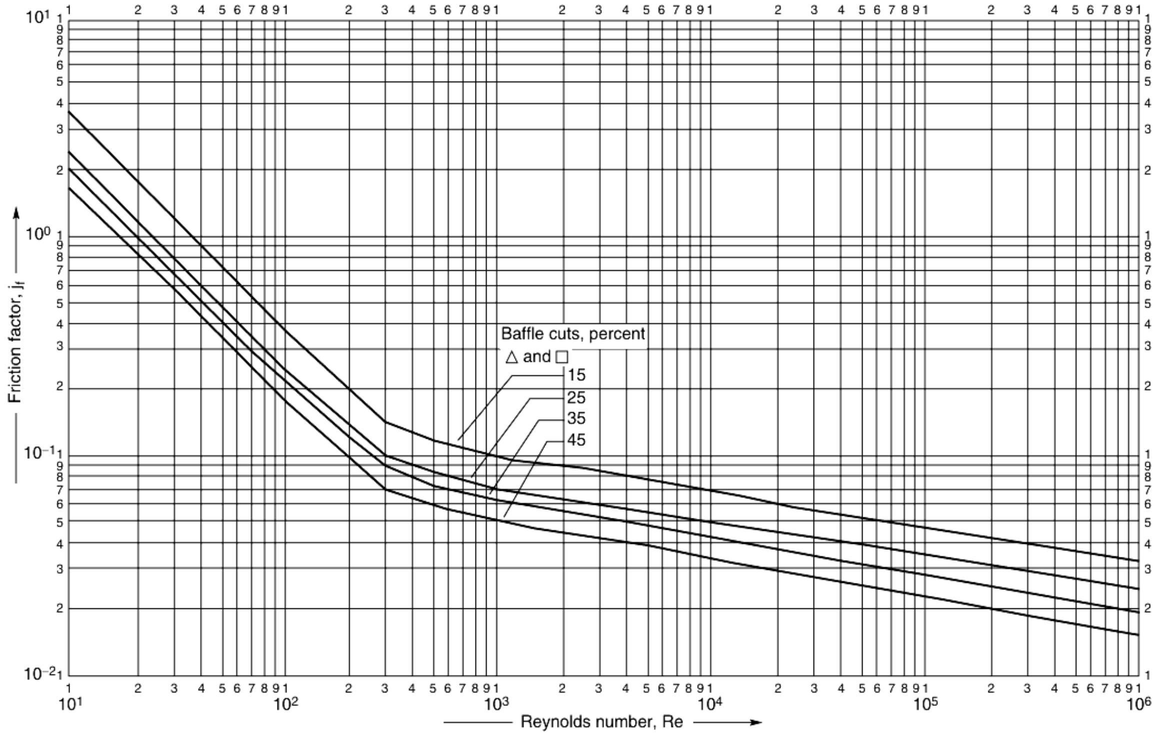


Figure 21 Shell Side Friction Factor

Shell-side Friction Factor = $f_s = 0.047$

Pressure Drop is calculated by using the following formula, neglecting the viscosity correction term,

$$\Delta Ps = 8\, j_f \left(\frac{Ds}{de}\right) \left(\frac{L}{lB}\right) \frac{\rho us2}{2} \left(\frac{\mu}{\mu w}\right)^{-0.14}$$

$\Delta P_s = 4.22$ psi

Tube side:

For calculating the pressure drop, first we must find the tube side friction factor based on the Reynold's number on the tube side using the following graph,

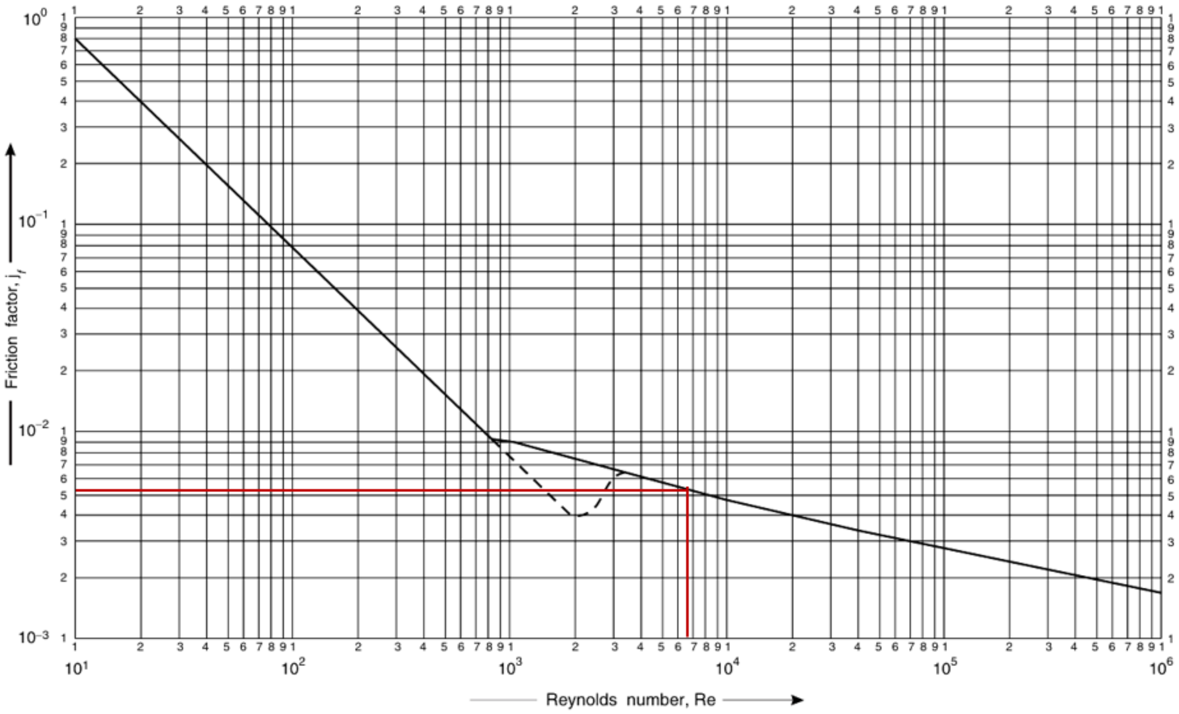


Figure 22 Tube Side Friction Factor

Tube-side Friction Factor = $f_t = 0.004$

Pressure Drop is calculated by using the following formula, neglecting the viscosity correction term,

$$\Delta P_t = N_p \left[8\, j_f \left(\frac{L}{d_i}\right) \left(\frac{\mu}{\mu_w}\right)^{-m} + 2.5\right] \frac{\rho u_t^2}{2}$$

$\Delta P_t = 0.06$ psi

From the pressure drop calculations at shell and tube side, we can conclude that our design is feasible since the pressure drop is within the permissible limit (ΔP < 10psi)

6.4 Reactor R-104:

A Continuous Stirred Tank Reactor (CSTR) is a common type of reactor used in industrial processes for chemical reactions, particularly in the chemical and biochemical industries. The design of a CSTR is crucial for ensuring efficient and safe operation, optimal product yield, and effective control of reaction conditions. This section provides an overview of the fundamental principles, key design considerations, and essential components involved in designing a CSTR.

6.4.1 Significance:

CSTRs are designed to operate continuously, with reactants being continuously fed into the reactor and products being continuously removed. This continuous operation makes CSTRs ideal for large-scale production processes where steady-state conditions are desired. The well-mixed environment within a CSTR ensures uniform reactant concentration and temperature throughout the reactor, which is beneficial for controlling reaction kinetics and maximizing conversion rates.

6.4.2 Basic Principle:

The operation of a CSTR is based on the following key principles:

6.4.2.1 Continuous Flow:

Reactants are introduced into the reactor at a constant rate, and products are removed at the same rate, maintaining a constant volume within the reactor.

6.4.2.2 Uniform Mixing:

The reactor contents are continuously stirred to ensure homogeneous mixing, leading to uniform temperature and concentration profiles.

6.4.2.3 Steady-State Operation:

In steady-state operation, the concentration of reactants and products remains constant over time, assuming constant flow rates and reaction conditions.

6.4.3 Key Design Consideration:

Designing an effective CSTR involves several critical considerations:

6.4.3.1 Reactor Volume:

Determining the appropriate reactor volume to achieve the desired conversion and residence time.

6.4.3.2 Stirring and Mixing:

Ensuring adequate mixing to maintain uniform conditions, which may involve selecting appropriate impeller types and configurations.

6.4.3.3 Heat Transfer:

Designing for effective heat removal or addition to maintain the desired reaction temperature, which may involve incorporating jackets or internal coils.

6.4.3.4 Material of Construction:

Choosing materials that can withstand the chemical environment and operating conditions, such as temperature and pressure.

6.4.3.5 Safety and Control:

Implementing safety measures and control systems to manage reaction conditions and prevent runaway reactions or other hazards.

6.4.3 Design Calculations:

6.4.3.1 Design Equation:

$$V = \frac{F_{A0}X}{-r_a}$$

Where,

V = Reactor Volume

F_{A0} = Initial Molar Flow of Component A

X = Conversion

r_a = Rate of Reaction

6.4.3.2 Reactions:

Reaction 1: $C_9H_6N_2O_2 + 2C_2H_2O_2 \longrightarrow C_{13}H_{10}N_2O_6$

Conversion (TDI to Polyurethane) = 97%

Reaction 2: $C_9H_6N_2O_2 + 2H_2O \longrightarrow 2CO_2 + C_7H_{10}N_2$

Conversion (TDI to CO_2) = 70%

6.4.3.3 Reactor Specifications:

Table 41 Reactor R-104 Specifications

Reactor R-104 Specifications	
Type	CSTR
Flow Rate (kg/hr)	42,193
Temperature (^oC)	25
Pressure (bar)	120
Catalyst	Triethylamine
Blowing Agent	CO_2

6.4.3.4 Design Procedure:

1. The rate equation for the main reaction and its reaction kinetics are available through literature.
2. Calculation of Reactor Volume using the concept of rate to maximum conversion.
3. Calculation of residence time through the formula:
   $t = \frac{V}{vo}$
4. Calculation of Reactor height and diameter from the formula of volume of reactor and taking $\frac{H}{D} = 2$

6.4.3.5 Calculated Parameters:

Table 42 Reactor R-104 Calculated Parameters

Parameters	Value
Residence time (hr)	0.43
Reactor Volume (m^3)	7.7
Height of Reactor (m)	7.3
Diameter of Reactor (m)	3.64

CHAPTER 7

SIMULATION

7.1 Simulation Tool:

Polyurethane is a versatile polymer used in a wide range of applications, including foams, coatings, adhesives, and elastomers. The design of a polyurethane production plant involves complex chemical processes and requires careful consideration of reaction kinetics, thermodynamics, and process dynamics. Aspen PLUS simulation software was used as the simulation software to simulate the whole process because of the unavailability of desired components (Carbamates, trifluoroethanol) in ASPEN Hysys.

7.2 Purpose and Significance:

The purpose of this simulation is to design an efficient and economically viable polyurethane production plant using Aspen Plus. By simulating the entire process, from raw material inputs to final product outputs, we can gain valuable insights into the operational parameters, optimize process conditions, and identify potential bottlenecks or inefficiencies.

Using Aspen Plus for the design of a polyurethane plant offers several significant advantages:

7.2.1 Design and Optimization:

Engineers and designers can use it to test various design iterations and construct virtual prototypes. This iterative method aids in design optimization and raises the caliber of finished goods.

7.2.2 Economic Evaluation:

When compared to real prototyping and testing, simulating complicated systems or processes can result in considerable cost and time savings.

7.2.3 Analysis and Prediction:

It makes it possible to create virtual representations of actual systems or procedures. Before putting these systems into practice in the real world, we can use simulations to forecast and examine their behavior.

7.2.4 Performance Evaluation:

It enables us to assess and contrast how well various processes or systems perform under diverse circumstances. It could aid in manufacturing process optimization.

7.2.5 Visualization and Communication:

It frequently offers graphical depictions of intricate data and models, which facilitate the comprehension and dissemination of results.

7.2.6 Safety and Environmental Impact:

Enables the evaluation of safety and environmental aspects, such as the potential for hazardous emissions and waste generation.

7.3 Process Modeling:

Develop a comprehensive process model that includes all key unit operations involved in the production of polyurethane.

7.3.1 Parameter Optimization:

Optimize process parameters to achieve the highest possible efficiency and product quality.

Economic Analysis: Perform a detailed economic analysis to evaluate the cost-effectiveness of the proposed plant design.

7.3.2 Sensitivity Analysis:

Conduct sensitivity analysis to understand the impact of varying process parameters on overall plant performance.

7.3.3 Environmental and Safety Evaluation:

Assess the environmental impact and safety aspects of the process to ensure compliance with regulatory standards.

7.4 Simulation Flowsheet:

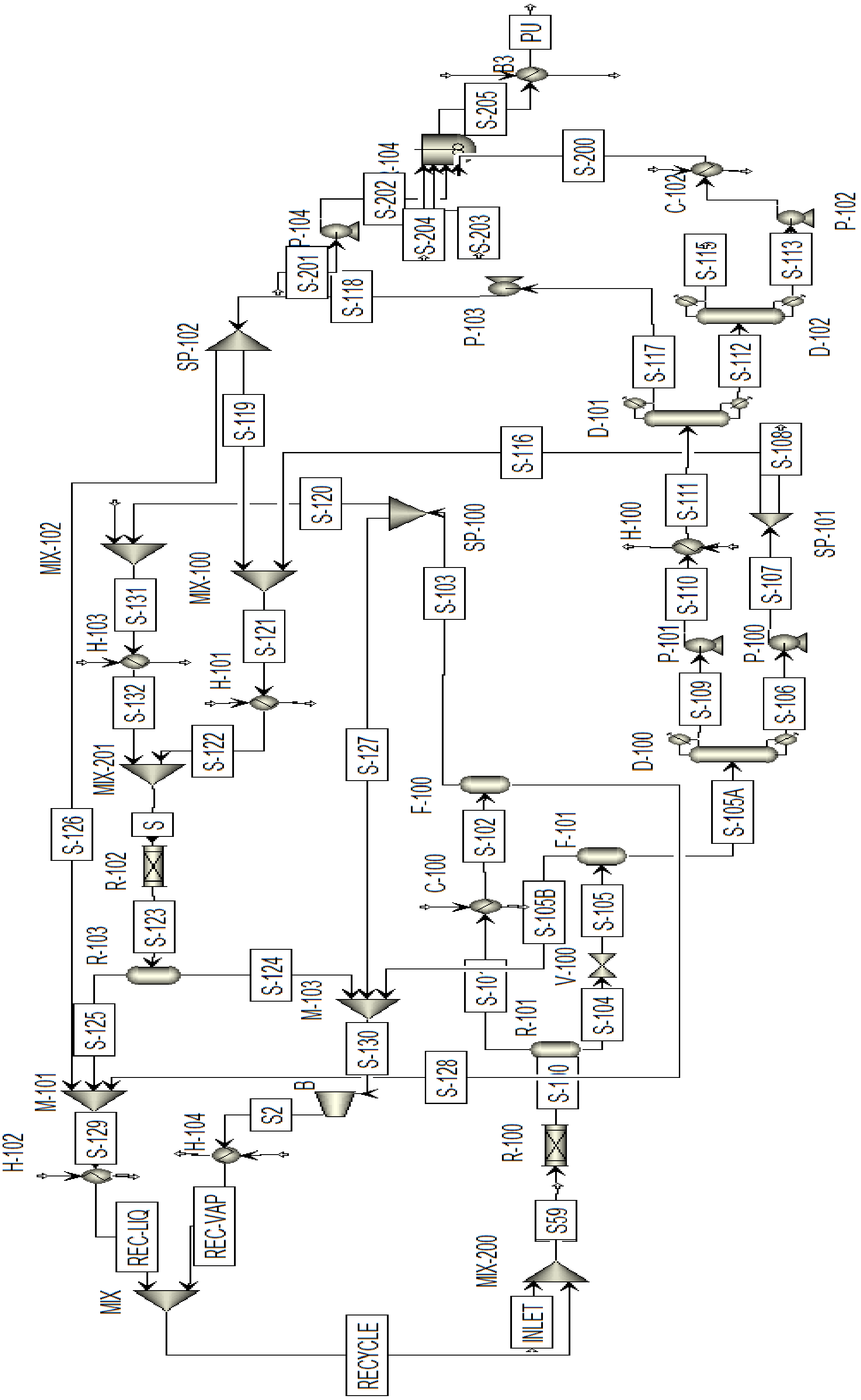
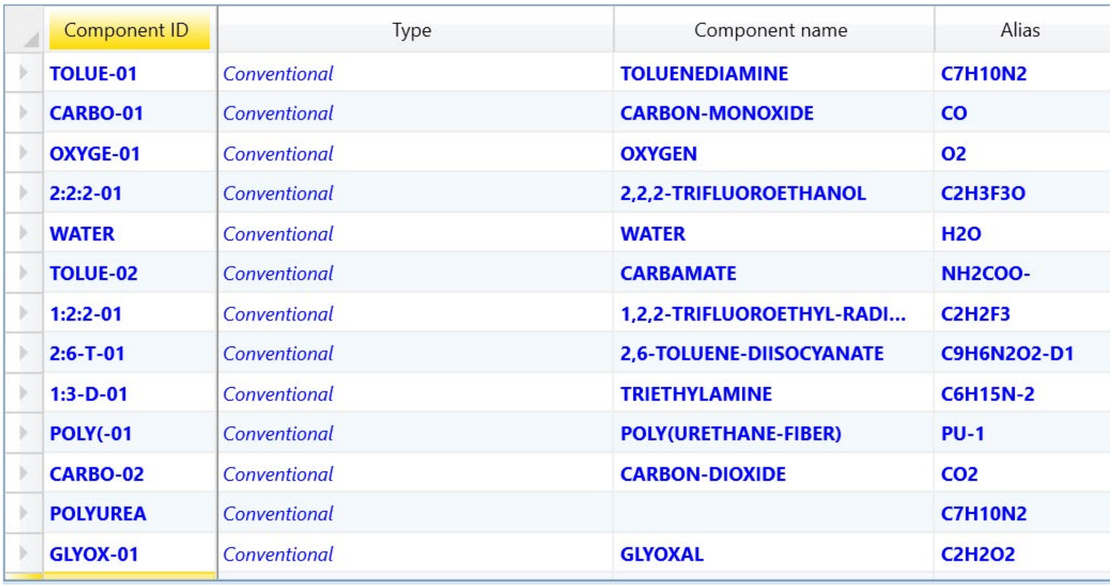


Figure 23 Simulation Flowsheet

7.5 Components:



Component ID	Type	Component name	Alias
TOLUE-01	Conventional	TOLUENEDIAMINE	C7H10N2
CARBO-01	Conventional	CARBON-MONOXIDE	CO
OXYGE-01	Conventional	OXYGEN	O2
2:2:2-01	Conventional	2,2,2-TRIFLUOROETHANOL	C2H3F3O
WATER	Conventional	WATER	H2O
TOLUE-02	Conventional	CARBAMATE	NH2COO-
1:2:2-01	Conventional	1,2,2-TRIFLUOROETHYL-RADI...	C2H2F3
2:6-T-01	Conventional	2,6-TOLUENE-DIISOCYANATE	C9H6N2O2-D1
1:3-D-01	Conventional	TRIETHYLAMINE	C6H15N-2
POLY(-01	Conventional	POLY(URETHANE-FIBER)	PU-1
CARBO-02	Conventional	CARBON-DIOXIDE	CO2
POLYUREA	Conventional		C7H10N2
GLYOX-01	Conventional	GLYOXAL	C2H2O2

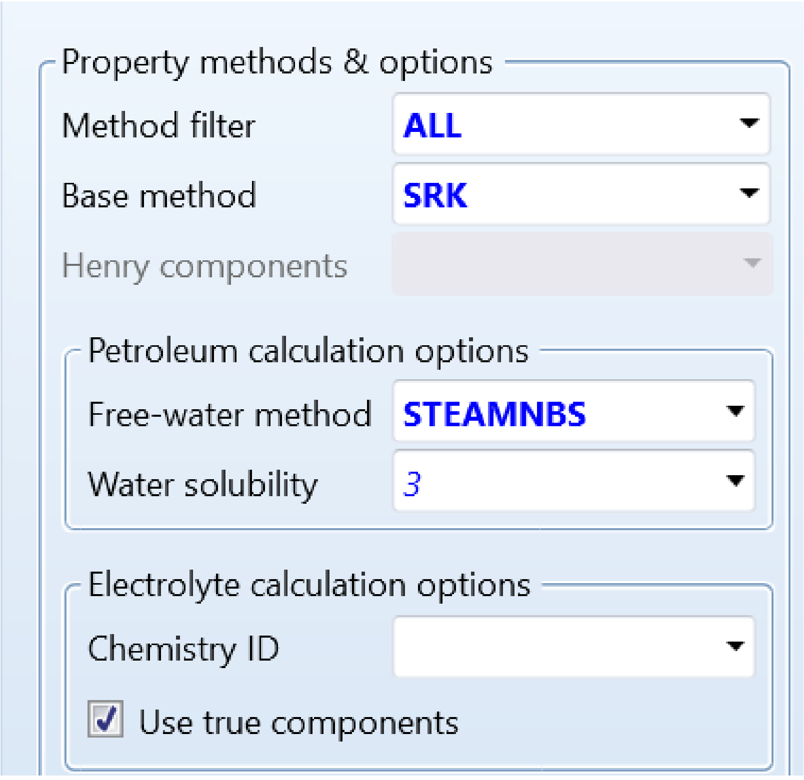
Figure 24 Components List

The following steps are followed to add components in Aspen PLUS:

1. Open Aspen PLUS Software.
2. Create New workbook.
3. Click on the components in the properties environment. Click on the Find tab below component list.
4. Type the name of the component or respective formula and then click on the Find Now button.
5. Select the component you want to add. Then click on the Add Selected Compounds button.
6. Those components that are not present in the simulation software are defined manually.
7. Same procedure is followed to add all components.

7.6 Property Package:

SRK property package was used in the simulation of our process. To give precise thermodynamic and physical property data required for modeling, simulating, and optimizing chemical processes, property packages are introduced to Aspen Plus.



Property methods & options

Method filter: ALL

Base method: SRK

Henry components:

Petroleum calculation options

Free-water method: STEAMNBS

Water solubility: 3

Electrolyte calculation options

Chemistry ID:

☑ Use true components

Figure 25 Property package

They allow users to maximize process performance, achieve realistic simulation results, and guarantee compliance with industry standards and experimental data. The SRK (Soave-Redlich-Kwong) fluid package in Aspen Plus is a thermodynamic model used to predict the behavior of fluids, particularly in terms of phase equilibrium and properties.

The SRK equation of state is an extension of the original Redlich-Kwong equation of state, which was modified by Giorgio Soave to better predict the behavior of real gases, especially at high pressures and temperatures.

7.7 Sections of Simulation:

The overall simulation flowsheet is divided into three major sections:

1. Toluene Diisocyanate Production Section
2. Separation Section of TDI from unreacted reactants
3. Polyurethane Production Section

7.7.1 Toluene Diisocyanate Production Section:

This section includes the reaction of toluene diamine, oxygen, and carbon monoxide in the presence of solvent trifluoroethanol to produce toluene diisocyanates in two reactors. Initially production of TDI from reactants was first carried out in R-100. Then the unreacted reactants are separated and then added to the second reactor R-102 for further utilization of reactants.

7.7.1.1 Flowsheet of Toluene diisocyanate production section:

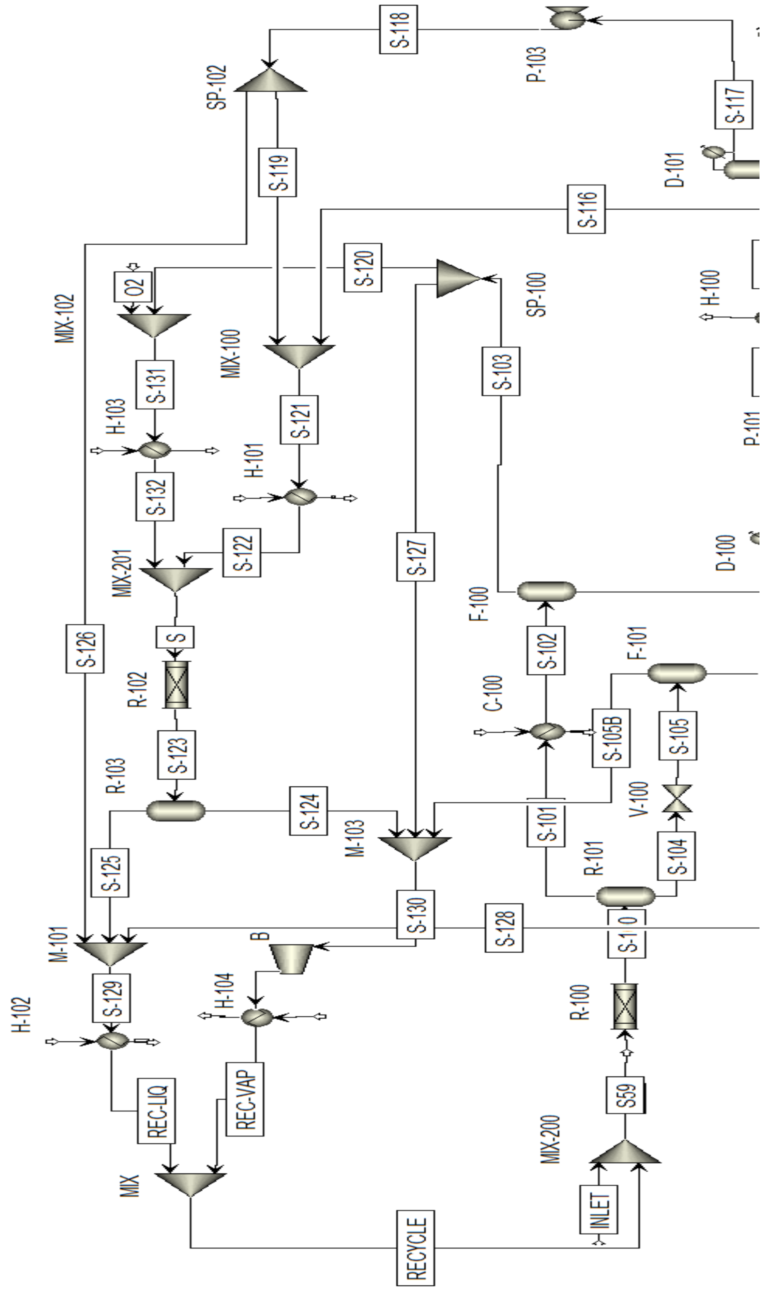
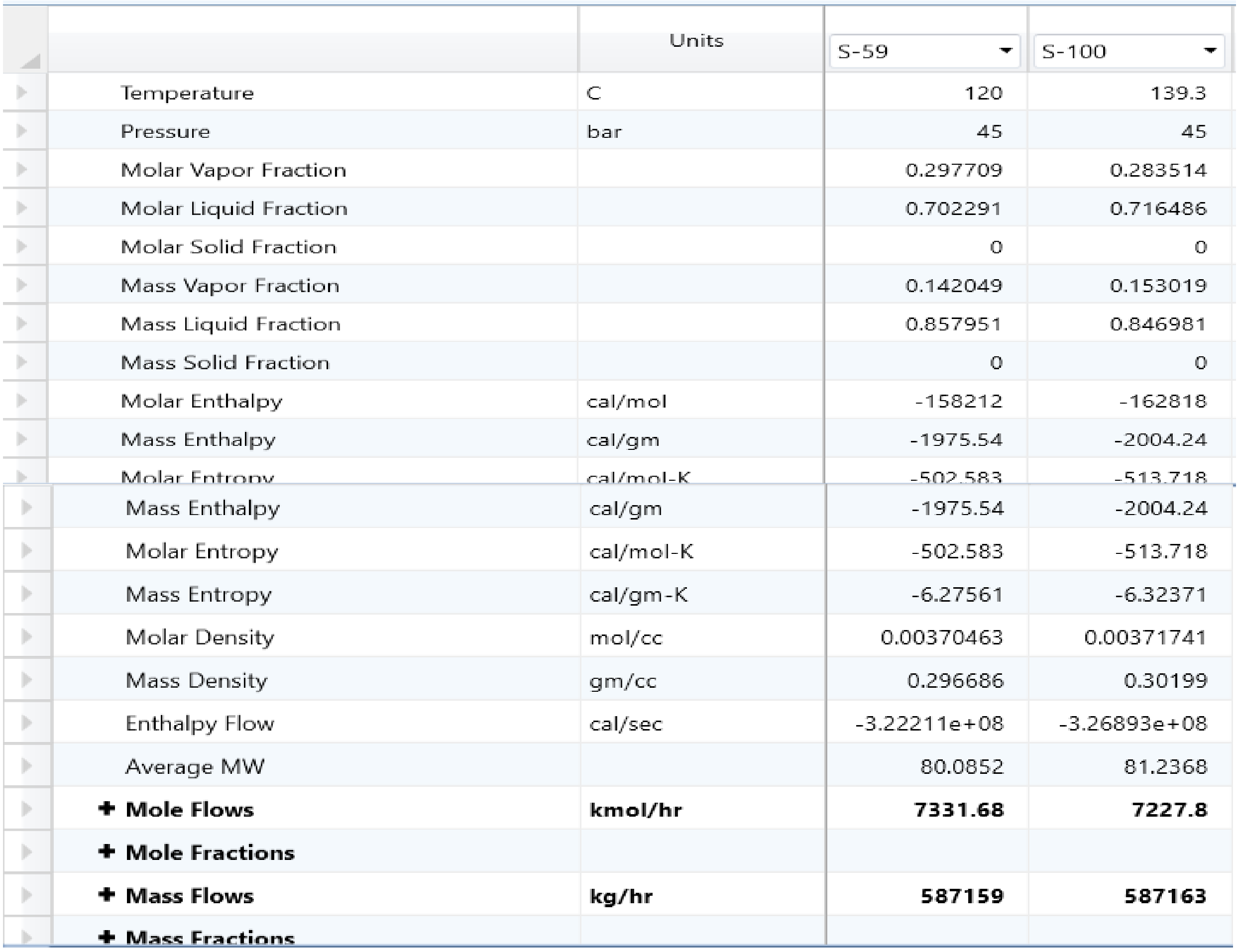


Figure 26 Flowsheet for Toluene diisocyanate production section

7.7.1.2 Stream Results for Toluene diisocyanate production section:



	Units	S-59	S-100
Temperature	C	120	139.3
Pressure	bar	45	45
Molar Vapor Fraction		0.297709	0.283514
Molar Liquid Fraction		0.702291	0.716486
Molar Solid Fraction		0	0
Mass Vapor Fraction		0.142049	0.153019
Mass Liquid Fraction		0.857951	0.846981
Mass Solid Fraction		0	0
Molar Enthalpy	cal/mol	-158212	-162818
Mass Enthalpy	cal/gm	-1975.54	-2004.24
Molar Entropy	cal/mol-K	-502.583	-513.718
Mass Entropy	cal/gm-K	-6.27561	-6.32371
Molar Density	mol/cc	0.00370463	0.00371741
Mass Density	gm/cc	0.296686	0.30199
Enthalpy Flow	cal/sec	-3.22211e+08	-3.26893e+08
Average MW		80.0852	81.2368
+ Mole Flows	**kmol/hr**	**7331.68**	**7227.8**
+ Mole Fractions			
+ Mass Flows	**kg/hr**	**587159**	**587163**
+ Mass Fractions			

Figure 27 Stream Results for Toluene diisocyanate production

7.7.2 Separation Section of TDI from unreacted reactants:

In this section, unreacted reactants from reactor R-100 are separated through a series of distillation columns. In the first column D-100, the solvent is mainly separated from other reactants and products. In the second column D-101, the unreacted oxygen, carbon monoxide and carbamates got separated. In the third column D-102, the final product TDI is separated from wastewater.

7.7.2.1 Flowsheet of Separation section:

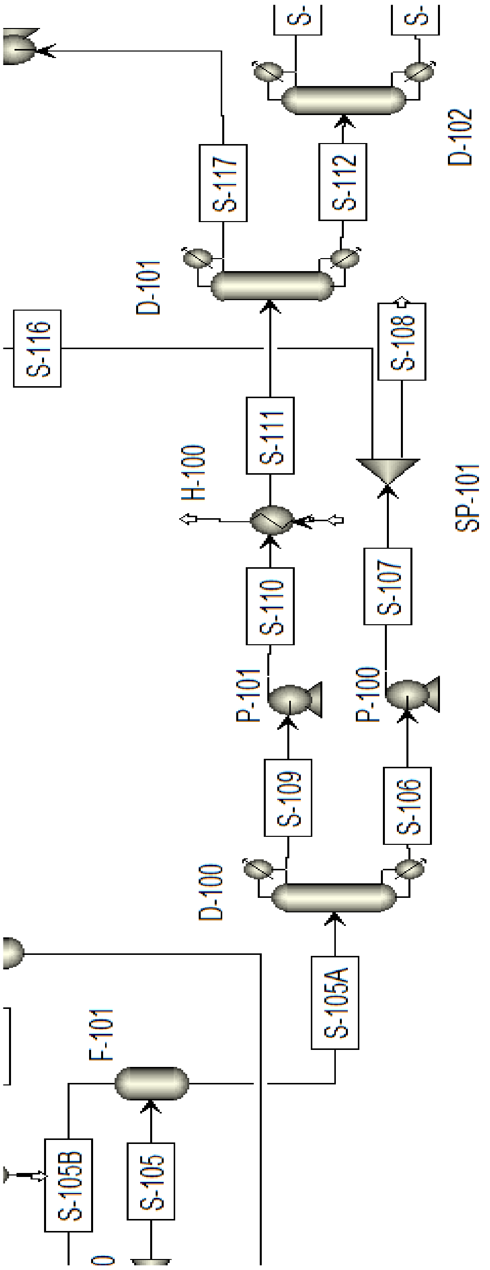
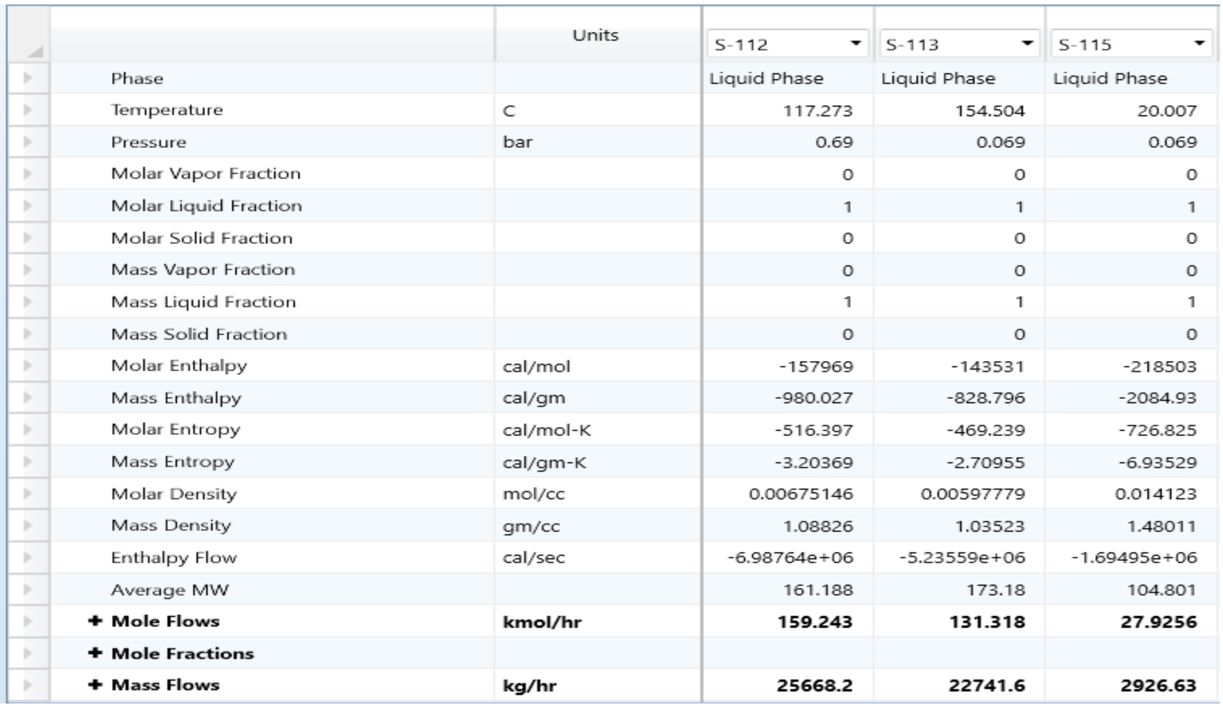


Figure 28 Flowsheet of Separation Section

7.7.2.2 Stream Results for Separation section:



	Units	S-112	S-113	S-115
Phase		Liquid Phase	Liquid Phase	Liquid Phase
Temperature	C	117.273	154.504	20.007
Pressure	bar	0.69	0.069	0.069
Molar Vapor Fraction		0	0	0
Molar Liquid Fraction		1	1	1
Molar Solid Fraction		0	0	0
Mass Vapor Fraction		0	0	0
Mass Liquid Fraction		1	1	1
Mass Solid Fraction		0	0	0
Molar Enthalpy	cal/mol	-157969	-143531	-218503
Mass Enthalpy	cal/gm	-980.027	-828.796	-2084.93
Molar Entropy	cal/mol-K	-516.397	-469.239	-726.825
Mass Entropy	cal/gm-K	-3.20369	-2.70955	-6.93529
Molar Density	mol/cc	0.00675146	0.00597779	0.014123
Mass Density	gm/cc	1.08826	1.03523	1.48011
Enthalpy Flow	cal/sec	-6.98764e+06	-5.23559e+06	-1.69495e+06
Average MW		161.188	173.18	104.801
+ Mole Flows	**kmol/hr**	**159.243**	**131.318**	**27.9256**
+ Mole Fractions				
+ Mass Flows	**kg/hr**	**25668.2**	**22741.6**	**2926.63**

Figure 29 Result Stream for Separation Section

7.7.3 Polyurethane Production Section:

This section includes the reaction of toluene diisocyanate and polyol in the presence of catalyst (triethylamine). The side reaction also occur in which toluene diisocyanate reacts with water to form CO_2. This CO_2 then act as a blowing agent in the foam manufacturing process.

7.7.3.1 Flowsheet of Polyurethane production section:

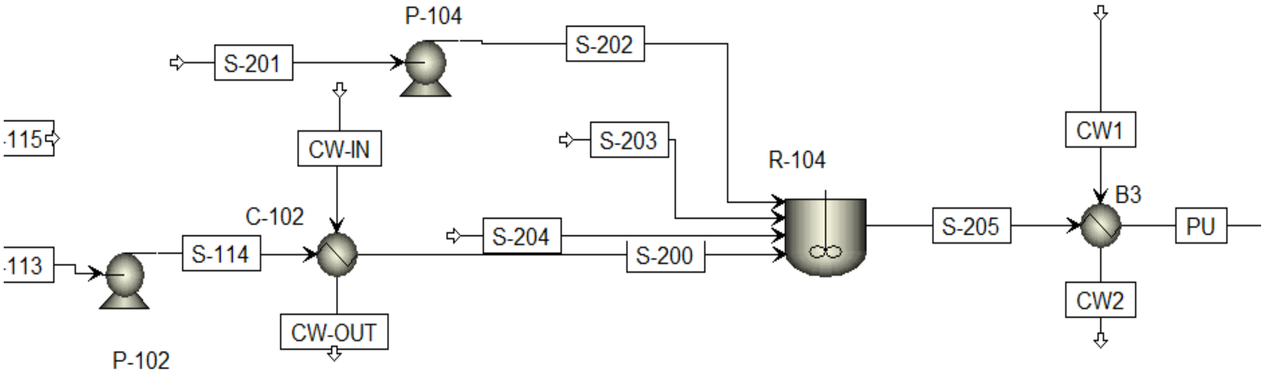
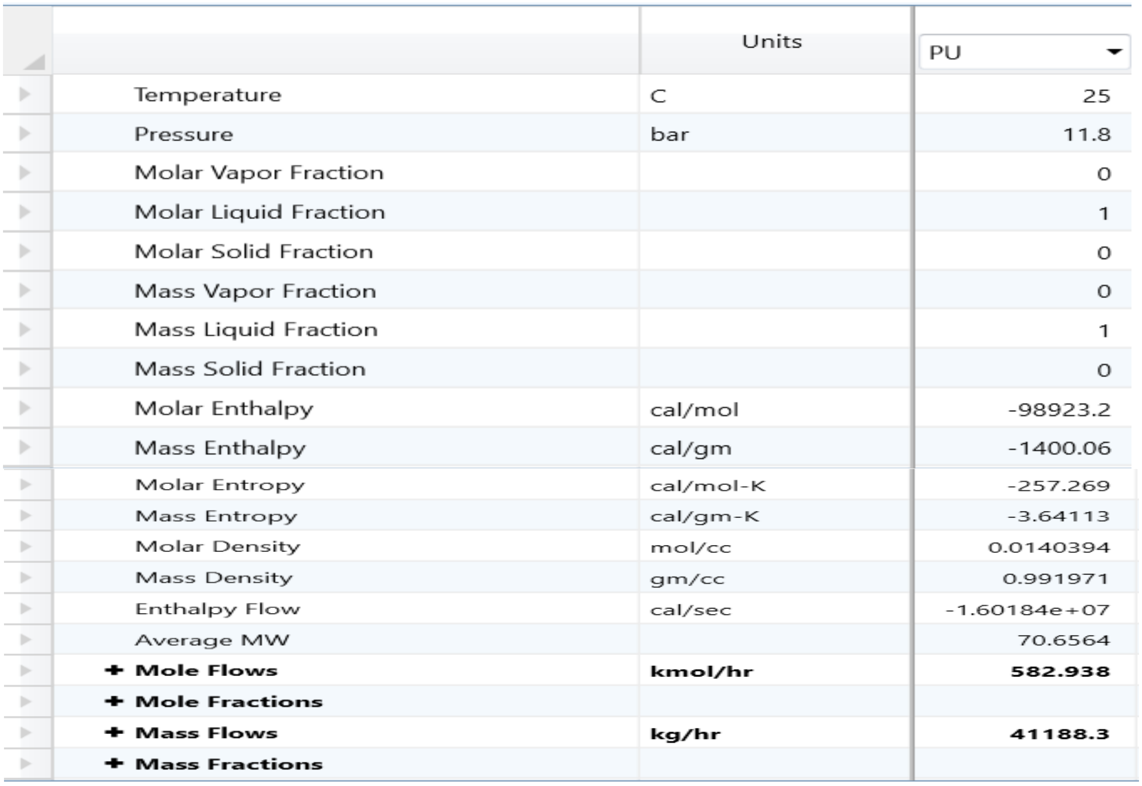


Figure 30 Flowsheet for Polyurethane Production

7.7.3.2 Stream Results for Polyurethane production section:



	Units	PU
Temperature	C	25
Pressure	bar	11.8
Molar Vapor Fraction		0
Molar Liquid Fraction		1
Molar Solid Fraction		0
Mass Vapor Fraction		0
Mass Liquid Fraction		1
Mass Solid Fraction		0
Molar Enthalpy	cal/mol	-98923.2
Mass Enthalpy	cal/gm	-1400.06
Molar Entropy	cal/mol-K	-257.269
Mass Entropy	cal/gm-K	-3.64113
Molar Density	mol/cc	0.0140394
Mass Density	gm/cc	0.991971
Enthalpy Flow	cal/sec	-1.60184e+07
Average MW		70.6564
+ Mole Flows	**kmol/hr**	**582.938**
+ Mole Fractions		
+ Mass Flows	**kg/hr**	**41188.3**
+ Mass Fractions		

CHAPTER 8

INSTRUMENTATION

In the instrumentation and control phases of the process, control methods are used to ensure that the production of TDI from TDA and then production of polyurethane from TDI and polyols is happening in a way that is both efficient and effective. A few of the attributes that may be tracked and managed with the aid of control systems are temperature, pressure, flow rate, and concentration.

8.1 Ratio Controller:

A ratio controller is an important component in many control systems, especially in industrial automation and processes where precise control of the ratio of two variables is required. This is a summary of ratio controller theory. Fundamentally, a ratio controller is used to maintain a particular ratio between two variables, usually identified as the process variable, or PV, and the set point, or SP. To maintain a consistent PV to SP ratio, the controller continually modifies the manipulated variable (MV). A ratio controller's control algorithm is made to determine the necessary MV using the PV and SP values as of right now. In order to change the MV in accordance with the intended ratio, the actual ratio (PV/SP) must be compared to it.

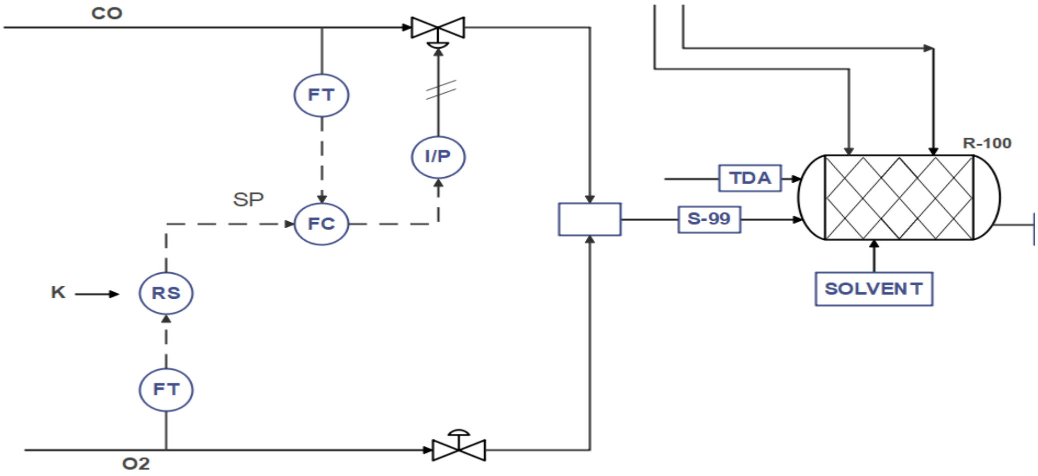


Figure 31 Ratio Controller

Ratio control in this context involves adjusting the flow rates of CO2 and O2 using control valves to achieve and maintain a desired ratio between their concentrations in the process stream. The control strategy for ratio control typically involves continuously monitoring the concentrations of CO2 and O2 in the process stream using sensors. These measurements are then compared to a setpoint ratio, and the control system calculates the required adjustments to the flow rates of each gas to maintain this ratio. By precisely adjusting the flow rates of each gas using control valves, these systems ensure that the desired ratio is maintained, contributing to product quality, process efficiency, and safety.

8.2 Temperature Controller:

In industrial processes where precise temperature control is essential, temperature controllers play a vital role in maintaining temperatures close to setpoints. Let's delve into the theoretical framework of how temperature controllers achieve these using terms such as Temperature Transmitter (TT), Temperature Controller (TC), and I/P (current to pneumatic) -converter. The TT is a sensor that measures the process temperature and converts it into an electrical signal, typically a voltage or current proportional to the temperature. The TC is the brain of the temperature control system. It receives the temperature signal from the TT and compares it to the setpoint temperature entered by the operator or specified by the process requirements. The temperature control system operates in a closed-loop feedback configuration, where the measured temperature from the TT provides feedback to the TC. The TC continuously adjusts the control output based on this feedback to maintain the process temperature close to the setpoint.

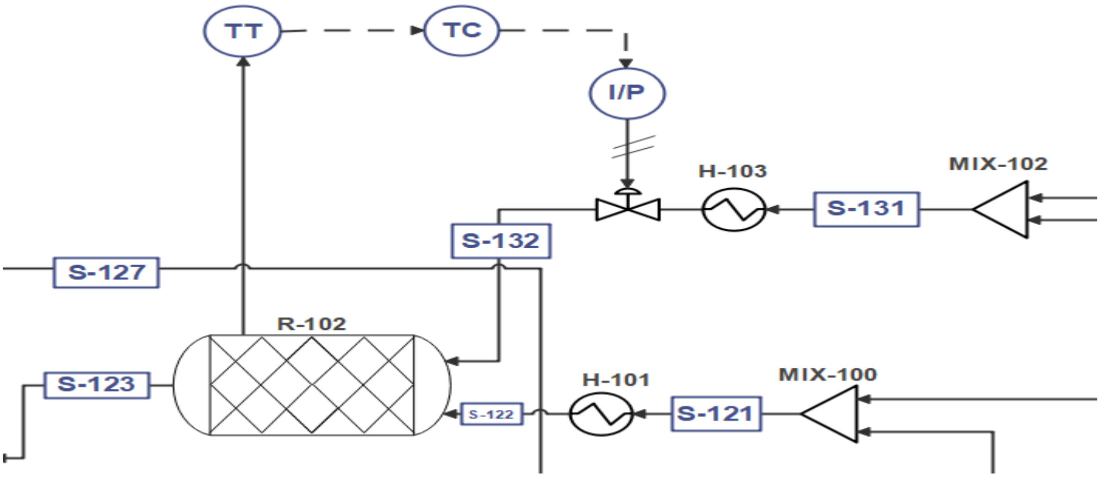


Figure 32 Temperature Controller

8.3 Pressure Controller:

A pressure control system typically comprises three primary components: a Pressure Transmitter (PT), a Pressure Controller (PC), and a final control element, often a control valve or regulator. These components work together to maintain the pressure within a desired range by continuously monitoring and adjusting the process pressure. The PT is a sensor that measures the process pressure and converts it into an electrical signal, typically a voltage or current proportional to the pressure. The PC is the central component of the pressure control system responsible for regulating the process pressure.

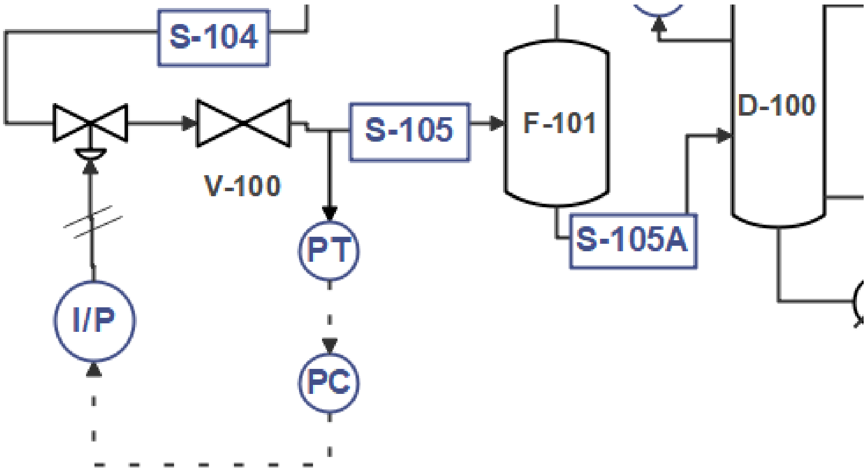


Figure 33 Pressure Controller

It receives the pressure signal from the PT and compares it to the desired setpoint pressure, which is typically entered by the operator or specified by the process requirements.

8.4 Level Controller:

A level control system typically consists of two primary components: a Level Transmitter (LT) and a Level Controller (LC). These components work together to monitor the level of polyurethane in a tank or vessel and adjust the flow rates of incoming or outgoing material to maintain the level at a setpoint.

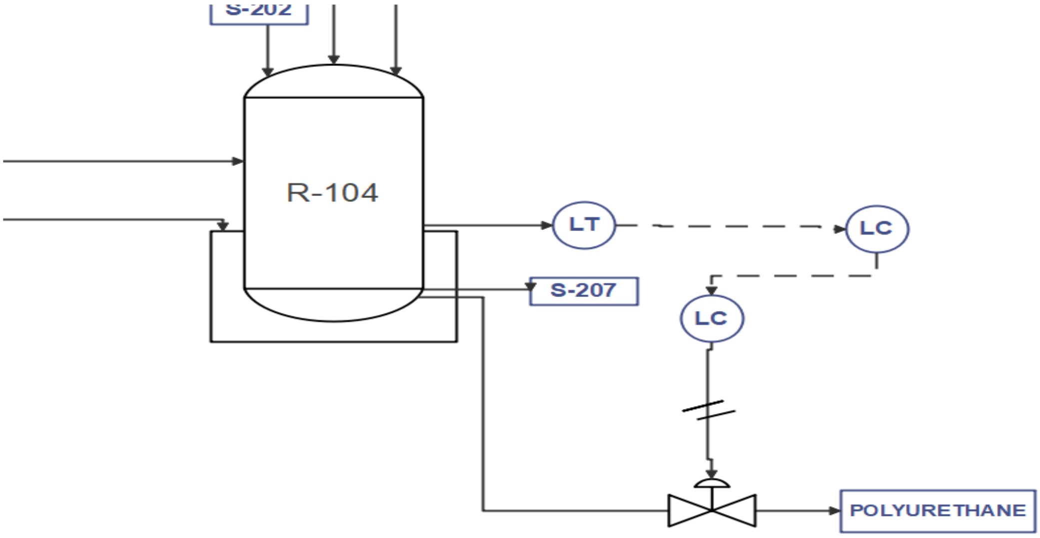


Figure 34 Level Controller

The LT is a sensor responsible for continuously measuring the level of polyurethane in the tank or vessel. Various types of level sensors may be used depending on the specific requirements of the application, including ultrasonic, radar, capacitance, or hydrostatic sensors. The LT provides real-time feedback to the LC regarding the current level of polyurethane. The LC is the central component of the level control system, tasked with regulating the level of polyurethane to the desired setpoint. It receives the level signal from the LT and compares it to the setpoint level entered by the operator or specified by the process requirements. The LC calculates the error, which is the difference between the setpoint and the measured level, and determines the corrective action needed to minimize this error. The level control system operates in a closed-loop feedback configuration, where the measured level from the LT provides feedback to the LC. The LC continuously adjusts the control output based on this feedback to maintain the level of polyurethane within the desired range.

CHAPTER 9

ECONOMIC ANALYSIS

Cost estimation and economic analysis are the most important yet complicated aspects of setting up a plant. Industrial plants, like the one being discussed in our thesis, are designed to produce products on a very large scale. To maximize the profits generated, the plant investment needs to be minimized. Hence, costing is of utmost importance especially because it is a crucial part of the feasibility analysis, which helps in the selection of the manufacturing process to be used.

The estimation of design cost is the fiscal description of the different costs related to the plant, based on total investment. Working capital and fixed capital make up the total investment. Fixed capital is the overall cost required for erection of a plant that is functional and ready to be set up. This cost is paid for the installation of equipment and will eventually wind up as the salvage value. Whereas working capital is the additional funds that would be needed to ensure that the plant is up and running. All these values, along with the detailed economic analysis are shown in the tables given below.

9.1 Distillation Column:

Trays type = Bubble caps
No. of trays = 38
Diameter of column = 4.09 m
Height of column = 22.8 m
Pressure = 7 bar
Vessel material = Carbon steel
Cost of Vessel = Bare Cost * Pressure Factor * Type Factor
= $ 40,000 (1) (1.1)
= $ 44,000

Cost of Plates = 20.62(Bare Cost * Material Factor)

= $ 82,480

Total Cost of Column= $ 126,480

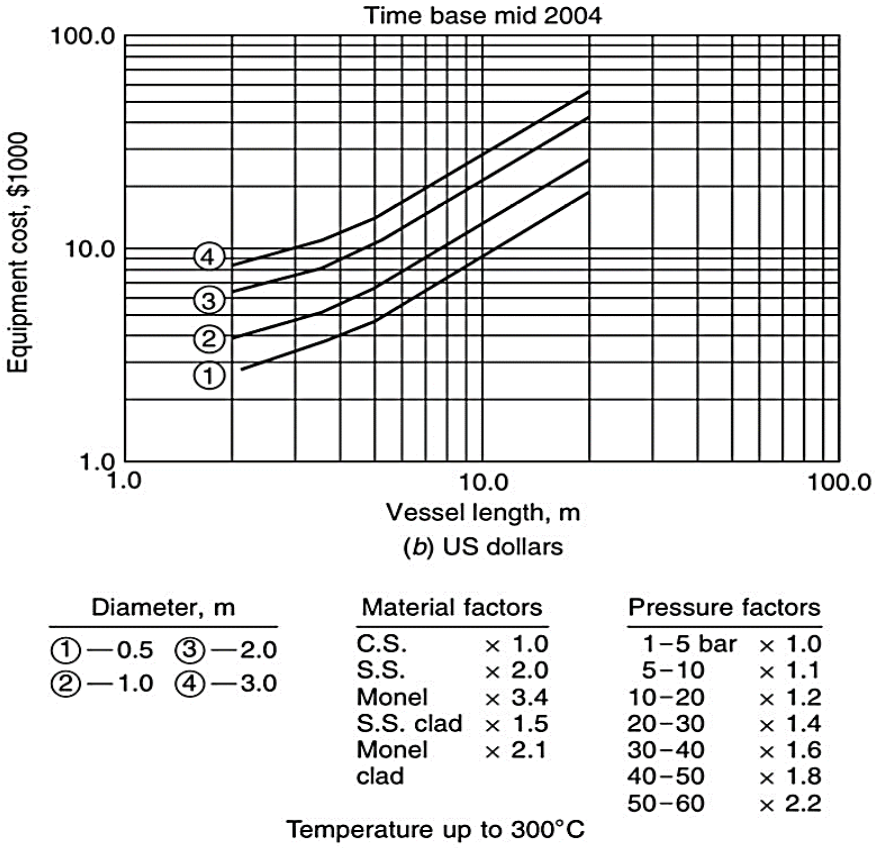


Figure 36 Cost of Distillation Column

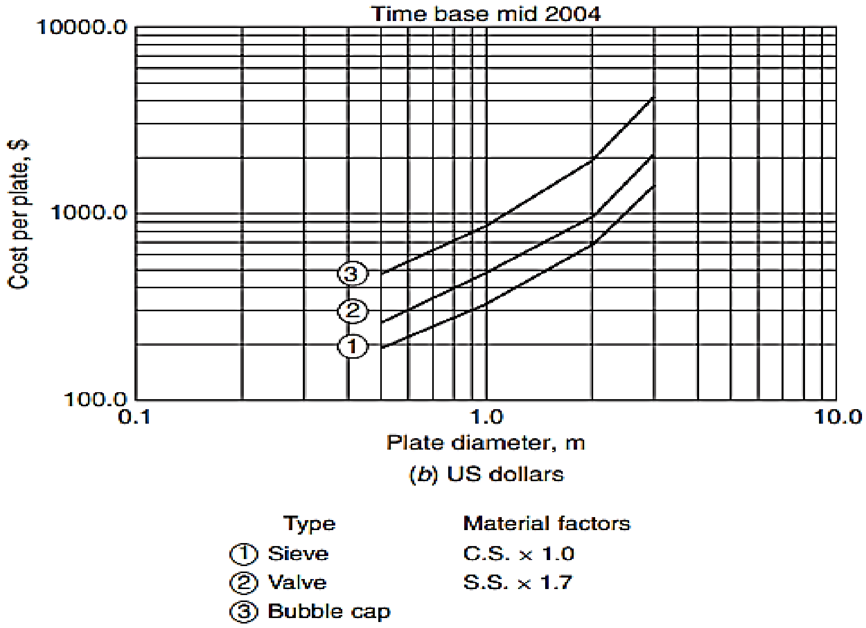


Figure 35 Cost of Column Packing

9.2 Pump:

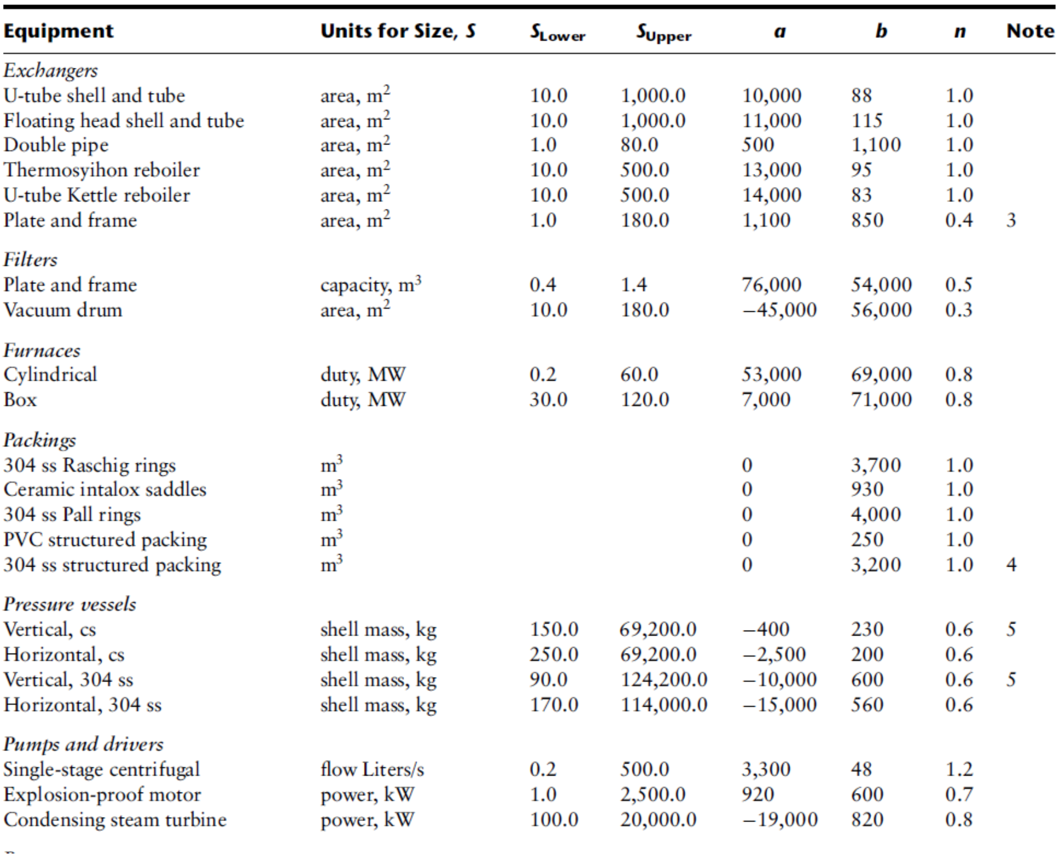
Purchased equipment cost = a+b*Sn*

From table 6.6 in Coulson Richardson’s Chemical Engineering Series Volume 6,

a= $3300

n = 0.8

S = *driver power in kW* = 0.7726 *kW Ce* = 3300+48 × 1.140.8 = $3356.17



Equipment	Units for Size, S	S_{Lower}	S_{Upper}	a	b	n	Note
Exchangers							
U-tube shell and tube	area, m^2	10.0	1,000.0	10,000	88	1.0	
Floating head shell and tube	area, m^2	10.0	1,000.0	11,000	115	1.0	
Double pipe	area, m^2	1.0	80.0	500	1,100	1.0	
Thermosyihon reboiler	area, m^2	10.0	500.0	13,000	95	1.0	
U-tube Kettle reboiler	area, m^2	10.0	500.0	14,000	83	1.0	
Plate and frame	area, m^2	1.0	180.0	1,100	850	0.4	3
Filters							
Plate and frame	capacity, m^3	0.4	1.4	76,000	54,000	0.5	
Vacuum drum	area, m^2	10.0	180.0	−45,000	56,000	0.3	
Furnaces							
Cylindrical	duty, MW	0.2	60.0	53,000	69,000	0.8	
Box	duty, MW	30.0	120.0	7,000	71,000	0.8	
Packings							
304 ss Raschig rings	m^3			0	3,700	1.0	
Ceramic intalox saddles	m^3			0	930	1.0	
304 ss Pall rings	m^3			0	4,000	1.0	
PVC structured packing	m^3			0	250	1.0	
304 ss structured packing	m^3			0	3,200	1.0	4
Pressure vessels							
Vertical, cs	shell mass, kg	150.0	69,200.0	−400	230	0.6	5
Horizontal, cs	shell mass, kg	250.0	69,200.0	−2,500	200	0.6	
Vertical, 304 ss	shell mass, kg	90.0	124,200.0	−10,000	600	0.6	5
Horizontal, 304 ss	shell mass, kg	170.0	114,000.0	−15,000	560	0.6	
Pumps and drivers							
Single-stage centrifugal	flow Liters/s	0.2	500.0	3,300	48	1.2	
Explosion-proof motor	power, kW	1.0	2,500.0	920	600	0.7	
Condensing steam turbine	power, kW	100.0	20,000.0	−19,000	820	0.8	

Figure 37 Pump Costing

9.3 Heat Exchanger:

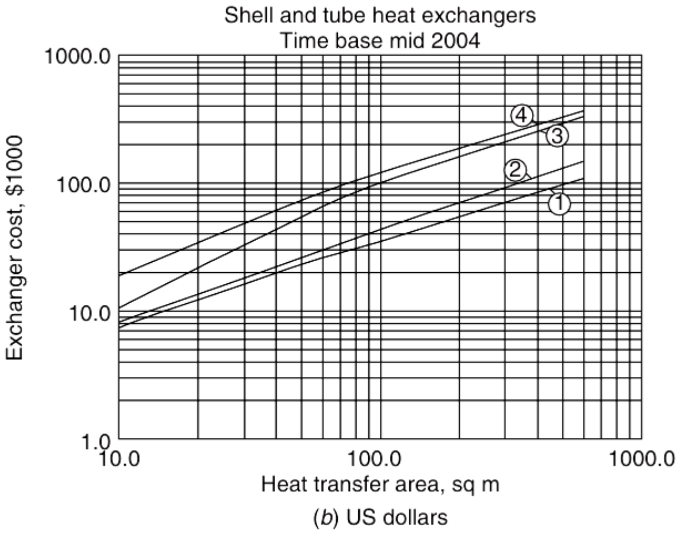
Heat Transfer Area = 77.31 m3

Type of Heat Exchanger = Shell and Tube (Floating Head)

Material of Shell and Tubes = Carbon Steel (Shell), Stainless Steel (Tubes)

Pressure Factor = 1.0

Following graph is used for the costing of heat exchanger,



Materials		
	Shell	Tubes
①	Carbon steel	Carbon steel
②	C.S.	Brass
③	C.S.	Stainless steel
④	S.S.	S.S.

Pressure factors	
1–10 bar	× 1.0
10–20	× 1.1
20–30	× 1.25
30–50	× 1.3
50–70	× 1.5

Type factors	
Floating head	× 1.0
Fixed tube sheet	× 0.8
U tube	× 0.85
Kettle	× 1.3

Figure 38 Cost of Heat Exchanger

Cost of H-X = Bare Cost*Pressure Factor*Type Factor

= $ 20,000 (1)(1)

Cost of H-X = $ 20,000

9.4 Continuous Stirred Tank Reactor:

Operating Pressure = 1 atm

Reactor Volume = 7.71 m3

Material = Carbon Steel

Purchase cost of CSTR:

C_e= C S^n

Where:

Ce = Purchase cost of equipment

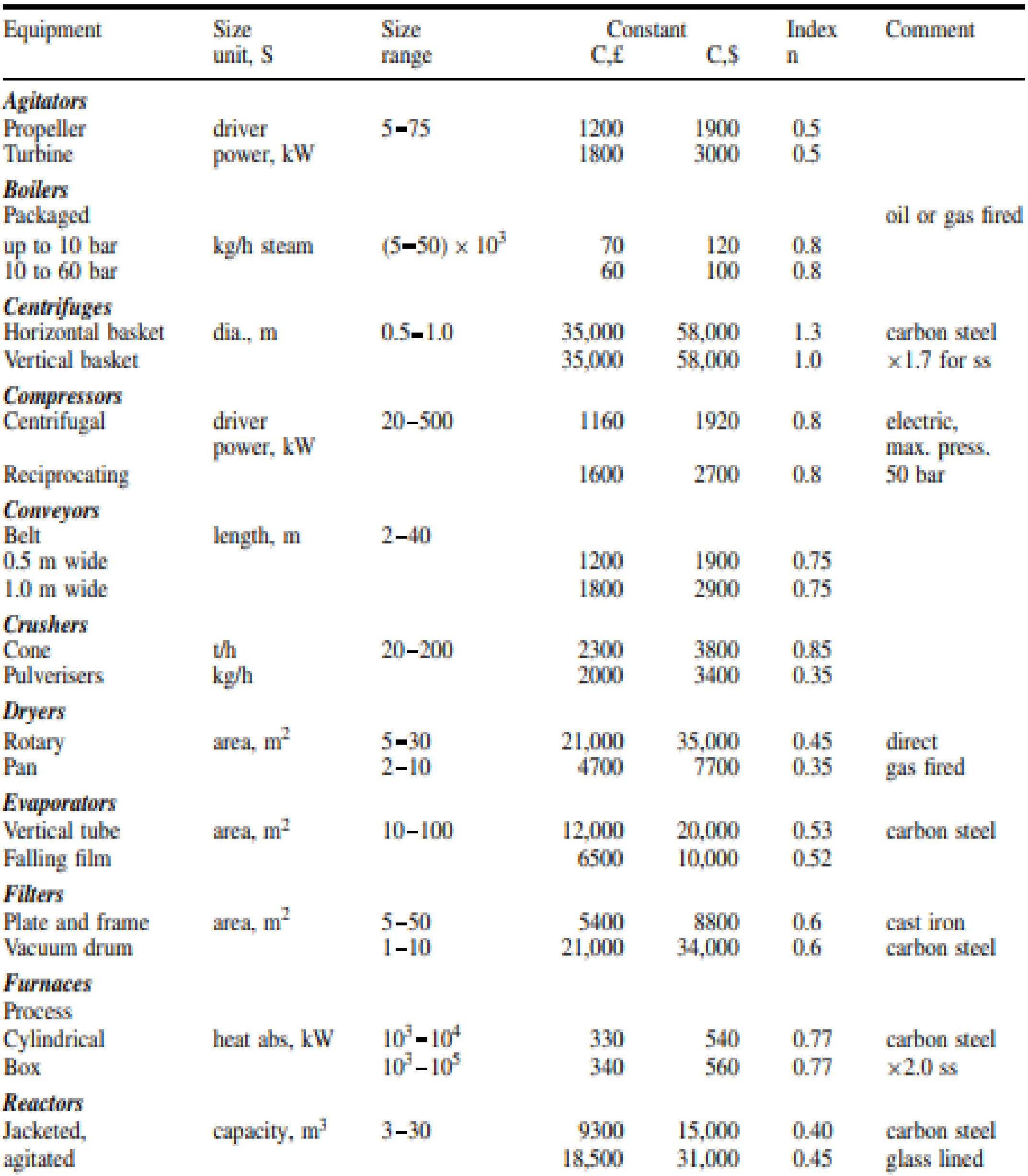
C = Cost constant

S = Characteristics size parameter

n = Index

$C_e = 15000\ (7.71)^{0.4}$

C_e= \$ 33,955



Equipment	Size unit, S	Size range	Constant		Index n	Comment
			C,£	C,$		
Agitators						
Propeller	driver	5–75	1200	1900	0.5	
Turbine	power, kW		1800	3000	0.5	
Boilers						
Packaged						oil or gas fired
up to 10 bar	kg/h steam	$(5–50) \times 10^3$	70	120	0.8	
10 to 60 bar			60	100	0.8	
Centrifuges						
Horizontal basket	dia., m	0.5–1.0	35,000	58,000	1.3	carbon steel
Vertical basket			35,000	58,000	1.0	×1.7 for ss
Compressors						
Centrifugal	driver power, kW	20–500	1160	1920	0.8	electric, max. press.
Reciprocating			1600	2700	0.8	50 bar
Conveyors						
Belt	length, m	2–40				
0.5 m wide			1200	1900	0.75	
1.0 m wide			1800	2900	0.75	
Crushers						
Cone	t/h	20–200	2300	3800	0.85	
Pulverisers	kg/h		2000	3400	0.35	
Dryers						
Rotary	area, m^2	5–30	21,000	35,000	0.45	direct
Pan		2–10	4700	7700	0.35	gas fired
Evaporators						
Vertical tube	area, m^2	10–100	12,000	20,000	0.53	carbon steel
Falling film			6500	10,000	0.52	
Filters						
Plate and frame	area, m^2	5–50	5400	8800	0.6	cast iron
Vacuum drum		1–10	21,000	34,000	0.6	carbon steel
Furnaces						
Process						
Cylindrical	heat abs, kW	$10^3–10^4$	330	540	0.77	carbon steel
Box		$10^3–10^5$	340	560	0.77	×2.0 ss
Reactors						
Jacketed,	capacity, m^3	3–30	9300	15,000	0.40	carbon steel
agitated			18,500	31,000	0.45	glass lined

Figure 39 Cost of Continuous Stirred Tank Reactor

9.5 Packed Bed Reactor:

Cost of PBR = Cost of Vessel + Cost of Catalyst

$Cost\ of\ catalyst\ (USD\ per\ gram) = 41.4$

Mass of catalyst (gram) = 553397071.5

Cost of Vessel = 197630.84

Total cost of Reactor (\$) = 22910836391

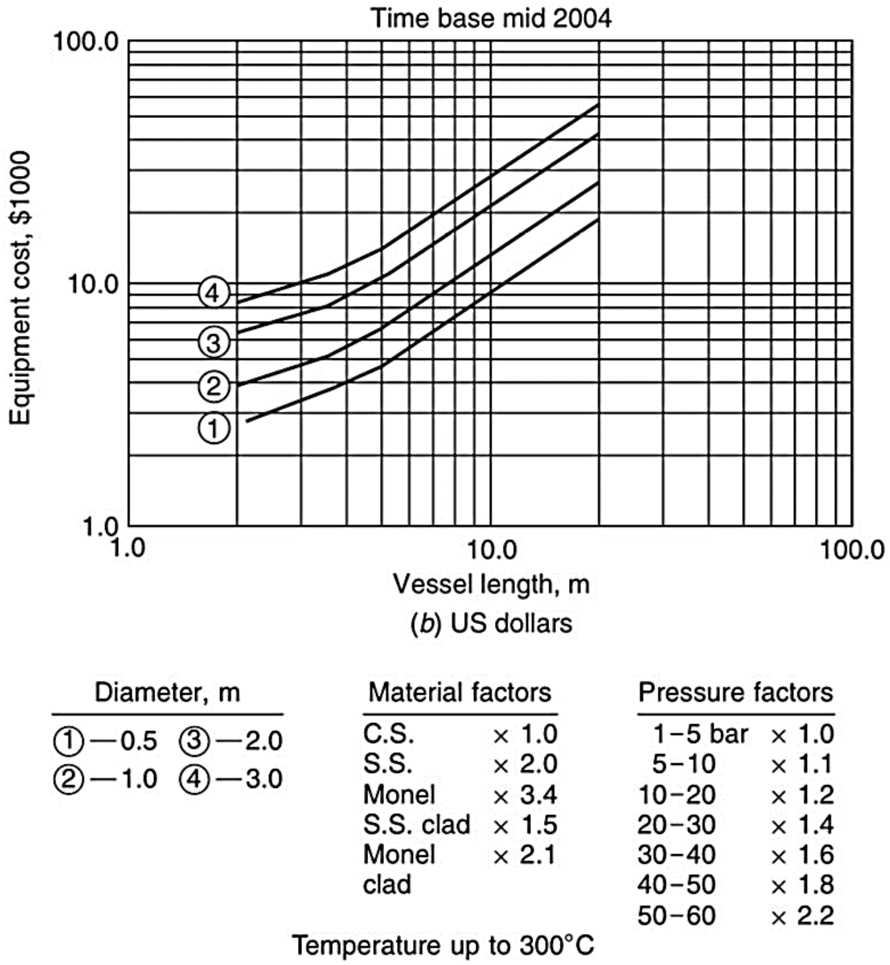


Figure 40 Cost of Packed Bed Reactor

9.6 Total Purchase Cost of Equipment:

Table 43 Total Purchase Cost

EQUIPMENT	COST (dollars)
Reactor 1	22910836
Reactor 2	56239289
Distillation column 1	888008.7
Distillation column 2	158707
Distillation column 3	155000
CSTR	33955
Pumps (5)	69393.5

Heaters (5)	278500
Coolers (2)	53300
Phase separators (2)	42175
Reboilers (3)	42000
Condensers (3)	35000
PCE	**16635574**
Index ratio	2.0571

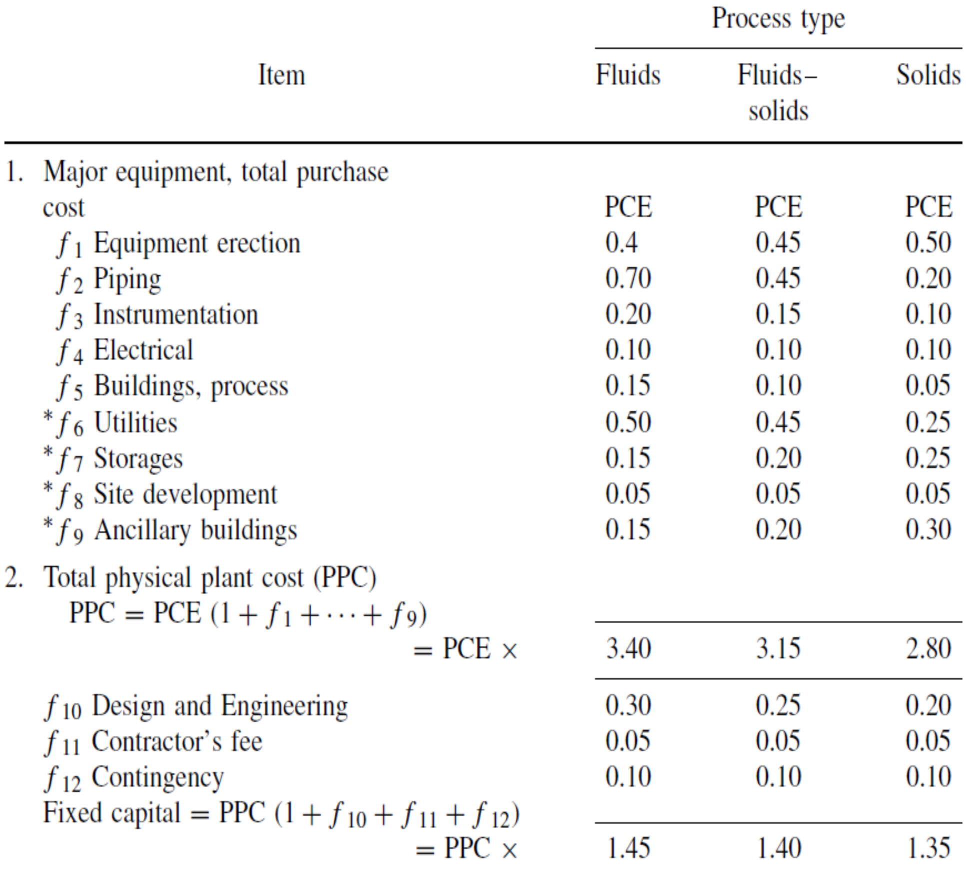
9.7 Total Plant Purchase Cost:

Purchased Cost of Equipment (PCE) = $16635574

Physical Plant Cost (PPC) = PCE*3.25

= $ 16635574 *3.25

= $ 54065618.1



Item	Process type		
	Fluids	Fluids–solids	Solids
1. Major equipment, total purchase cost	PCE	PCE	PCE
f_1 Equipment erection	0.4	0.45	0.50
f_2 Piping	0.70	0.45	0.20
f_3 Instrumentation	0.20	0.15	0.10
f_4 Electrical	0.10	0.10	0.10
f_5 Buildings, process	0.15	0.10	0.05
$^*f_6$ Utilities	0.50	0.45	0.25
$^*f_7$ Storages	0.15	0.20	0.25
$^*f_8$ Site development	0.05	0.05	0.05
$^*f_9$ Ancillary buildings	0.15	0.20	0.30
2. Total physical plant cost (PPC) $\text{PPC} = \text{PCE}\,(1 + f_1 + \cdots + f_9)$ $= \text{PCE} \times$	3.40	3.15	2.80
f_{10} Design and Engineering	0.30	0.25	0.20
f_{11} Contractor's fee	0.05	0.05	0.05
f_{12} Contingency	0.10	0.10	0.10
Fixed capital $= \text{PPC}\,(1 + f_{10} + f_{11} + f_{12})$ $= \text{PPC} \times$	1.45	1.40	1.35

Figure 41 Factors for the Calculation of Plant Purchase Cost

9.8 Total Capital Investment:

Fixed Capital Cost = PPC (1.45)

Fixed Capital Cost = $ 783951471.3

Working Capital Cost is 5% of Fixed Capital Cost. So,

Working Capital Cost= $ 39197573.57

Total Investment required for project = $ 82314904.9

9.9 Annual Operating Cost:

9.9.1 Variable Cost:

9.9.1.1 Raw Material Cost:

Total Cost of TDA ($) = 203904.35

Total Cost of TFE ($) = 273311.99

Total Cost of CO ($) = 621677.93

Total Cost of O_2 ($) = 1495.84

Total cost of Polyol ($/hr) = 378.89667

Total Raw Material Cost = $ 96685687

9.9.1.2 Miscellaneous Material Cost:

Cost of Miscellaneous Material = 10% of raw materials cost

Cost of Miscellaneous Material ($) = 3919757.4

9.9.1.3 Utilities Cost:

Chilled water Cost:

Chilled water requirement (kg/hr) = 1.06E+06

Cost of Chilled water (c/t) = 8

Total Cost ($ per hr) = 6211.96712

Steam Cost:

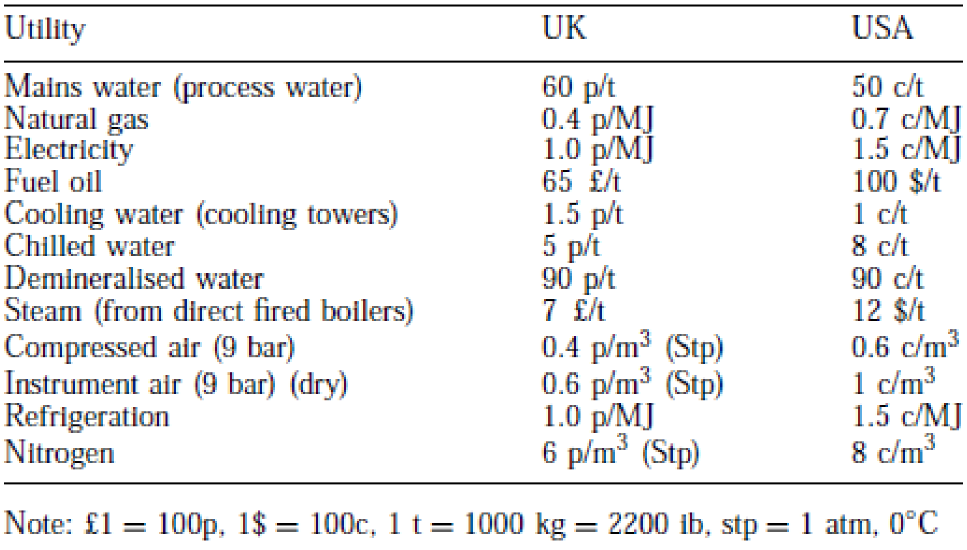
Steam Requirement (kg/hr) = 7.74E+07

Cost of steam ($/t) = 12

Total Cost ($/hr) = 9.29E+05

Total Cost of Utilities ($/hr) = 9.35E+05

Total Cost of Utilities ($/yr) = 8190704832



Utility	UK	USA
Mains water (process water)	60 p/t	50 c/t
Natural gas	0.4 p/MJ	0.7 c/MJ
Electricity	1.0 p/MJ	1.5 c/MJ
Fuel oil	65 £/t	100 $/t
Cooling water (cooling towers)	1.5 p/t	1 c/t
Chilled water	5 p/t	8 c/t
Demineralised water	90 p/t	90 c/t
Steam (from direct fired boilers)	7 £/t	12 $/t
Compressed air (9 bar)	0.4 p/m^3 (Stp)	0.6 c/m^3
Instrument air (9 bar) (dry)	0.6 p/m^3 (Stp)	1 c/m^3
Refrigeration	1.0 p/MJ	1.5 c/MJ
Nitrogen	6 p/m^3 (Stp)	8 c/m^3

Note: £1 = 100p, 1$ = 100c, 1 t = 1000 kg = 2200 ib, stp = 1 atm, 0°C

Figure 42 Cost of Utilities

Total Variable Cost ($) = 18251249.4

9.9.2 Fixed Cost:

Table 44 Fixed Cost

Fixed Costs		
4.Maintenance	5-10% of fixed capital	$ 39197574
5.Operating Labor	From manning estimates	$ 40000
6.Laboratory Costs	20-30% of (5)	$ 8000
7.Supervision	20-30% of (5)	$ 8000
8.Plant Overheads	50% of item (5)	$ 20000
9.Capital Charges	10% of fixed capital	$ 78395147
10.Insurance	1% of fixed capital	$ 7839514.7
11.Local Taxes	2% of fixed capital	$ 15679029
12.Royalties	1% of fixed capital	$ 7839514.7

Total Fixed Cost = $ 33153927.4

9.9.3 Annual Operating Cost:

Sales Expense = N/A

General Overheads = 66307854.38

R&D = N/A

Sub-total = 66307854.38

Annual Operating Cost = 397847126.3

9.10 Total Annual Revenue:

Mass of Polyurethane = 282093374.4 kg/yr

Cost ($ per kg) = 3.2

Total Annual Revenue = 90269879.1

9.11 Annual Cash Flow:

Annual Cashflow = Annual Revenue – Annual Production Cost

Annual Cash Flow = 504851671.8/yr

9.12 Payback Period:

Payback period = Total Capital Investment / Annual Cashflow

Payback period = 1.63yr

9.13 Rate of Return:

Rate of return = (1/payback period) *100

Rate of return = 61.33%

CHAPTER 10

HAZOP ANALYSIS

Hazard and Operability Analysis, or HAZOP, is a thorough and methodical approach to risk assessment that follows a set of guidelines. It is essential for maintaining a plant's safe and effective functioning while putting workers' health first. HAZOP helps sustain consistent manufacturing of desired products by putting in place a variety of procedures, which eventually improves the process's overall profitability.

10.1 HAZOP on Continuous Stirred Tank Reactor:

Table 45 HAZOP Study on CSTR

Study Node	Design Intent	Process Parameter	Guide Word	Causes	Consequences	Actions
Reactor R-104	Polyurethane Production	Flow	No/Low	Malfunction of flow control valves, loss of feed due to leaks or blockages, Inaccurate measurement of reactant feed	Incomplete reaction, reduced production rate, Formation of undesired by-products, Risk of catalyst deactivation or fouling.	Install flow alarms, Temperature sensors at outlet and implementation of control for flow rates of streams.

			High	Inlet valve malfunctioning, Operator error in setting flow rates, Inaccurate measurement of reactant feed	Increased reaction rates leading to potential over-pressurization, Risk of runaway reaction or uncontrolled temperature rise, Formation of undesired by-products	Check and repair/ replace faulty valves, install pressure release valves, Install temperature alarms.
			Reverse	Reversal of pump direction, Failure of check valves, Sudden pressure drops	Contamination of upstream equipment, Risk of reactor contamination, Potential damage to pump seals.	Install automatic sensors and control devices, Check, and repair/ replace faulty check valves

Study Node	**Design Intent**	**Process Parameter**	**Guide Word**	**Causes**	**Consequences**	**Actions**
Reactor R-104	Polyurethane Production	Pressure	Low	Failure of pressure control valves, Loss of reactants or products due to leaks, Insufficient feed rates or reaction rates	Low production rates, Formation of undesirable by-products, Risk of process contamination due to air or moisture ingress	Implement redundant pressure control valves and leak detection systems, enhance operator training, Develop procedures for emergency shutdown and

						containment in case of pressure loss.
			High	Malfunction of pressure control valves, Failure of pressure relief systems, Excessive feed rates or reaction rates.	Risk of vessel rupture or explosion.	Install redundant pressure control valves and relief systems, Implement automatic shutdown systems, Regular inspection and maintenance of pressure relief devices.

Study Node	**Design Intent**	**Process Parameter**	**Guide Word**	**Causes**	**Consequences**	**Actions**
Reactor R-104	Polyurethane Production	Temperature	Low	Failure of heating system, Malfunction of temperature control equipment, Insufficient heat transfers due to fouling or blockage in	Reduced reaction rates, lower productivity, Formation of undesirable by-products, Risk of material freezing in the reactor or downstream equipment.	Implement redundant heating systems or emergency heating sources, Regular inspection and cleaning of heat exchangers to prevent fouling, implement process controls to adjust heating

				heat exchangers		rates and maintain optimal reaction temperatures.
			High	Failure of cooling system, Malfunction of temperature control equipment, Excessive reaction rates	Risk of thermal runaway, Increased reaction rates, Potential damage to equipment due to overheating	Install backup cooling systems for redundancy, adjust reactant feed rates to control reaction rates within safe limits

10.2 HAZOP on Pump:

A hazard and operability study are used for systematic, critical, examination of operability of a process. It can be applied to a process design or operating plant to find out the potential hazards that may arise from deviations that occur instead of intended design conditions.

As the pump is the very first equipment the feed enters, it is necessary that it is functioning properly to avoid any complication further in the process.

Table 46 HAZOP Study on Pump

Study Node	Design Intent	Process Parameter	Guide Word	Causes	Consequences	Actions
Pump	Transfer fluids at high pressure	Flow	No	Blocked pipelines, pump failure	Line overpressure, pump overheating	Proper monitoring of pumps and installation of alarms on valve
			High	Too high shaft power	More energy consumption	Check and decrease the speed of shaft rotation, check operating procedures.
			Less	low rotational speed of shaft, improper suction at the inlet, partial opening of downstream valve	Pump overheating and damaging pump.	Check and increase speed of shaft rotation, install control system to change valve opening according to flow

Study Node	**Design Intent**	**Process Parameter**	**Guide Word**	**Causes**	**Consequences**	**Actions**
Pump	Transfer fluids at high pressure	Pressure	Low	Pump failure, power outage, shaft failure, faulty pressure sensor	Cavitation	Maintenance procedures
			High	Operating fault, Faulty pressure sensor	Explosion, deterioration of bearings	Install high pressure alarms

10.3 HAZOP on Heat Exchanger:

Table 47 HAZOP Study on Heat Exchanger

Study Node	**Design Intent**	**Process Parameter**	**Guide Word**	**Causes**	**Consequences**	**Actions**
H-100	Heating Process Stream	Flow	Low	Line Blockage, Valve failure	No heat transfer, Higher temperature of product gas	Install flow alarms, Temperature sensors at outlet and implementation of control for flow rates of streams

			High	Failure of inlet valve to close	Less than required temperature of exiting stream achieved. High pressure on shell side. Incomplete Heat Exchange	Install temperature alarms. Install flow meter. High Pressure alarms for safety consideration
			Reverse	Blockage in shell or tubes outlet	No heat exchange	Install automatic sensors and control devices. Install check valves

Study Node	**Design Intent**	**Process Parameter**	**Guide Word**	**Causes**	**Consequences**	**Actions**
H-100	Heating Process Stream	Pressure	Low	Leakage in the shell Leakage in tubes	Improper Heat Exchange	Install low-pressure indicator. Check for leakages

			High	Product line blockage Higher temp leading to high Pressure	Improper flow/heat exchanger shell or tubes might leak or blast	Install a high-pressure alarm. Install PSV's

Study Node	Design Intent	Process Parameter	Guide Word	Causes	Consequences	Actions
H-100	Heating Process Stream	Temperature	Low	Low heating supply Temperature	Improper Heat Exchange	Install controllers
			High	High heating supply Temp	Required outlet temp is not achieved	Install high flow temperature and flow alarm

CONCLUSION

We were able to optimize the design of polyurethane plant from polyols and isocyanates by introducing a new phosgene free route for toluene diisocyanate production. The expansion helps to reduce the toxicity of isocyanates by altering its production route. This has resulted in additional annual revenue generation of $90 million.

Our work includes material and energy balance, equipment design, process simulation, instrumentation, economic analysis, and safety considerations. The precise tracking of all reactants and products is ensured by these balances on each unit operation. To meet the specific needs of the process and ensure efficiency and safe operation, comprehensive design calculations are needed for critical equipment such as heat exchangers, distillation columns, and reactors. The entire process was modeled using sophisticated simulation techniques to forecast the behavior under different operating situations. This assisted in determining any bottlenecks and adjusting the process parameters. To maintain the desired operating conditions, important control strategies were devised, such as ratio control, temperature control, and pressure control. This guarantees the industrial process's efficiency and stability. A comprehensive economic assessment was carried out to determine the project's viability. Potential hazards in the process were identified and mitigated with the use of a Hazard and Operability Study (HAZOP). To guarantee the safety of the workers and the facility, this examination is essential.

The thesis concludes that the proposed phosgene free route has emerged as a promising solution to tackle environmental concerns associated with isocyanates production. The continuous production and consumption of toluene diisocyanate reduce the environmental hazards, safety concerns and handling problems. It highlights the significance of further research, innovation and collaboration to improve the viability, scalability and general use of less toxic isocyanate production as a key driver in the transition toward sustainable future.

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