DESIGN OF 150 TONNES/DAY PRODUCTION OF GREEN AMMONIA PLANT

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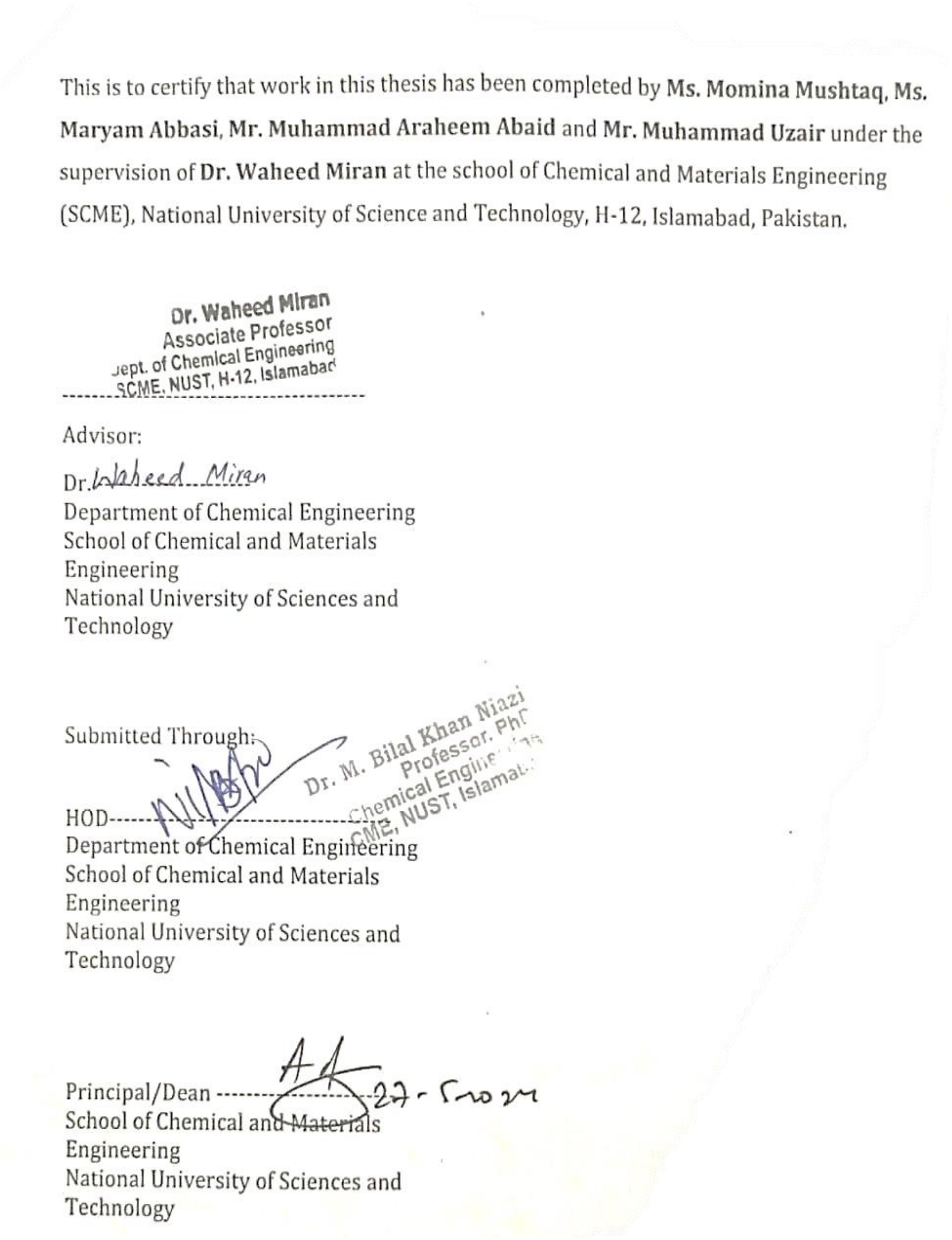

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DEDICATION

This Thesis is dedicated to our parents, for their unwavering support and belief in us. To our friends for their love and encouragement and to our mentors here at SCME, whose guidance has been invaluable throughout this journey.

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First and foremost, we are truly grateful to Allah Almighty for His countless blessings and guidance, which provided us with the strength and patience to complete this thesis.

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Authors

ABSTRACT

Ammonia, with annual production of about 176 million tonnes, is a key component of many fertilizers. The conventional Haber-Bosch process for ammonia production relies on nonrenewable resources (natural gas) which are rapidly depleting. In addition, it contributes to about 1.8% of global carbon emissions annually causing serious environmental problems.

A significant amount of work has been done in exploring the alternatives for the conventional process and green ammonia emerges as a prominent contender. The purpose of this project is to address the above-mentioned challenges and develop an eco-friendly process utilizing renewable raw materials and energy resources.

The project proposes the production of 150 tonnes/day of green ammonia from green hydrogen and nitrogen. Green hydrogen is produced via water electrolysis using a Proton Exchange Membrane Electrolyzer. Water is split into hydrogen and oxygen gas using electricity produced from renewable resources (solar and wind). Nitrogen is separated from air via Pressure Swing Adsorption. Carbon molecular sieve is used as the adsorbent that selectively absorbs oxygen from air leaving behind the pure nitrogen gas. Hydrogen and nitrogen are then reacted in a fixed bed reactor to produce ammonia. This catalyst driven exothermic reaction is carried out under high pressures and moderate temperatures. The ammonia produced as the result can be stored and utilized as a fuel or for production of different fertilizers.

Use of such sustainable methods for ammonia production can help address major environmental problems and contribute to the net zero carbon future.

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CHAPTER 1

INTRODUCTION

1.1 Problem Statement

Most used method for ammonia production worldwide developed in 20th century is Haber-Bosch process. One of the major drawbacks of this method is that it relies on non-renewable energy sources. Natural gas (CH_4) and coal are mainly used as a raw material for ammonia production and generation of energy and electricity. Both are finite resources and are being depleted at an alarming rate.

In addition, the use of fossil fuels is a major source of emission of greenhouse gases. There is a large amount of net-Carbon release in the environment mainly in form of Carbon dioxide. Approximately 1.8 to 2% of the total carbon emissions comes from ammonia synthesis. This is posing serious threats to the environment including global warming and climate change.

1.2 Purpose of Study

The object is to study alternative methods to produce hydrogen and nitrogen for ammonia synthesis that can help combat the harmful effects of traditional ammonia production process. These are the methods that make use of renewable resources and avoid carbon emission into the atmosphere. One such alternative is the production of ‘Green Hydrogen’ and ‘Green Ammonia’.

Green Hydrogen refers to hydrogen produced using renewable resources via processes that avoid the emission of greenhouse gases. This hydrogen is playing an important role in reaching the goal of net zero carbon future.

Green Ammonia refers to the ammonia produced from green hydrogen, and renewable energy sources like wind and solar. This is mainly used as a clean fuel and for synthesis of different fertilizers.

1.3 Brief Introduction of Products

Major products produced in this project are Green Hydrogen and Nitrogen (intermediate products) and Ammonia (final product). A brief introduction and major uses of each are given below.

1.3.1 Green Hydrogen

Hydrogen is a colorless, odorless and highly flammable gas present in abundance in the universe. It is commonly found in water and organic matter. It has different types each represented by a color. Major types include grey hydrogen, brown hydrogen, blue hydrogen and green hydrogen. These names are based on the method adopted for its production. Unlike grey hydrogen, which is produced from natural gas and is responsible for carbon emissions, green hydrogen is produced using renewable raw materials and energy sources and emits no greenhouse gases. Green hydrogen finds various applications in daily life, some of which are listed below.

Chemical Production: Green hydrogen is a major feedstock for production of green ammonia and methanol.

Transportation: It can serve as a clean fuel to power vehicles, proving a zero-emission alternative to the traditional diesel and gasoline engines. It is commonly used in trains, ships and heavy-duty trucks.

Industrial Uses: It can be used as fuel for processes that are energy intensive and require high operating temperature such as cement manufacturing. It can also replace use of coke and coal in steel production.

Oil Refinery: Hydrogen is commonly used in some basic processes of oil refineries such as desulphurization and hydrocracking.

Energy Storage: It can be used to store large amounts of renewable energy that can be converted into different forms for easy usage.

1.3.2 Nitrogen

Nitrogen, making up almost 78% of the total air in earth's atmosphere, is a tasteless colorless and odorless element. It is found in gaseous form in nature and is known to be inert under normal conditions. Nitrogen finds many applications in different processes, some of which are listed below.

Industrial Chemical Production: Nitrogen is a major raw material in ammonia production. It is also used in the production of other fertilizers, nitric acid, explosives, nylon and dyes.

Food Industry: Liquid nitrogen is used in preservation of food items usually by freezing.

Medical Applications: It can be used in different cryogenic applications such as preservation of cells and other biological organisms.

Purging: It is performed to avoid explosions in equipments by displacing the oxygen present in them using some inert gas**.** Nitrogen is the most common inert gas used for purging storage tanks, reactor vessels and pipes.

1.3.3 Ammonia

Ammonia (NH_3) is one of the most crucial chemicals that is produced within the chemical industry. It is conventionally produced via the Haber-Bosch process by reacting Hydrogen and Nitrogen gas in presence of catalyst. Being one of the most widely produced chemicals in the world, great work has been done to ensure that the production of Ammonia is as efficient as possible, giving the maximum possible yield at the lowest possible cost. Ammonia plays a vital role in different sectors due to its versatile applications. Some of which are listed below.

Fertilizer Production: Ammonia's most significant contribution is in the agricultural sector, where it serves as a vital nitrogen source for fertilizers, enhancing soil fertility and crop production. Some of the major fertilizers produced from ammonia are Urea, Ammonium Nitrate, Ammonium Phosphate and Ammonium Sulphate.

Industrial Chemical Production: Ammonia is also an important contributor in the production of various industrial chemicals, including those used in making nitric acid, plastics, synthetic fibers like nylon and resins, textiles, and pharmaceuticals.

Cleaning: It is also used in household and industrial cleaning products, especially glass cleaners and surface cleaners. Ammonia's ability to tackle stubborn stains and dissolving grease and grime makes it a preferred ingredient in cleaning solutions.

Refrigeration: Ammonia's role in refrigeration, especially within the food and beverage industry, highlights its utility in preserving freshness through cooling and freezing, as it has excellent thermal properties and a minimal environmental footprint.

Textile Industry: The textile sector utilizes ammonia in processing and dyeing fabrics, ensuring better colors adhesion and smooth textiles finish. It is also used in textile finishing process as a pH adjuster.

Food Industry: Ammonia is used in meat processing as an antimicrobial agent to control growth of bacteria in meat. It also finds its use as a leavening agent and acidity regulator.

Water treatment: Ammonia is used with chlorine as a disinfectant in water treatment plants providing protection against microbial regrowth. It is also used to adjust the pH level of water especially where water is too acidic.

CHAPTER 2

LITERATURE REVIEW

2.1 Different Techniques for Ammonia Synthesis

There are several techniques available for the synthesis of ammonia. Some of which are at experimental level and some are well developed and commonly used in the industry. Each has its own pros and cons . some if the major techniques are listed below.

2.1.1 Biomass Gasification

Biomass gasification for ammonia production encompasses a series of steps. Different biomass sources, including wood, crop residues, or organic waste, are utilized as raw materials. The gasification process occurs under controlled conditions with restricted oxygen supply, generating a synthetic gas (syngas) primarily composed of hydrogen (H_2) and carbon monoxide (CO). The subsequent stages involve the purification and conditioning of the syngas, aimed at eliminating impurities like sulfur compounds and tar, while ensuring compliance with downstream processing requirements. Post-cleaning, the conditioned syngas serves as the feedstock for the Haber-Bosch process, a well-established technique for ammonia synthesis. Here, nitrogen from the air reacts with hydrogen in syngas to produce ammonia (NH_3).

Gasification operates within the temperature range of 700 to 1,500 degrees Celsius. Gasification Pressure is variable, often elevated to enhance gas yields and reaction rates. Catalysts based on iron or ruthenium may be employed to facilitate ammonia synthesis at lower temperatures and pressures. (Martín & Sánchez, 2024)

Drawbacks: Major drawbacks include inconsistent feedstock quality, potential emissions of tar and particulates, and the need for advanced gas cleaning systems to ensure the purity of the syngas. Additionally, the process may face challenges in achieving high efficiency and cost competitiveness compared to traditional methods.

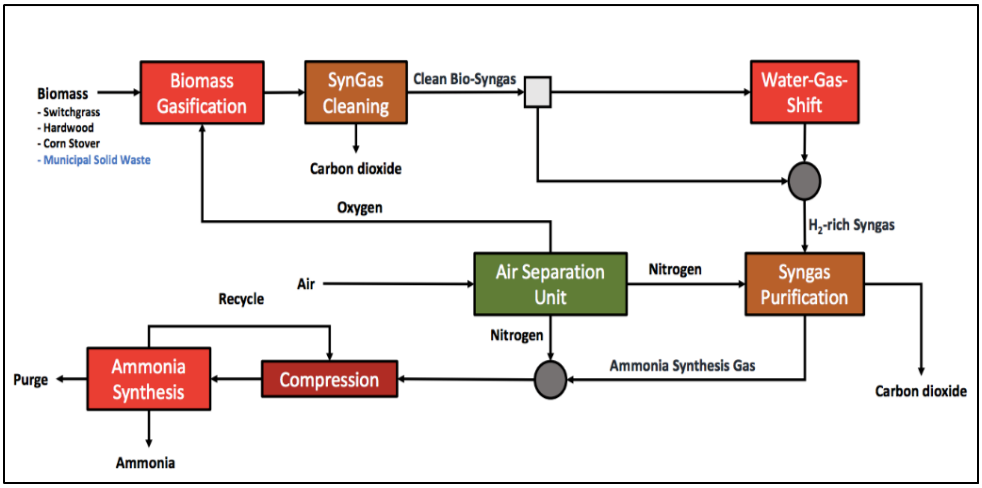

Figure 2.1 Biomass gasification process for ammonia synthesis

2.1.2 Electrochemical Process

Ammonia synthesis through electrochemical processes involves the direct reduction of nitrogen (N_2) and protons (H^+) to form ammonia (NH_3) using renewable electricity. The process requires lower temperatures and pressures compared to traditional methods, potentially offering energy efficiency advantages.

An electrochemical device employs electrical energy for a chemical reaction, comprising two electrodes, an anode (positive) and a cathode (negative). At anode the hydrogen is broken down to produce H^+ ions and release electrons. This ion moves towards cathode where they are combined with nitrogen to produce ammonia. The electrolyte facilitates ion passage between electrodes and can be either aqueous or solid. While aqueous electrolytes pose a challenge due to the necessity for low operating temperatures, which can impede reaction kinetics.(Juangsa et al., 2021)

Drawbacks: The challenges include developing efficient electrocatalysts for nitrogen reduction and addressing issues related to cell stability and selectivity. While electrochemical ammonia synthesis shows promise for sustainable production, further research and technological advancements are needed to overcome these challenges and make it a commercially viable alternative.

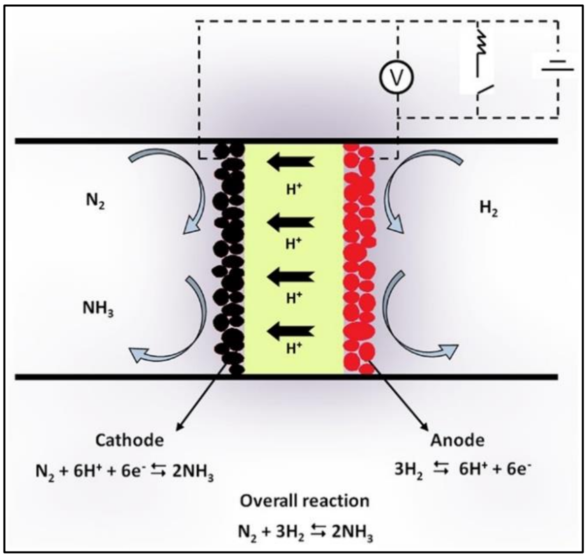

Figure 2.2 Electrochemical production of Ammonia

2.1.3 Water Electrolysis and Air Separation

Water electrolysis is another method that can lead to the production of ammonia. Electricity obtained from renewable resources is used to break down water into hydrogen and oxygen. The oxygen can be vented into air or used for other processes while hydrogen is used in ammonia production. Nitrogen is generally separated from air. The hydrogen and nitrogen are then combined using the Haber-Bosch process or electrochemical cell to produce ammonia.

Drawbacks: Some of the electrolyzes used in this process are still at experimental level and more research is needed to make them mature. The huge requirement of electricity from renewable resources and its high price is also an obstacle in large amount of ammonia production from this process.

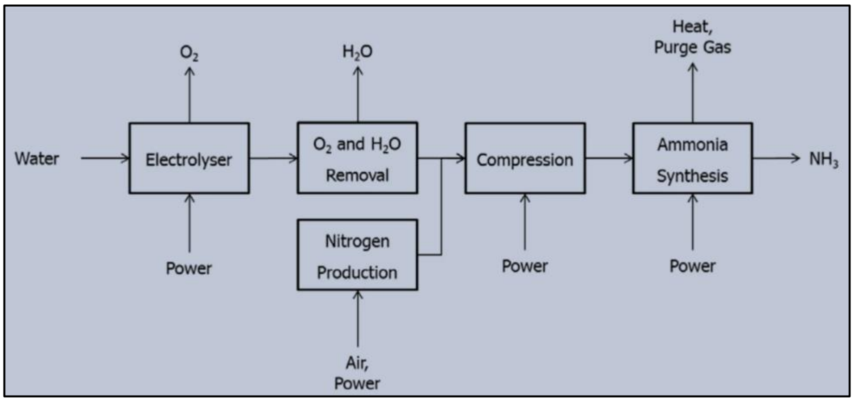

Figure 2.3 Water electrolysis and Air separation for Ammonia production

2.1.4 Steam Methane Reforming

Conventionally ammonia is produced by Haber-Bosch process, coupled with steam methane reforming (SMR). During SMR, methane reacts with steam to generate carbon monoxide and hydrogen. SMR operates at high temperatures, typically around 800°C to 1000°C, to facilitate the endothermic reaction.

Hydrogen produced is then combined with nitrogen in the presence of an iron catalyst under moderate temperature (400-500°C) and high pressure (150-300 atm). This chemical reaction yields ammonia (NH_3). The high pressure facilitates the conversion, while the iron catalyst enhances the reaction rate. The produced ammonia is then separated and collected for further use.

Drawbacks: It is energy-intensive, requiring high temperatures and pressures to drive the reaction. Also, the process relies on non-renewable natural gas as a hydrogen source, contributing to carbon emissions.

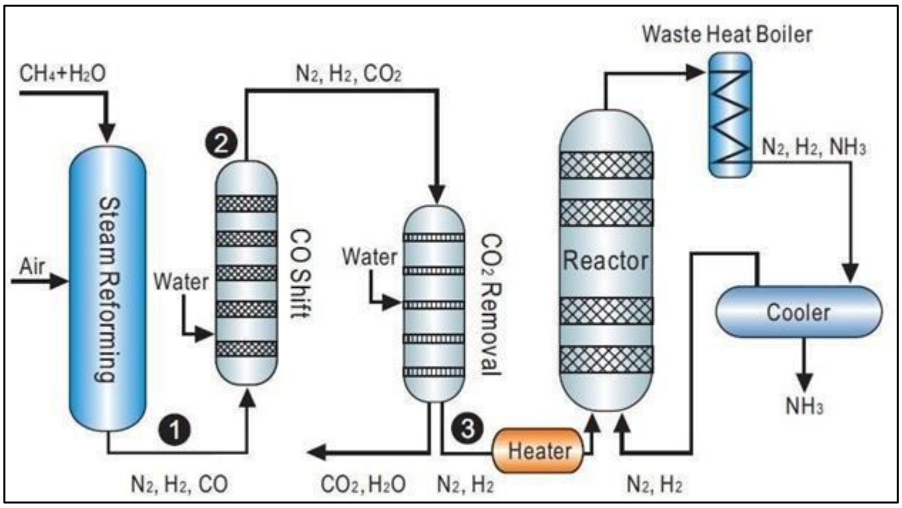

Figure 2.4 Steam Methane Reforming and other steps in Ammonia production

CHAPTER 3

PROCESS SELECTION AND DESCRIPTION

In the initial phase, several publishing materials were read extensively to understand the nature of Green Hydrogen and Green Ammonia, as these were the primary objectives of the project. Several methodologies were studied before finalizing the processes to produce hydrogen and nitrogen. All other methodologies were excluded either because of a lack of efficiency and high operating cost, or because they led to the production of hydrogen type other than green hydrogen (Ayub et al., 2024).

Detailed process selection and description is given below.

3.1 Hydrogen Production

3.1.1 Process Selection

To produce ammonia fertilizer through a clean and green process an important reagent required is green hydrogen. Electrolysis is a promising option for carbon free hydrogen production .Three major Electrolysis were considered for this process (Guo et al., 2019)

- Alkaline Electrolysis
- Solid Oxide Electrolysis
- Polymer Exchange Membrane Electrolysis

After an in-depth study of these Electrolyzer, PEM electrolysis process was selected due to following reasons:

- High purity hydrogen production (99.99%)
- Easy operation in low temperature and pressure conditions
- High efficiency and faster response time
- Compact design and structure

3.1.2 Process Description

For PEM electrolysis, Proton Exchange Membrane PEM Electrolyzer is used. A PEM Electrolyzer (like a cell) consists of Anode , Cathode separated by a solid polymer electrolyte membrane. During the electrolysis reaction water is split into its constituent parts on either side of polymer exchange membrane. (Rashid et al., 2015), (Carmo et al., 2013)

When direct voltage is applied to the PEM Electrolyzer highly pure water at the anode is oxidized to produce oxygen, protons, and electrons. Protons selectively move across the positive ion exchange membrane (hydrogen ions) while electrons flow through the external circuit towards cathode.

- **Anode Reaction:**

  $H_2O \rightarrow 1/2O_2 + 2H^+ + 2e^-$

At the cathode hydrogen ions combine with the electrons to produce hydrogen gas

- **Cathode Reaction:**

  $2H^+ + 2e^- \rightarrow H_2$

The hydrogen gas produced is then dried and fed into ammonia reactor.

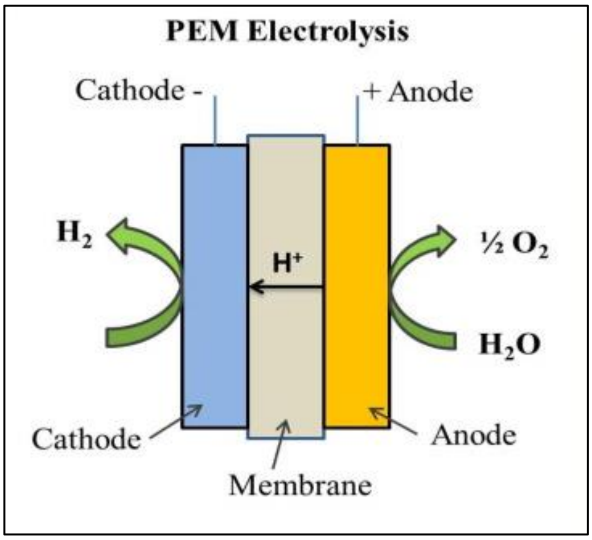

Figure 3.1 PEM Electrolyzer

3.2 Nitrogen Separation

3.2.1 Process Selection

For the separation of nitrogen from air three major processes were taken under consideration.

- Membrane Air separation
- Cryogenic Air separation
- Pressure Swing Adsorption

After performing literature review PSA was chosen for nitrogen separation due to the following reasons

- Simple Operation
- Cost effectiveness
- High performance under ambient temperature
- High regeneration rate
- Low energy intensity

3.2.2 Process Description

Pressure Swing Adsorption PSA is an economical and reliable non cryogenic method used to separate nitrogen gas (in high purity) from air.

In PSA, gaseous species are separated under pressure based on their molecular characteristics and affinity for an adsorbent material. It is based on the principle of adsorption. Adsorption is a surface-based procedure during which agas, or liquid molecules adhere on the surface of the absorbent and a film of adsorbing material is created on the surface of adsorbent. (Ivanova & Lewis, 2012)

PSA system uses specialized adsorbent materials such as zeolites, molecular sieves, activated carbon as a trap, ideally adsorbing the target gas species at high pressure.The process then shifts toward low pressure to desorb the adsorbed material (oxygen) hence the name pressure swing adsorption. Main components of PSA system include two adsorption towers filled with adsorbent material, filters, and a storage tanks. (Lemcoff, 1999)

Two main simultaneous processes that occur in the PSA adsorption towers for nitrogen generation are:

- Separation
- Regeneration

Separation Process

The adsorbent selected for nitrogen generation in this process is Carbon molecular sieve CMS, a strong and chemically inert material that captures mainly oxygen gas under high pressure. Air under ambient conditions passes through the filter system. It is then compressed and enters one of the two adsorption towers. CMS has a high affinity to adsorb Oxygen while leaving Nitrogen untouched, allowing it to pass through easily. This process continues till the adsorbent gets saturated.

Regeneration Process

The first column reaching its maximum capacity for adsorbing results in the desorbing phase, in which the pressure of the column is reduced, and Oxygen is separated out from the carbon molecular sieves and is vented out from the column.

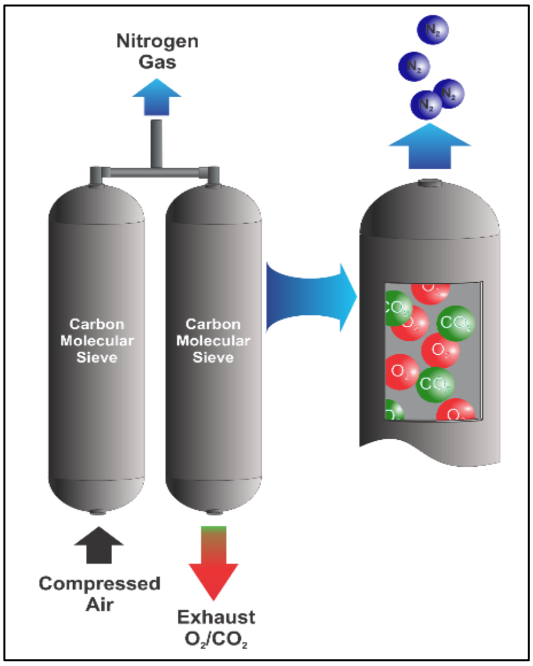

Figure 3.2 Pressure Swing Adsorption of Air

3.3 Ammonia Synthesis

3.3.1 Process Selection

To produce ammonia from nitrogen and hydrogen produced in the previous steps, the **Haber Bosch process** is used. As it is the most used process and is already being utilized at FFC for ammonia synthesis.

3.3.2 Process Description

Nitrogen and hydrogen are compressed and heated to reach the temperature and pressure suitable for the Haber process.

Ammonia synthesis reaction is as follows:

$$N_2 + 3H_2 \leftrightarrow 2NH_3$$

It is a reversible exothermic reaction which occurs in the presence of iron catalyst under the suitable temperature of approximately 400-450 °C and the atmospheric pressure of 150-300 bar.

The Ammonia produced is cooled, liquified and stored while some the unreacted gases (inert) are purged to lower their buildup and most of them are recycled to achieve the desire ammonia productivity. (Moulijn et al., 2013)

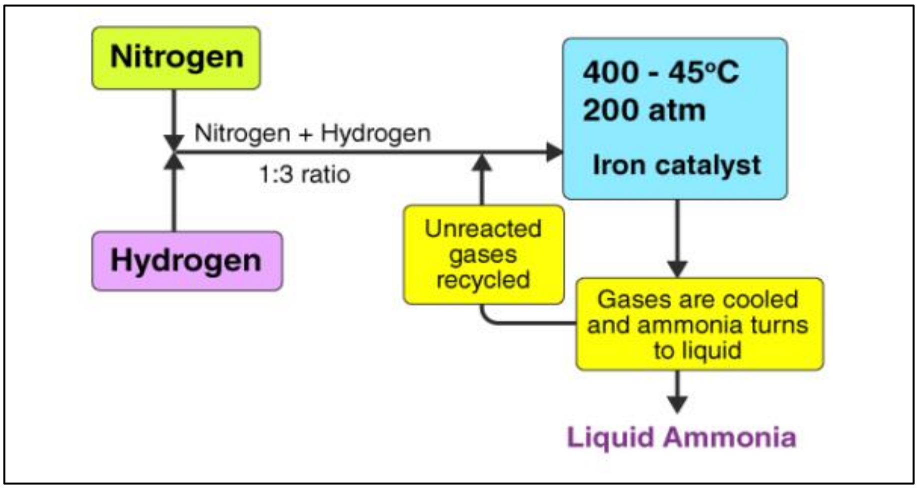

Figure 3.3 Ammonia production via Haber Bosch

3.4 Process Flow Diagram

The proposed Process Flow Diagram is shown below

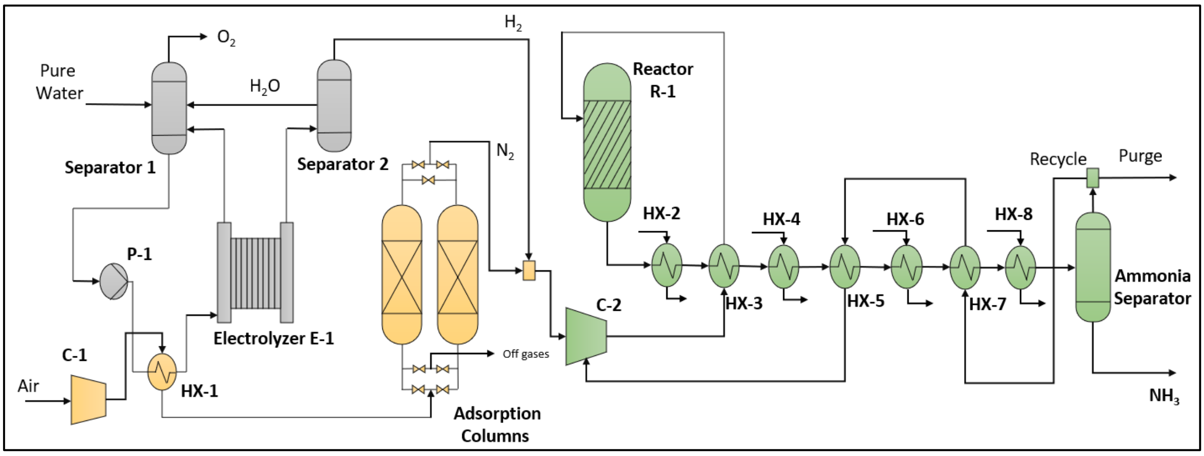

Figure 3.4 Process Flow Diagram

CHAPTER 4

MATERIAL BALANCE

4.1 Basis

The basis for the material balance is taken to be 150 tonnes of ammonia produced per day.

4.2 General Mass Balance

Mass in – Mass out + Generation – Consumption = Accumulation

- **Steady state non-reactive system**:

Mass in = Mass out

DOF = No of unknown variables – No of independent Equ- additional info

- **Steady state Reactive system**:

Mass in + Generation - Consumption = Mass out

DOF = No of unknown variables + No of reactions – No of independent Equation – additional info

4.3 Component Wise Material Balance

Balance for each component present in the system is given below:

4.3.1 Electrolyzer

Pure water is split into hydrogen and oxygen by applying electrical energy in PEM Electrolyzer using proton conducting polymer as an electrolyte.

Oxygen is generated at the anode side. While Hydrogen is produced at cathode side.

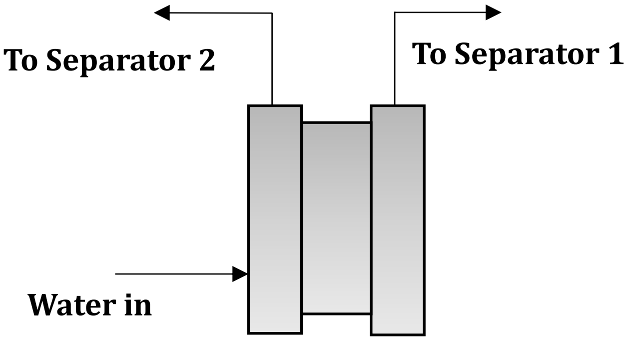

Figure 4.1 PEM Electrolyzer

Reactions and Equations used are mentioned below:

At Anode: $\mathbf{H_2O \rightarrow 2H^+ + ½\, O_2 + 2e^-}$

H_2O req = $\frac{H+Generated}{Conversion\times 2}$

At Cathode: $\mathbf{2H^+ + 2e^- \rightarrow H_2}$

H+ req = H_2 Produced × 2

Table 4.1Material balance for PEM Electrolyzer

MATERIAL BALANCE			
Components	**Water in**	**Separator 2 in**	**Separator 1 in**
	kg/h	kg/h	kg/h
Water	16900	2113	2113
Oxygen	0	11260	traces
Hydrogen	0	traces	1419
	16900	13373	3532

4.3.2 Separator 1

This separates hydrogen and water. Hydrogen is sent for ammonia formation and water is sent to water storage tank. For further purification of hydrogen dryer can be used.

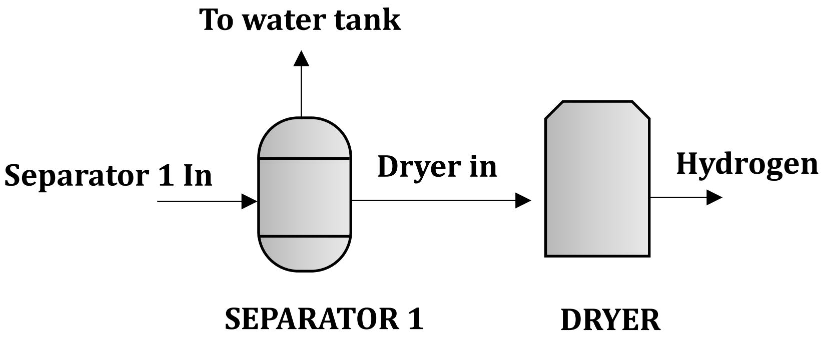

Figure 4.2 Separator 1 and dryer

Equation used are mentioned below:

- Hydrogen in (dryer) = efficiency of Separator × Hydrogen in(separator)
- Efficiency of separator = 99%
- Purity of hydrogen at dryer outlet = 99.9%

Table 4.2 Material balance for Separator1 and Dryer

MATERIAL BALANCE				
Components	**Separator 1 in**	**To water Tank**	**Dryer in**	**Hydrogen**
	kg/h	kg/h	kg/h	kg/h
Water	2113	2092	21.1	1.3
Oxygen	traces	traces	traces	traces
Hydrogen	1419	14.2	1405	1405
	3532	2106	1426	1406

4.3.3 Separator 2

This separator serves 2 purposes. It separates oxygen and water and acts as a water storage tank. The oxygen is vented into air and the water along with fresh water is fed to the Electrolyzer.

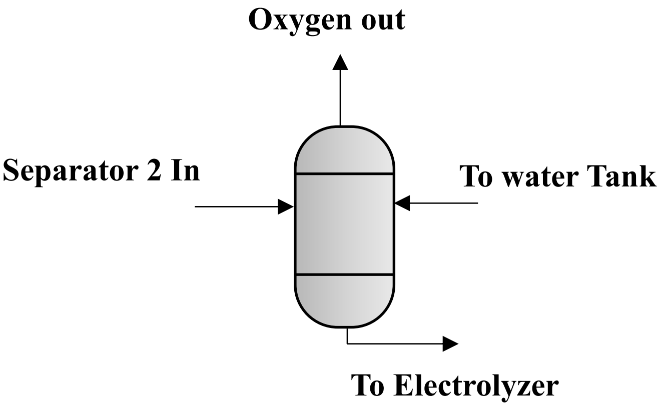

Figure 4.3 Separator 2

Equation used are mentioned below:

- Oxygen out = efficiency of Separator × Oxygen in
- Efficiency of separator = 99%

Table 4.3 Material balance for Separator 2

MATERIAL BALANCE			
Components	**Separator 2 in**	**To water Tank**	**Oxygen out**
	kg/h	kg/h	kg/h
Water	2113	2092	21.1
Oxygen	11260	traces	11147
Hydrogen	traces	traces	traces
	13373	2092	11168

4.3.4 Air Filter

Filter removes any solid particles from the air to purify it for smooth operation of adoption columns.

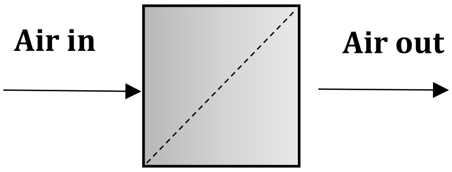

Figure 4.4 Air Filter

Composition of air used is as follows:

N_2= 78%

O_2 = 21%

Inert = 1%

Equation used is mentioned below:

- Air Required= Nitrogen produced/0.78

Table 4.4 Material Balance for Air Filter

MATERIAL BALANCE		
	Air in	**Air Out**
	kg/h	kg/h
Nitrogen	9300	9300
Oxygen	2860	2860
inert	170	170
Solid particles	Traces	-
	12330	12330

4.3.5 Adsorption ColumnS

Equations used are mentioned below:

Nitrogen purity= 99.8%

Nitrogen Recovery = 70%

(Ruthven et al., 1994)

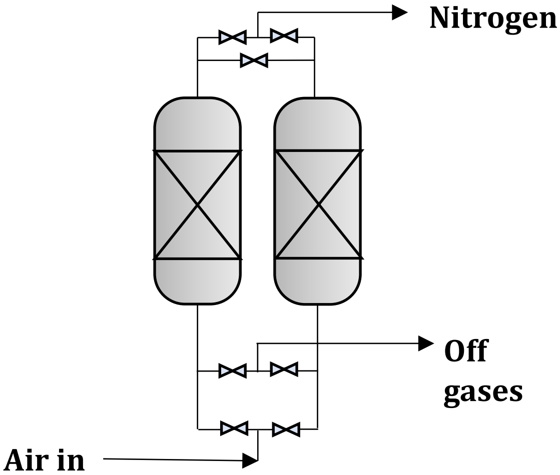

Figure 4.5 Adsorption Columns

Table 4.5 Material Balance for Adsorption Columns

MATERIAL BALANCE			
Components	**Air in**	**Nitrogen**	**Off gases**
	kg/h	kg/h	kg/h
Nitrogen	9300	6506	2790
O_2 +inert	3030	154	2870
	12330	6660	5660

4.3.6 Ammonia Reactor

Fresh feed (containing hydrogen produced from electrolysis and nitrogen from PSA) and recycle stream are mixed. This mixed stream is then fed to the ammonia reactor.

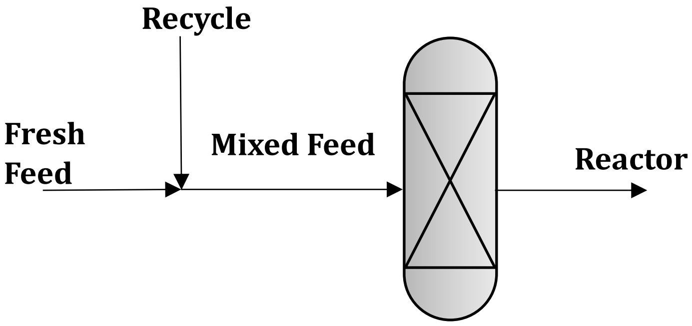

Figure 4.6 Ammonia Reactor

Equations used are mentioned below:

- Mixed Feed = Recycle + Fresh Feed

Ammonia Synthesis Reaction: $N_2 + 3 H_2 \leftrightarrow 2 NH_3$

- N_2 out = N_2 in – N_2 consumed = N_2 in – (N_2 in × conversion)
- H_2 out = H_2 in – H_2 consumed = H_2 in – (N_2 consumed × 3)
- NH_3 out = NH_3 in + NH_3 generated = NH_3 in + (N_2 consumed × 2)

Conversion = 30%

Table 4.6 Material balance for Ammonia Reactor

MATERIAL BALANCE				
Components	**Fresh Feed F**	**Recycle R**	**Mixed feed M**	**Reactor out**
	kg/h	kg/h	kg/h	kg/h
Nitrogen	6506	11019	17524	12276
Hydrogen	1405	2379	3784	2649
Ammonia	-	1318	1318	7711
	7911	14716	22626	22626

4.3.7 Ammonia Separator

This separates the liquid ammonia from the unreacted gases. Part of unreacted gases is purged, and rest is recycled back to ammonia reactor.

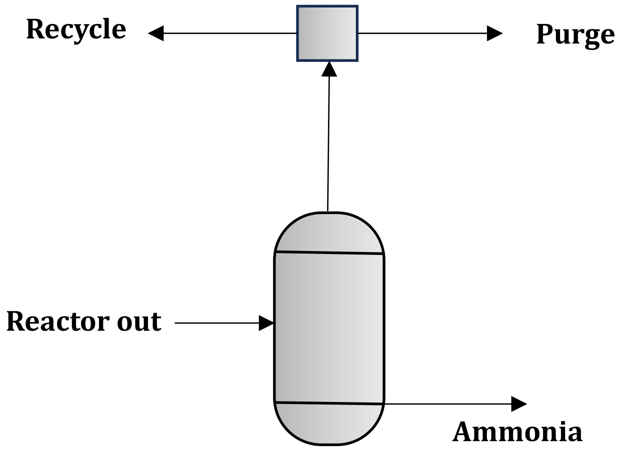

Figure 4.7 Ammonia Separator

Equations used are mentioned below:

- Product (ammonia)= 150 ton/day
- Product purity = 99.8%

Table 4.7 Material Balance for Ammonia Separator

MATERIAL BALANCE				
Components	**Reactor Out**	**Ammonia**	**Recycle**	**Purge**
	kg/h	kg/h	kg/h	kg/h
Nitrogen	122767	5.1	11019	1244
Hydrogen	2649	1.1	2379	269
Ammonia	7711	6244	1318	149
	22626	6250	14716	1661

CHAPTER 5

ENERGY BALANCE

5.1 General Energy Balance

For open system:

$$\Delta H + \Delta E_k + \Delta E_p = Q - W_s$$

$\Delta E_k = 0$

$\Delta E_p = 0$

$$\Delta H = Q - W_s$$

Where, $\Delta H = \Delta U + W_{flow}$

W_s = shaft work

Q = Heat

5.2 Component Wise Energy Balance

5.2.1 Water Pump

A pump is used to raise the pressure of Electrolyzer feed water from 1 bar to 30 bar.

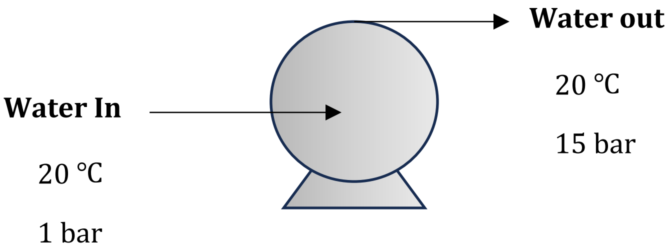

Figure 5.1 Water Pump

Pump duty is calculated using the following relation. Adiabatic efficiency of pump is taken as 75 % (assuming no temperature rise)

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

Table 5.1 Energy Balance for Water pump

ENERGY BALANCE			
Properties	**Units**	**Water In**	**Water Out**
Temperature	°C	20	20
Pressure	bar	1	15
Density	kg/m^3	1000	1000
Mass flow rate	Kg/h	16904	16904
Adiabatic Efficiency		0.75	
Pump Duty	kW	8.77	

5.2.2 Electrolyzer

Electrical energy consumption for the Electrolyzer is given by the following equation:

$$\boldsymbol{Q = \frac{\dot{m}H_2 * HHV_{H_2}}{\eta_{electrolyzer}}}$$

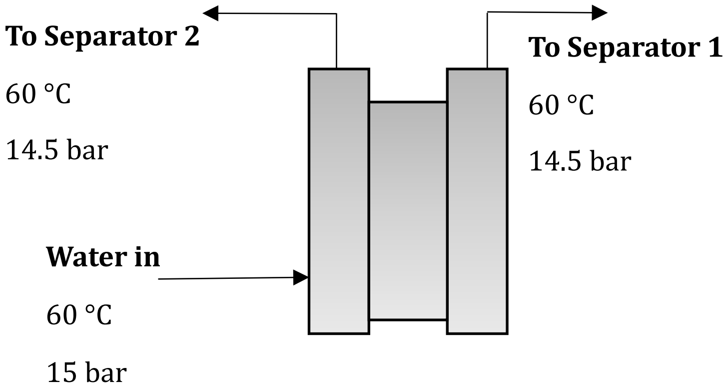

Figure 5.2 PEM Electrolyzer

For 75 % Electrolyzer efficiency,

39.39 kWhkg HHV_{H_2}(Higher heating value of H_2)

1405 kg/h H_2 (mass flow rate of H2 produced) Energy required is calculated.

Also Specific energy consumption is given by

$$\boldsymbol{SEC = \frac{Q_{IN}}{\dot{m}H_2}}$$

Table 5.2 Energy Balance for PEM Electrolyzer

ENERGY BALANCE			
Properties	**Units**	**Electrolyzer in**	**Electrolyzer out**
Temperature	°C	60	60
Pressure	bar	15	14.5
Efficiency		0.75	
Qin	kW	73000	
SEC	kWh/kg	52	

5.2.3 Multistage Compressors

Compressors are used for compression of gases within the process. Intercoolers are installed after each compressor unit to reduce compressor duty and proper functioning. (Sinnott et al., 2005)

The polytropic work for each stage is given by.

$$\mathbf{W=\frac{Z*R*T1}{MW}\left(\frac{n}{n-1}\right)\left((P_2/P_1)^{n/(n-1)}-1\right)}$$

Where, Z is Compressibility factor

n is Polytropic exponent given by

$$n = \frac{\Upsilon Ep}{\Upsilon \mathrm{Ep} - \Upsilon + 1}$$

Mw is Molecular weight

Ep is polytropic efficiency.

$\Upsilon = Cp/(Cp - R)$

P2 and P1 are pressure at inlet and outlet

Two main compressors are used in this process. Detailed calculations for each are shown below:

- **Two Stage Air Compressor**

This is used for compressing the air before entering the adsorption column.

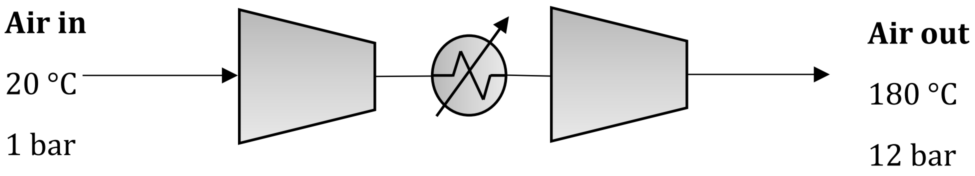

Figure 5.3 Two Stage Air Compressor

Table 5.3 Energy balance for Two stage Compressor

ENERGY BALANCE					
Properties	**Units**	**Stage 1**		**Stage 2**	
		Air in	**Air out**	**Air in**	**Air out**
Temperature	°C	25	180	**45**	180
Pressure	bar	1	3.54	3.54	12
Flowrate	kg/h	12300	12300	12300	12300
Avg ϒ		1.403		1.409	
Actual Work	kW	630		650	
Total Work	kW	**1280**			

- **Four Stage Feed Compressor**

This compresses the ammonia reactor feed to the desired pressure.

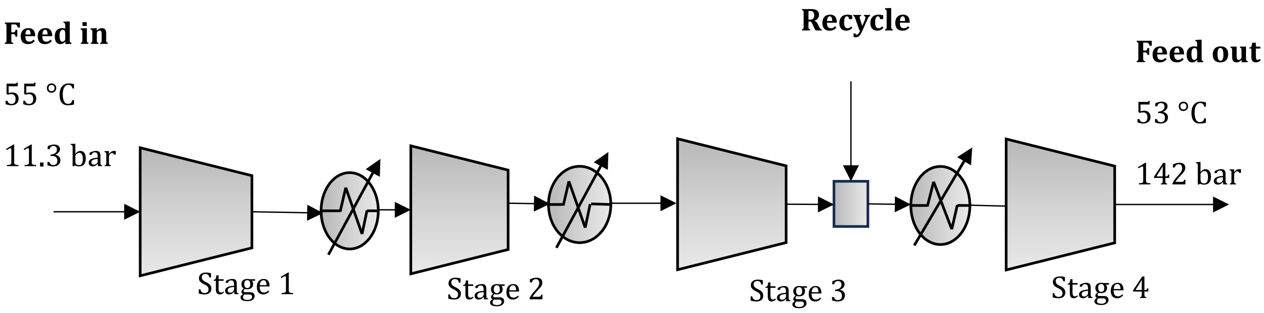

Figure 5.4 Four Stage Feed Compressor

Table 5.4 Energy Balance for 4 stage Feed Compressor

ENERGY BALANCE									
Properties	**Units**	**Stage 1**		**Stage 2**		**Stage 3**		**Stage 4**	
		Feed in	**Feed out**	**Feed in**	**Feed out**	**Feed in**	**Feed out**	**Feed in**	**Feed out**
Temperature	°C	55	182	45	176	45	180	35	53
Pressure	bar	11.3	25.6	25.6	58	58	132	132	142
Flowrate	kg/h	7910	7910	7910	7910	7910	7910	22630	22630
Avg ϒ		1.413		1.419		1.432		3.295	
Actual Work	kW	978		958		979		203	
Total Work	kW	**3118**							

5.2.4 Adsorption Column

The temperature and pressure conditions for inlet and outlet streams are shown in the figure.

The equation used is

$Q = m C_p \Delta T$

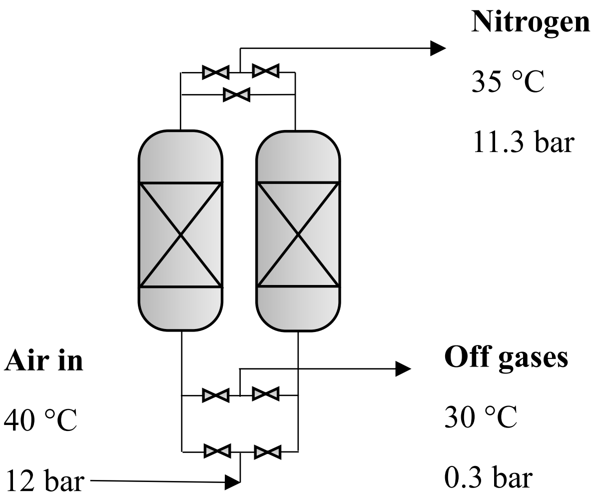

Figure 5.5 Adsorption Columns

Table 5.5 Energy balance for Adsorption Column

ENERGY BALANCE				
Properties	**Units**	**Air in**	**Nout**	**off gases**
Temperature	°C	40	35	30
Pressure	bar	12	11.3	0.3
Cp	kJ/kg °C	1.006	1.042	0.8887
Mass Flow Rate	Kg/h	12330	6660	5660
Heat Flow	kW	51.7	19.3	7.0
Heat Absorbed	kW	25.4		

5.2.5 Ammonia Reactor

As single chemical reaction is involved Heat of Reaction method is used for reactor's energy balance.

The reference state for the enthalpy change of products and reactant is taken as 25C and 1 bar at which $\Delta\widehat{H_r}$ is known.

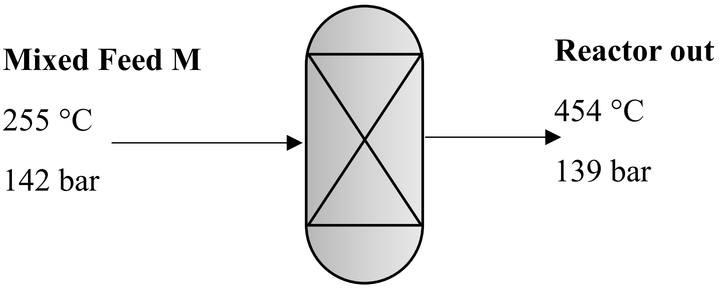

Figure 5.6 Ammonia Reactor

General equation for heat of reaction method

$$\Delta\dot{H} = \dot{\xi}\Delta\widehat{H_r} + \sum \dot{n}_{out}\,\widehat{H}_{out} - \sum \dot{n}_{in}\,\widehat{H}_{in}$$

Where, ξ is the extent of reaction given by

$$\xi = \frac{\left|n_{N_2,out} - n_{N_2,in}\right|}{\left|v_{N_2}\right|}$$

Table 5.6 Energy Balance for Ammonia Reactor

ENERGY BALANCE							
Properties	**Units**	**Reactor In**			**Reactor out**		
		N_2	**H_2**	**NH_3**	**N_2**	**H_2**	**NH_3**
Enthalpy $\hat{H}$	**kJ/kmol**	6.7×10^3	6.6×10^3	9.1×10^3	1.3×10^4	1.3×10^4	1.8×10^4
Flow rate (n)	**kmol/h**	626	1877	77	438	1314	453
$\Sigma(n.\hat{H})$	**kJ**	17.32×10^6			30.27×10^6		
Extent of reaction	**kmol/h**	188					
$\Delta\hat{H}\dot{r}$	**kJ/kmol**	-9.5×10^4					
ΔH	**kW**	-1.38×10^3					

5.2.6 Heat Exchangers

Heat exchangers are used to exchange heat between two fluids. The amount of heat released by the hot fluid is equal to the amount of heat absorbed by the cold fluid. This is given by:

$$\mathbf{\Delta H_{hot} = \Delta H_{cold}}$$

$$m_1\ C_{p,1}\ \Delta T_1 = m_2\ C_{p,2}\ \Delta T_2$$

The energy balance for the exchangers used in the process is given below.

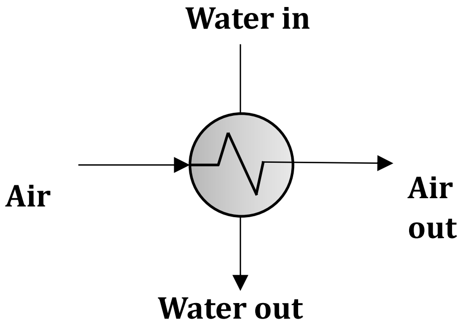

Figure 5.7 HX-1

Table 5.7 Energy Balance for HX-1

ENERGY BALANCE					
Properties	**Units**	**Water in**	**Water out**	**Air in**	**Air out**
Temperature	°C	25	60	180	40
Pressure	bar	30	30	12	12
Flowrate	kg/h	16904	16904	8626	8626
Avg Cp	kJ/ kg°C	4.17		1.036	
Q	kW	485		-485	

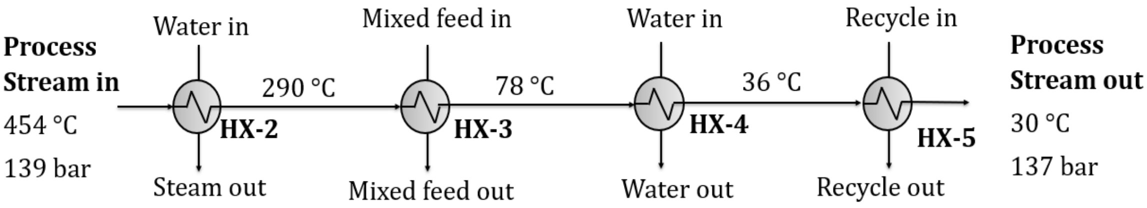

Figure 5.8 Heat Exchangers (HX-2 to HX-5)

Table 5.8 Energy balance for HX-2

ENERGY BALANCE					
HX-2					
Properties	**Units**	**Water in**	**Steam out**	**Process S in**	**Process S out**
Temperature	°C	25	179	454	290
Pressure	bar	10	9.5	139	138.5
Flowrate	kg/h	7700	7700	22626	22626
Avg Cp	kJ/kg°C	2.017		3.23	
Q	kW	3360		-3360	

Table 5.9 Energy balance for HX-3

ENERGY BALANCE					
HX-3					
Properties	**Units**	**M in (1)**	**M out (1)**	**Process S in**	**Process S out**
Temperature	**°C**	90	246	290	78
Pressure	**bar**	142	141.5	138.5	138
Flowrate	**kg/h**	22630	22630	22626	22626
Avg Cp	**kJ/kg°C**	4.1		3.15	
Q	**kW**	4060		-4060	

Table 5.10 Energy balance for HX-4

ENERGY BALANCE					
HX-4					
Properties	**Units**	**Water in**	**Water out**	**Process S in**	**Process S out**
Temperature	**°C**	25	45	78	36
Pressure	**bar**	1	1	138	137.5
Flowrate	**kg/h**	50400	50400	22626	22626
Avg Cp	**kJ/kg°C**	4.18		3.15	
Q	**kW**	857		-857	

Table 5.11 Energy balance for HX-5

ENERGY BALANCE					
HX-5					
Properties	**Units**	**Recycle in**	**Recycle out**	**Process S in**	**Process S out**
Temperature	°C	13	21	36	30
Pressure	bar	134.5	134	137.5	137
Flowrate	kg/h	14716	14716	22626	22626
Avg Cp	kJ/kg°C	3.24		2.955	
Q	kW	111		-111	

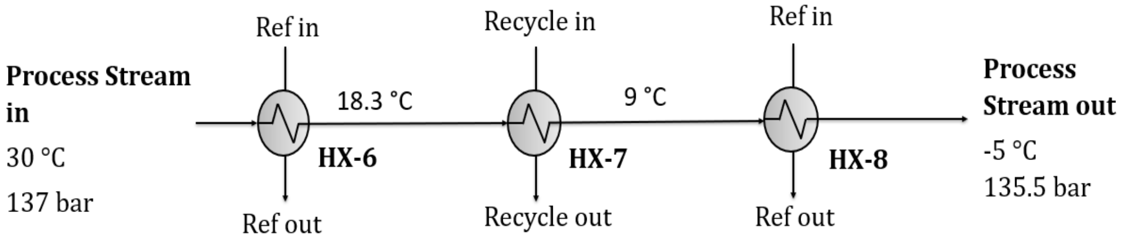

Figure 5.9 Evaporators and Heat Exchanger

Table 5.12 Energy balance for HX-6

ENERGY BALANCE			
HX-6			
Properties	**Units**	**Refrigerant in**	**Refrigerant out**
Temperature	°C	0.5	0.5
Pressure	bar	4.5	4.5
Flowrate	kg/h	27700	27700
Q	kW	9297	

Table 5.13 Energy Balance for HX-7

<table>
<tr><th colspan="6">ENERGY BALANCE</th></tr>
<tr><th colspan="6">HX-7</th></tr>
<tr><th>Properties</th><th>Units</th><th>Recycle in</th><th>Recycle out</th><th>Process S in</th><th>Process S out</th></tr>
<tr><th>Temperature</th><td>°C</td><td>-5</td><td>13</td><td>18.3</td><td>5.2</td></tr>
<tr><th>Pressure</th><td>bar</td><td>13240</td><td>13240</td><td>13900</td><td>13900</td></tr>
<tr><th>Flowrate</th><td>kg/h</td><td>14716</td><td>14716</td><td>22626</td><td>22626</td></tr>
<tr><th>Avg Cp</th><td>kJ/kg°C</td><td colspan="2">3.232</td><td colspan="2">2.924</td></tr>
<tr><th>Q</th><td>kW</td><td colspan="2">143</td><td colspan="2">-143</td></tr>
</table>

Table 5.14 Energy balance for HX-8

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<tr><th colspan="4">HX-8</th></tr>
<tr><th>Properties</th><th>Units</th><th>Refrigerant in</th><th>Refrigerant out</th></tr>
<tr><th>Temperature</th><td>°C</td><td>-8.9</td><td>-8.9</td></tr>
<tr><th>Pressure</th><td>bar</td><td>3</td><td>3</td></tr>
<tr><th>Flowrate</th><td>kg/h</td><td>29800</td><td>29800</td></tr>
<tr><th>Avg Cp</th><td>kJ/kg°C</td><td>250</td><td>1400</td></tr>
<tr><th>Q</th><td>kW</td><td colspan="2">953</td></tr>
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CHAPTER 6

EQUIPMENT DESIGN

6.1 Electrolyzer

PEM Electrolyzer is selected for Hydrogen production via water electrolysis (Barbir, 2005)

6.1.1 Designing Steps

Designing of PEM Electrolyzer involves following steps (Ifkovits et al., 2021)

- Total current required to produce the desired amount of Hydrogen (1418 kg/h) is calculated using Faraday's Law for electrolysis.

  Operating conditions: 60°C and 15 bar

  $$\text{Total Current: } I_{total} = F * mH_2 * n$$

  Where,
  F is Faraday's constant
  mH_2 is Molar flow rate of hydrogen produced in mole/s
  n is number of electrons taking part in the reaction

  $$\boldsymbol{I_{total} = 96485 * 197 * 2 = 38015090\ A}$$

- Calculating the total voltage of the cells by taking a sum of all four voltages namely activation overpotential, ohmic overpotential, concentration overpotential and reversible overpotential.

  $$\boldsymbol{V_{cell} = V_{concentration} + V_{ohmic} + V_{reversible} + V_{activation}}$$

i. Activation overpotential is associated with the activation energy barrier that must be exceeded to allow the electrochemical reactions at the electrodes.

$$V_{activation} = \frac{RT_o}{nF} * ln\frac{j}{j_o} = \frac{8.314 * 333}{2 * 96485} * ln\frac{2}{0.1}$$

$$\boldsymbol{V_{activation} = 0.0535\ V}$$

Where,

$R = 8.3145\ \frac{J}{Kelvin * Mole}$

$j_0\ (exchange\ current\ density) = 0.1\ \frac{A}{cm^2}$

$j\ (current\ density) = 4.15\ \frac{A}{cm^2} (From\ literature)$

ii. Ohmic overpotential arises from the resistance offered by the electrolyte (or more specifically the proton exchange membrane) to the flow of ions and the resistance in the electrodes and other constituent parts of the cell.

$V_{ohmic} = I * \frac{\rho}{2}$

$\boldsymbol{V_{ohmic}}$ **= 0.2544 V**

Where,

ρ is the thickness of the membrane= $1.125 * 10^{-6}\ m$

iii. The reversible cell potential is given by the thermodynamics of the water splitting reaction and is equal to approximately 1.23 V at standard conditions, which is minimum amount of energy which is needed for electrolysis reaction to take place.

$V_{reversible} = 1.229 - 0.9 * 10^{-3}(T_o - T)$

$\boldsymbol{V_{reversible} = 1.1975\ V}$

Where,

Process temperature (T_o)= 333 K

Room temperature (T)= 298 K

iv. Concentration overpotential refers to the overpotential occurring because of concentration gradients of reactants and products at the electrode surface.

$\boldsymbol{V_{concentration} = 0.4145\ V}\ (From\ literature)$

$Now\ V_{cell}$ is given by:

$$V_{cell} = 0.4145 + 0.2544 + 0.0535 + 1.1975$$

$$\boldsymbol{V_{cell} = 1.92\ V}$$

- By using the values for cell voltage and resistance, to calculate the current of one cell.

$$I_{cell} = \frac{V_{cell}}{R_{internal}}$$

Where,

$R_{internal} = 4.245 * 10^{-6}\Omega$

$$\boldsymbol{I_{cell} = 452350\ A}$$

- Calculating the number of cells, using the ratio of total heat produced by the Electrolyzer to the heat produced in a single cell.

$$n_{cells} = \frac{Q_{heat,electrolyzer}}{Q_{heat,cells}}$$

Where,

$Q_{heat,electrolyzer} = 73000\ kW\ (From\ energy\ balance)$

$Q_{heat,cells} = V_{cell} * I_{cell} = 1.92 * 452350 = 868.5\ kW$

$$\boldsymbol{n_{cells} = 84.05 \approx 84\ cells}$$

- Area of electrodes is calculated using the values obtained for current and current densities.

$$Area\ of\ Electrode = \frac{I_{total}}{j}$$

$$\boldsymbol{Area\ of\ Electrode = 109047\ cm^2 \approx 10.9\ m^2}$$

6.1.2 Results

Table 6.1 Results for Electrolyzer design.

Property	Units	Value
I_{total}	A	38015090
I_{cell}	A	452350
Area of Electrode	m^2	10.9
$V_{concentration}$	V	0.4145
V_{ohmic}	V	0.2544
$V_{activation}$	V	0.0535
$V_{reversible}$	V	1.1975
V_{cell}	V	1.92
$Q_{heat,\ cells}$	kW	868.5
n_{cells}		84

6.2 Ammonia Reactor

6.2.1 Assumptions

Following assumptions were taken for the designing of ammonia reactor.

REACTOR

- Adiabatic fix bed reactor type
- Axial flow of gas within reactor
- Three catalyst bed within reactor
- Operation is autothermal.
- indirect cooling mechanism using three heat exchangers.
- Single pass conversion 30%

CATALYST

- Magnetic Iron oxide catalyst
- Promotors Aluminum oxide (3%) , Potassium oxide (1%)
- The density of catalyst is 850 kg/m3.
- Void fraction is 0.4.
- The bulk density of catalyst is 2650 kg/m3.
- Diameter of catalyst particles is 0.003m

6.2.2 Available Information

Temperature of gas stream at the inlet and outlet of each bed

Table 6.2 Temperature conditions for gas stream

Specification	**Bed 1**	**Bed 2**	**Bed 3**
Inlet Temperature (C)	347.6	436.1	409.4
Outlet Temperature (C)	495.3	466.1	442.7

Assuming the conversion across each bed material balance was done and following results were obtained

Conversion for Bed 1 = 19%

Table 6.3 Bed 1 inlet conditions

Components	**Mol percent (%)**	**Mol Frac**	**Kmol/hr.**	**Kg/hr**
N2	24.25	0.2425	625.5785	17524.33
H2	72.75	0.7275	1876.735	3783.499
NH3	3	0.03	77.39115	1318.049
F	100	1	2579.705	22625.88

Conversion for Bed 2 =24%

Table 6.4 Bed 2 inlet conditions

Components	**Mol Percent (%)**	**Mol Frac**	**Kmol/hr.**	**Kg/hr**
N2	21.63628	0.216363	506.7186	14194.71
H2	64.90885	0.649089	1520.156	3064.634
NH3	13.45487	0.134549	315.111	5366.655
Rout	100	1	2341.985	22626

Conversion for Bed 3 =30%

Table 6.5 Bed 3 inlet conditions

Components	**Mol Percent (%)**	**Mol Frac**	**Kmol/hr.**	**Kg/hr**
N2	20.85785	0.208579	475.4396	13318.49
H2	62.57356	0.625736	1426.319	2875.459
NH3	16.56858	0.165686	377.6688	6432.078
Rout	100	1	2279.427	22626.03

6.2.3 Designing Steps

Following Steps were taken while solving each bed.

- To determine Volumetric flow rate first we need to determine Molar density.

  Molar density= $\frac{\boldsymbol{Pressure}}{\boldsymbol{Generalgas\ constant*temperature*Compressibility\ Factor}}$

  Then

  $$\boldsymbol{Average\ Density\ =\ Molar\ Density\ *\ Molecular\ weight}$$

  The molecular weight of gas stream can be calculated by multiplying molar mass of components with their mole fraction and adding them.

  Volumetric flowrate can be determined using formula.

  $\boldsymbol{Volumetric\ Flow\ rate\ =\ Mass\ flowrate\ of\ inlet\ stream/}$
  $\boldsymbol{Average\ Density}$

- Residence time can be determined using formula.

  $$\boldsymbol{T = Area\ under\ the\ curve * Initial\ Concentration\ of\ (N2)}$$

  N2 is the Limiting reactant.

  Area under the curve

  To Determine Area under the curve Graph is plotted by varying conversion and determining the value of 1/rate.

  Simple rate equation used is.

  $rate$ = $K\ [H]^2[N2]$

  K= rate constant

  It is calculated using equations:

  $lnk\ =\ -2.691122log(T) - 5.519265 * E - 5(\ T) + 1.848863 * E - 7\ (T\text{^}2)\ +$
  $2001.6/T\ + 2.68$

Dividing the answer with constant factor 17.09

[H2]=Concentration of Hydrogen

[N2]=Concentration of Nitrogen

Concentration of nitrogen and hydrogen is determined using formula.

$$\boldsymbol{Concentration\ =\ Initial\ Concentration\ *\ [(1-\ conversion)/(1+\ \in *\ Conversion)]}$$

Initial concentration of nitrogen and hydrogen is determined.

$$\boldsymbol{Co\ =\ (Initial\ Molar\ folwrate\ )/(Volumetric\ flow\ rate)}$$

$$\in = \frac{\boldsymbol{Total\ molar\ flow\ out - Total\ molar\ flow\ in}}{\boldsymbol{Total\ molar\ flow\ in}}$$

Calculations for each bed in detail are given below

For Bed 1

By varying the Conversion from 0 to 0.188 following results are obtained.

Graph is plotted between inverse of rate and conversion.

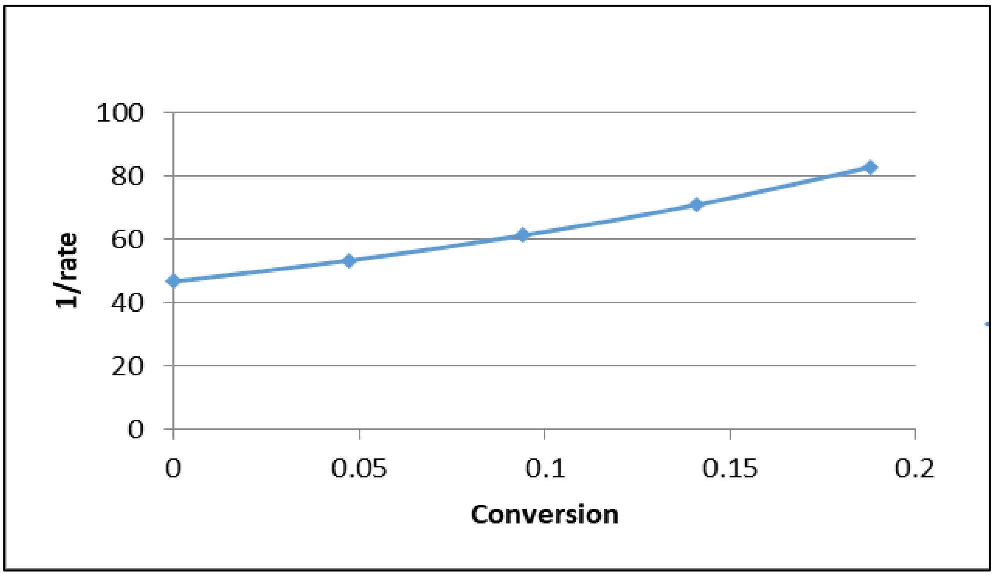


Figure 6.1 Inverse of rate vs Conversion - Bed 1

For Bed 2

We vary conversion from 0.189 to 0.241.

Table 6.6 Results for conversion from 0.189 to 0.241- Bed 2

Sr No	X	C_H	C_N	r_a	$1/r_a$
1	0.189	1.230248	0.410083	0.004381	228.2817
2	0.202	1.21095	0.40365	0.004178	239.3702
3	0.215	1.191639	0.397213	0.003981	251.1972
4	0.228	1.172314	0.390771	0.00379	263.8255
5	0.241	1.152976	0.384325	0.003606	277.3244

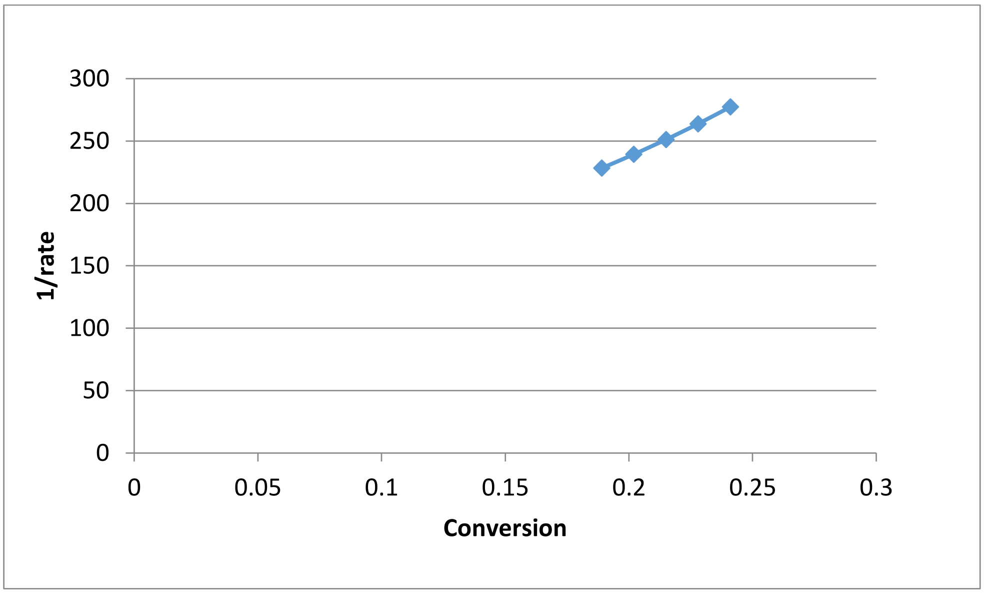


Figure 6.2 Inverse of rate vs Conversion - Bed 2

For Bed 3

By varying the Conversion from 0.242 to 0.3 following results are obtained

Table 6.7 Results for conversion from 0.189 to 0.241- Bed 2

Sr no	**X**	**C_H**	**C_N**	**r_a**	**$1/r_a$**
1	0.242	1.151518	0.383839	0.004173	239.6249
2	0.2565	1.130034	0.376678	0.003944	253.5533
3	0.271	1.108529	0.36951	0.003723	268.5975
5	0.285	1.087747	0.362582	0.003518	284.2891
6	0.3	1.065458	0.355153	0.003306	302.5062

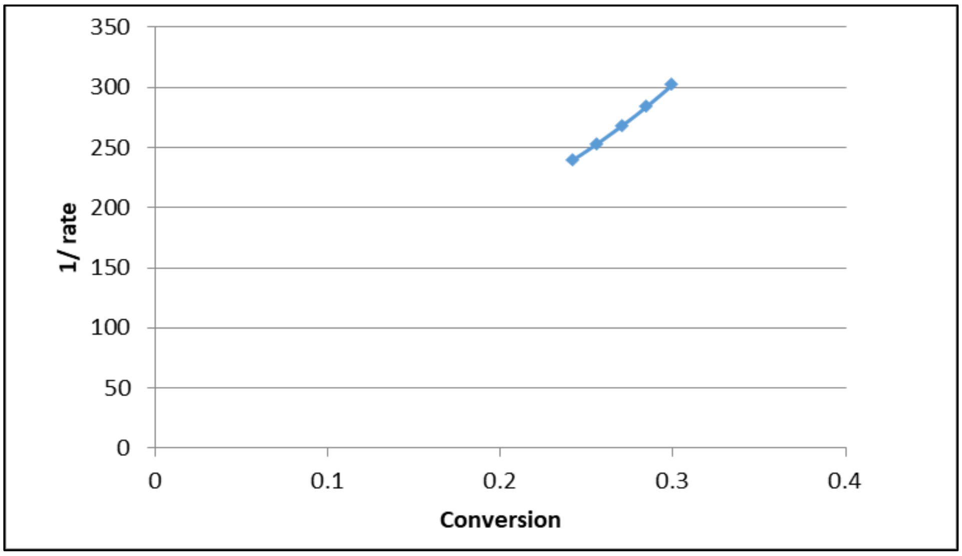


Figure 6.3 Inverse of rate vs Conversion - Bed 3

Area under the curve can be determined using formula.

$$\left(\frac{Yn+1+Yn}{2}\right) * (X(n+1) - Xn)$$

- To determine the volume of catalyst bed

$$Volume\ of\ Bed\ =\ Volumetric\ flow\ rate\ *\ Residence\ time$$

$$Actual\ Volume\ of\ bed\ =\ Volume\ of\ bed\ (1\ +\ void\ fraction)$$

- To determine Radius , Diameter, and length of bed

Considering bed as a cylinder

$$Actual\ Volume\ of\ Bed\ =\ pie\ *\ radius\text{^}2 *\ length$$

$(Length\ )/(Diameter\ )\ =\ 3$ (for catalyst bed)

$Diameter\ =\ 2\ *\ radius$

$Length\ of\ catalyst\ bed\ =\ 6\ *\ radius$

$Actual\ Volume\ of\ Bed\ =\ pie\ *\ 6\ *\ radius\text{^}3$

$Radius\ of\ bed\ =\ [(Volume\ of\ bed)/(pie\ *\ 6)]\text{^}1/3$

- To determine Mass of catalyst

$Mass\ \ =\ Bulk\ Density\ of\ Catalyst\ *\ Actual\ Volume\ of\ Bed$

- To determine Volume of catalyst bed

$Vol\ of\ Catalyst\ =\ Mass\ of\ Catalyst\ /\ Density\ of\ catalyst$

- Pressure Drop Calculation

Pressure drop is calculated using Ergun equation:

$\Delta P/\mathrm{L}$ = $(150 * (1 - void\ fraction)\text{^}2)/(Dp2 * void\ fraction\text{^}3) * \mathrm{V}s)$ + $(1.75 *(\mathrm{V}s2{*}density\ 1{-}void\ fraction)\ /(Dp{*}void\ fraction\text{^}3))$

Where,

Vs = superficial velocity

= volumetric flowrate/ area of cross section

6.2.4 Results

The results obtained by solving all above-mentioned equations are given below:

Table 6.8 Results for Reactor Design

Specification	**Catalyst Bed 1**	**Catalyst Bed 2**	**Catalyst Bed 3**
Molar Density (kgmol/m3)	2.54	2.32	2.41
Average Density (kg/m3)	2.23E+01	2.25E+01	2.39E+01
Volumetric Flow rate (m3/h)	1.01E+03	1.01E+03	9.46E+02
Initial Concentration of H2	1.85	1.51	1.51
Initial Concentration of N2 (kgmol/m3)	6.17E-01	5.03E-01	5.02E-01
$\in$	-0.09	-2.6711E-02	-3.29E-02
Residence time (s)	7.25	6.59	7.85
Actual Volume Of bed (m3)	2.9	2.6	2.9
Radius of catalytic bed (m)	0.5	5.15E-01	5.35E-01
Diameter of bed (m)	1.07	1.03	1.07
Length of catalyst bed (m)	3.2	3.1	3.2
Mass of catalyst (kg)	7573.9	6837.4	7659.31
Volume of catalyst (m3)	8.91	8.04	9.01
Pressure drop (bar)	0.40	0.448	0.375

6.3 Adsorption Column

6.3.1 Choice of adsorbent and its properties

The adsorbent used for PSA is Carbon molecular sieve CMS. Some of the important properties of CMS are given below (Green, 2007)

Table 6.9 Properties for CMS

Properties	
Porosity	0.5
Density	700 kg/m3
Adsorption Capacity	50% (0.5)

6.3.2 Assumptions

(Arnold & Stewart, 1998)

- The time for 1 cycle is 8 hours.
- Height to diameter ratio for adsorption column is 3:1

6.3.3 Designing Steps

- The adsorption capacity for any adsorbent is given by:

$$\boldsymbol{Adsorbent\ Capacity} = \frac{\textbf{mass of adsorbate}}{\textbf{mass of adsorbent}}$$

For nitrogen adsorbed in 1 cycle (8 working hours),

Mass of adsorbate = mass in – mass out

= (9294.71 – 6506.3) kg/hr * 8hr

Mass of adsorbate = 22307kg

Substituting values in above equation gives

$$\text{Mass of adsorbent} = \frac{\text{mass of adsorbent}}{\text{adsorbent Capacity}} = \frac{22307.2}{0.5}$$

Mass of adsorbent = 44614kg

- Volume for porous adsorbent is given by:

Volume of adsorbent = mass/ (density * porosity)

= 44614.4/ (700*0.5)

Volume of adsorbent = 127.5 m^3

- The diameter of cylindrical column is given by

Volume of cylindrical column = $\boldsymbol{\frac{\pi}{4} * D^2}$ *** H**

As Height to diameter = H:D = 3:1

$$= \frac{\pi}{4} * \ D^2 * 3 * D$$

$$= \ \frac{\pi}{4} * \ D^3 \ * 3$$

Diameter of adsorbent column = $\boldsymbol{\sqrt[3]{\frac{4*V}{3\pi}}}$

$$= \sqrt[3]{\frac{4*127.5}{3\pi}}$$

Diameter of adsorbent column = 3.7 m

Also,

Height of adsorbent column = 3*D

= 3* 3.7

Height of adsorbent column = 11.1m

With a compensation of about 1 ft above and 1 ft below the adsorbent column, the length of adsorption column is given by

Length of Adsorption Column =11.1 + 0.61m

Length of Adsorption column = 11.71 m

6.3.4 Results

Table 6.10 Results for Adsorption Column Design

Properties	Values
Mass of Adsorbate	22307 kg
Mass of Adsorbent	44614 kg
Volume of adsorbent	128 m^3
Column Length	11.7 m
Column Diameter	3.7 m

6.4 Heat Exchanger

6.4.1 Choice of Exchanger

Shell and Tube heat exchanger is used due to high flowrates. Counter-Current Flow is applied as outlet temperature of water is greater than outlet temperature of air.

6.4.2 Stream Condition

Water is placed at the tube side while air is present in the shell. Conditions and commonly used properties of both hot and cold fluid are given in the table below.

Table 6.11 Tube side specifications

TUBE SIDE	
Fluid	Water
Inlet Temperature (^{0}C)	25
Outlet Temperature (^{0}C)	60
Average cp (kJ/kgK)	4.180
Average Density (kg/m^3)	995
Average Viscosity (mNs/m^2)	0.8
Average Thermal Conductivity (W/m^{0}C)	0.59
Mass Flow Rate (Kg/hr)	16,904

Table 6.12 Shell side specifications

SHELL SIDE	
Fluid	Air
Inlet Temperature (^{0}C)	180
Outlet Temperature (^{0}C)	40
Average cp (kJ/kgK)	1.008
Average Density (kg/m^3)	0.922
Average Viscosity (mNs/m^2)	18.97 x 10^{-3}
Average Thermal Conductivity (W/m^{0}C)	0.028
Mass Flow Rate (Kg/hr)	8,626

Also, the Average Temperature of Water = (25+60)/2 = 45.2 ^{o}C

6.4.3 Designing Steps

Following are the main steps involved in designing of heat exchanger from ‘Chemical Engineering Design’ by R. K. Sinnott, J. M. Coulson and J. F. Richardson.

- **Heat Transfer Rate Q**

  $Q = m*Cp*\Delta T$
  $Q = (16904) * (4.180) * 35$
  $Q = 2473055.2$ kJ/h
  $Q = 2473055.2/3600$

  Q = 686.95kW

- **LMTD**

  $$\text{LMTD} = \frac{(180-60)-(40-35)}{\ln\frac{180-60}{40-35}}$$

  LMTD = 36.2 ^oC

- **Corrected LMTD**

  Corrected LMTD = F*LMTD
  Where,
  F= Correction Factor

$$\boldsymbol{R} = \frac{(\boldsymbol{T_{hot\ in}} - \boldsymbol{T_{hot\ out}})}{(\boldsymbol{t_{cold\ out}} - \boldsymbol{t_{cold\ in}})} = \frac{(180 - 40)}{(60 - 25)}$$

$$\boldsymbol{R} = 3.8$$

$$\boldsymbol{S} = \frac{(\boldsymbol{t_{cold\ out}} - \boldsymbol{t_{cold\ in}})}{(\boldsymbol{T_{hot\ in}} - \boldsymbol{t_{cold\ in}})} = \frac{(60 - 25)}{(190 - 25)}$$

$$\boldsymbol{S} = 0.226$$

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

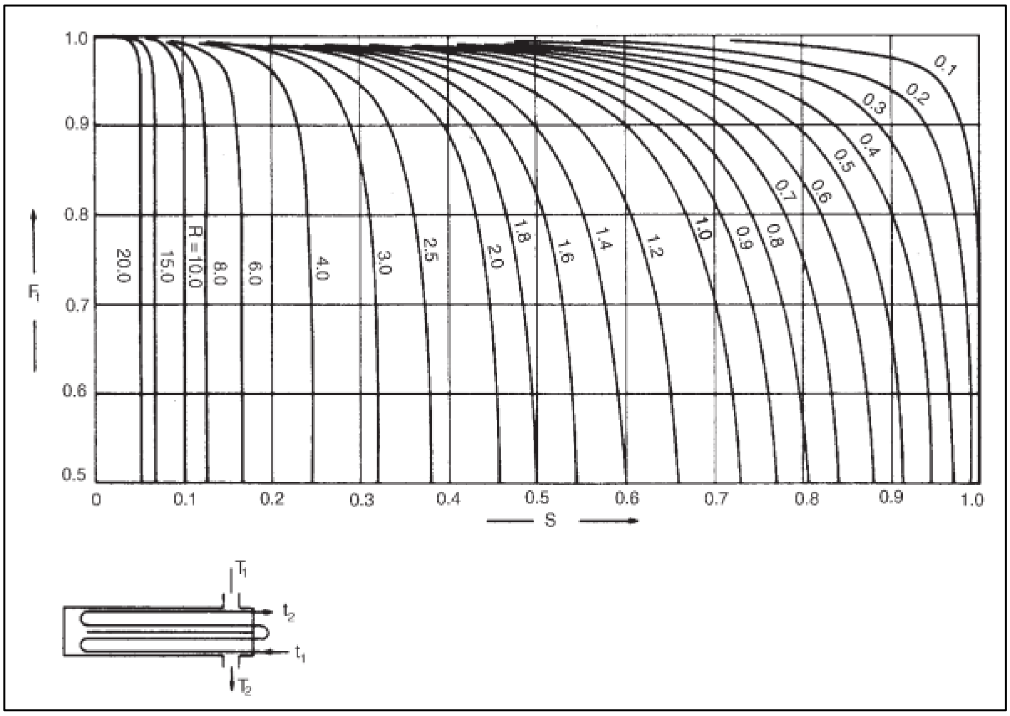


Figure 6.4 Temperature Correction factor

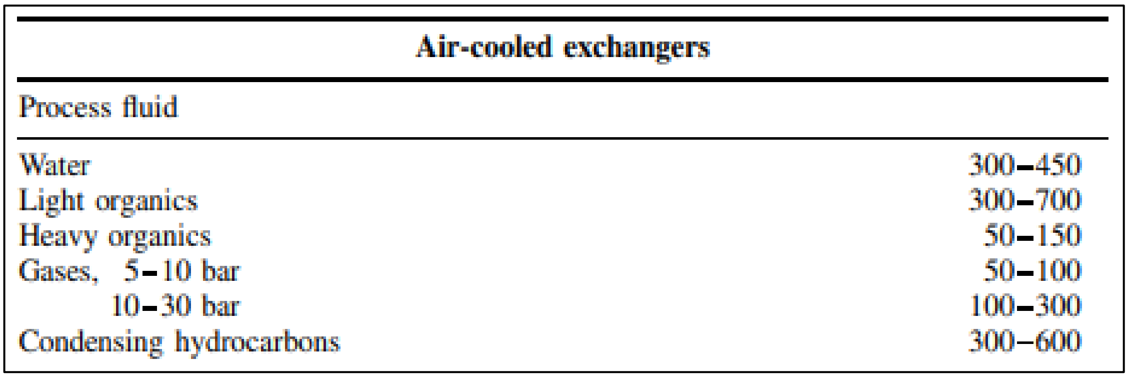
From the graph. F = 0.95
Corrected LMTD = F*LMTD
= 0.95 * 36.2

Corrected LMTD = 34.4 °C

- **Heat Transfer Area A**

Q = U*A*LMTD

U = Heat Transfer Coefficient
A = Heat Transfer Area



Air-cooled exchangers	
Process fluid	
Water	300–450
Light organics	300–700
Heavy organics	50–150
Gases, 5–10 bar	50–100
10–30 bar	100–300
Condensing hydrocarbons	300–600

Figure 6.5 Typical Overall coefficient

Assuming U = 440 W/m^2°C

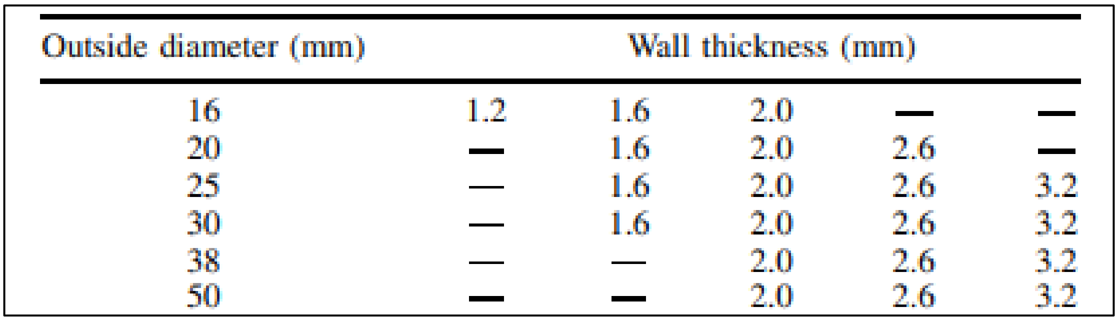
Also, the area is given by:

$A = \frac{Q}{U * LMTD}$

A = (686950)/(440*34.4)

A = 45.3 m^2

- **Tubes Specifications**



Outside diameter (mm)	Wall thickness (mm)				
16	1.2	1.6	2.0	—	—
20	—	1.6	2.0	2.6	—
25	—	1.6	2.0	2.6	3.2
30	—	1.6	2.0	2.6	3.2
38	—	—	2.0	2.6	3.2
50	—	—	2.0	2.6	3.2

Figure 6.6 Standard Dimensions for Steel tubes

The following values are used for steel tubes.

Outer Diameter = 50 mm , Tube Thickness = 2 mm , Inner Diameter = 48 mm

The pitch chosen for this type of heat exchanger is ***"Triangular Pitch",*** as shell side cleaning is not required frequently also the higher rates of the heat transfer provided by this type of pitch.
Tube Pitch = 1.25 * Outer Diameter

Pitch = 1.25 * 50

Pitch = 62.5 mm

Length of Tube = 9.90 m

Allow Tube Sheet Thickness of 0.05 m

Tube Length = 9.90 – 0.05

Tube Length = 9.85 m

Area of 1 tube = 9.85 * (50 x 10^{-3}) * Π

Area of 1 tube = 1.55 m^3

Number of tubes = $\frac{\text{Total Heat Transfer Area}}{\text{Area of 1 tube}}$

= 45.3/1.55

Number of tubes = 30 tubes

Tube Side Coefficient

Mean Water Temperature = (60 + 25)/2 = **42.5 ^{o}C**

Tube Cross Sectional Area = $\frac{\Pi}{4}$ * (50 x 10^{-3})^{2}

Tube Cross Sectional Area = 1.96 x 10^{-3} m^{2}

Tubes per pass = 30/8 = 3.75 = **4 tubes per pass**

Total Flow Area = 3.75 * (1.963 x 10^{-3})

Total Flow Area = 7.032 x 10^{-3} m^{3}

Flowrate of Water = 16904/3600 **= 4.6956 kg/s**

Water Mass Velocity = 4.6956/(7.032 x 10^{-3}) = **680 kg/m^{2}s**

Velocity of Water = 680/995

Velocity of Water = 0.7 m/s

di = 48 x 10^{-3} m

Viscosity of water = 0.8 mNs/m^{2}

Thermal conductivity = 0.59 W/m^{0}C

$$h^{i} = \frac{jh * Re * Pr0.33 * kF}{di}$$

Re = (density * u * di)/viscosity

Re = 41,790

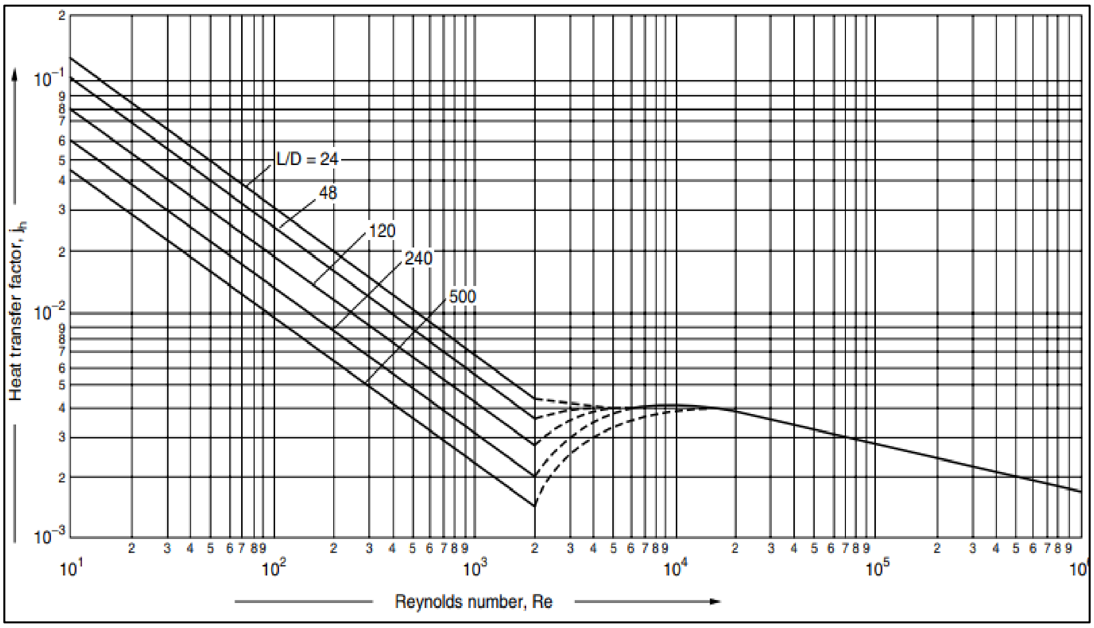


Figure 6.7 Tube side heat transfer coefficient

Jh = 3.9 x 10^{-2}

Pr = (cp * viscosity) / thermal conductivity

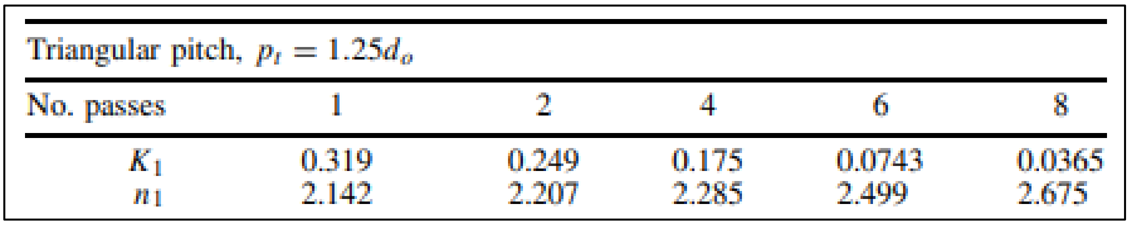
Pr = $(4.18 * 0.8 \times 10^{-3}) / 0.59$

Pr = 5.67×10^{-3}

hi = $\{(3.5 \times 10^{-2}) * (41790) * (5.67 \times 10^{-3})^{0.33} * (0.59)\} / (48 \times 10^{-3})$

Tube side Coefficient = hi = 3261 W/m^2°C

- **Shell Side Specifications**



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

Figure 6.8 Constants for Bundle Diameter Calculations

Bundle Diameter = D$_b$ = $62.5 * (\frac{30}{0.0365})^{1/2.675}$

Bundle Diameter = D$_b$ = 768 mm

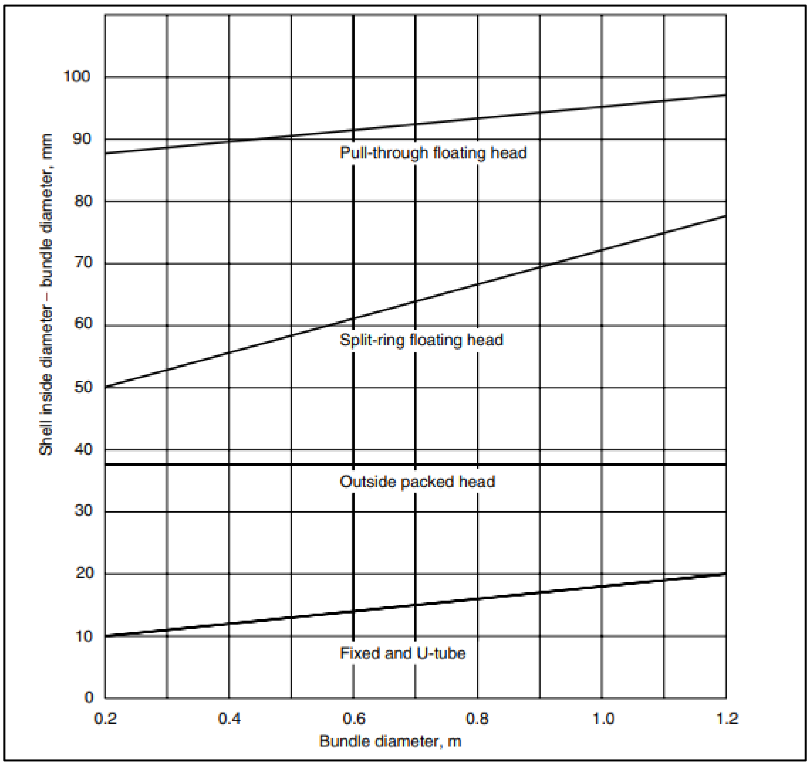


Figure 6.9 Shell bundle clearance.

Pull Through Floating Head Shell Inside Dia – Bundle Dia = 93 mm

Shell Inside Diameter = 859 mm = 0.859 m

Baffle Spacing = $D_s/2.5$

= 859/2.5

Baffle Spacing = 344 mm

Cross Flow Area = $A_s = \frac{(pt-do)*Ds*Lb}{pt}$

$$As = \frac{(63-50)*859*(0.000344)}{63}$$

Cross Flow Area = As = 0.061 m^2

Mass Velocity = G_s = (8626) / (3600 * 0.061)

Mass Velocity = G_s = 39 kg/m^{2}s

Equivalent Dia = de = (1.10 / do) * (pt^2 – 0.917 do^2)

de = (1.10/50) * (63^2 – 0.917(50)^2)

Equivalent Dia = de = 36.9 mm = 0.0369 m

Using specification of Air

Baffle Cut = 25%

Re = (Mass velocity * de) / viscosity

Re = (30 * 0.0369) / (18.97 x 10^{-6})

Re = 58,355

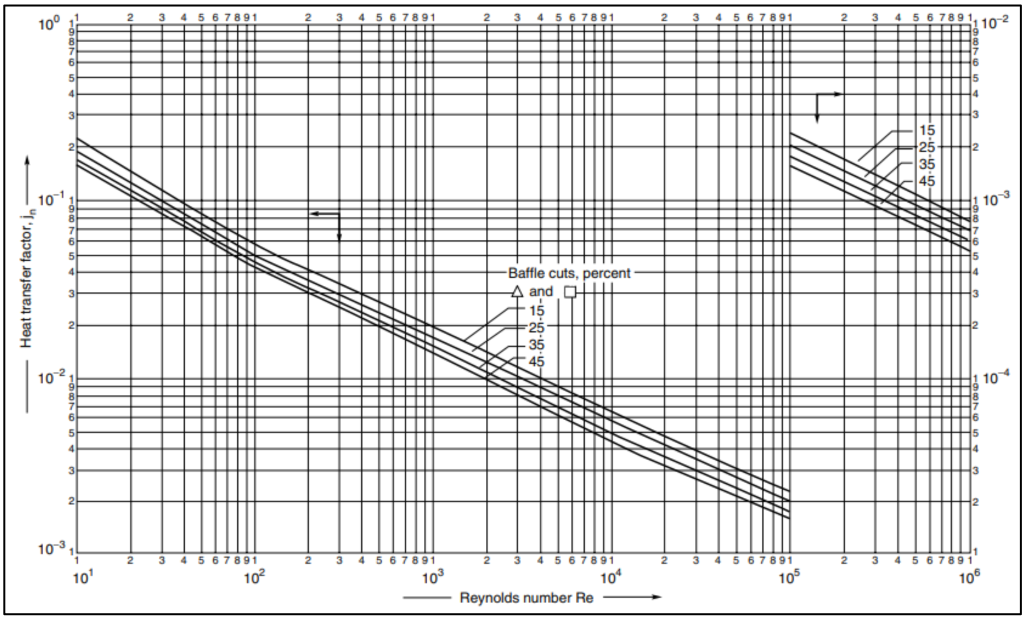


Figure 6.10 Shell side heat transfer coefficient

From the graph,

$$\mathbf{J_h = 2.5 \times 10^{-2}}$$

Pr = (heat capacity * viscosity) / (thermal conductivity)
Pr = {(1.008 * 1000) * (18.97 x 10^{-6})} / (0.028)

$$\mathbf{Pr = 0.68}$$

hs = (0.028 / 0.0369) * (2.5 x 10^{-2}) * (58355) * $(0.08)^{0.33}$

$$\mathbf{hs = 975\ W/m^{2\,o}C}$$

- **Overall heat transfer coefficient**

Fouling factor = 7500
Dirt coefficient = 5000

$$\frac{1}{\text{Uo}} = \frac{1}{\text{hs}} + \frac{1}{\text{fouling factor}} + \frac{(0.005)ln\frac{50}{48}}{2*45} + \frac{50}{48}\ \frac{1}{\text{inside dirt coefficient}} + \frac{50*1}{48*\text{hi}}$$

$$\mathbf{Uo = 585\ W/m^{2\,o}C}$$

*Which is above the assumed value of **440***

- **Tube Side Pressure Drop**

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

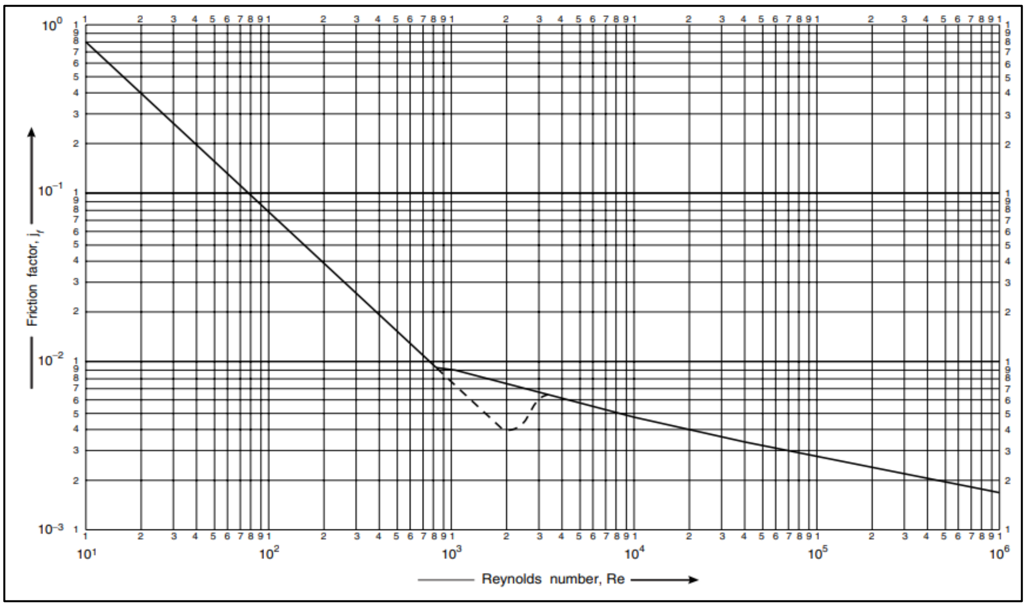


Figure 6.11 Tube side friction factor

ΔP = 24,182 N/m2 = 24.182 kPa = 3.48 psi = 0.24 bar

- **Shell Side Pressure Drop**

Linear Velocity = Gs / density = **30 m/s**
Number of Baffles = 5

l/lb = Number of Baffles + 1

l/lb = 6

Now, the pressure drop is given by:

$$\Delta P_s = 8 j_f \left(\frac{D_s}{d_e}\right)\left(\frac{L}{l_B}\right)\frac{\rho u_s^2}{2}\left(\frac{\mu}{\mu_w}\right)^{-0.14}$$

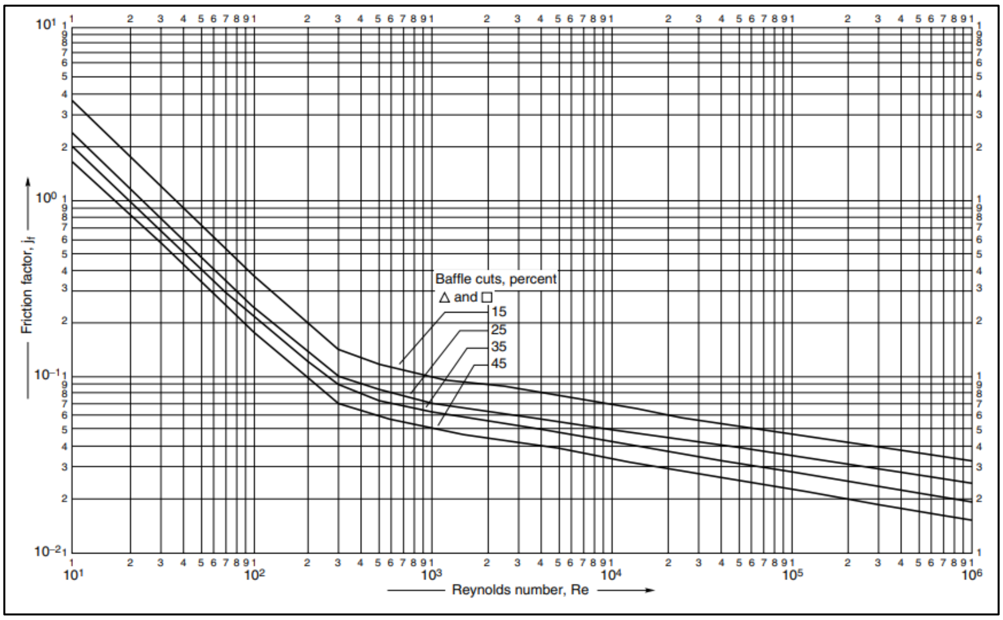


Figure 6.12 Shell side friction factor

ΔP = 29,257 N/m2 = 29.3 kPa = 4.3 psi = 0.30 bar

6.4.4 Results

Table 6.13 Results for Heat Exchanger design

Property	Unit	Value
HEAT DUTY	kJ/hr	2,473,055
LMTD	^0C	34.4
Area	m^2	45.3
U^o	$W/m^{2o}C$	585
Tubes		
Number		30
Length	m	9.85
Outer diameter	m	0.05
Pitch	m	0.0625
Passes		8
Jh		3.9×10^{-2}
h_i	$W/m^{2o}C$	3261
Pressure drop	psi	3.48
Shell		
Inner diameter	m	0.859
Baffle Spacing	m	0.344
Passes	-	2
Jh	-	2.5×10^{-2}
h_s	$W/m^{2o}C$	975
Pressure drop	psi	4.3

CHAPTER 7

SIMULATION

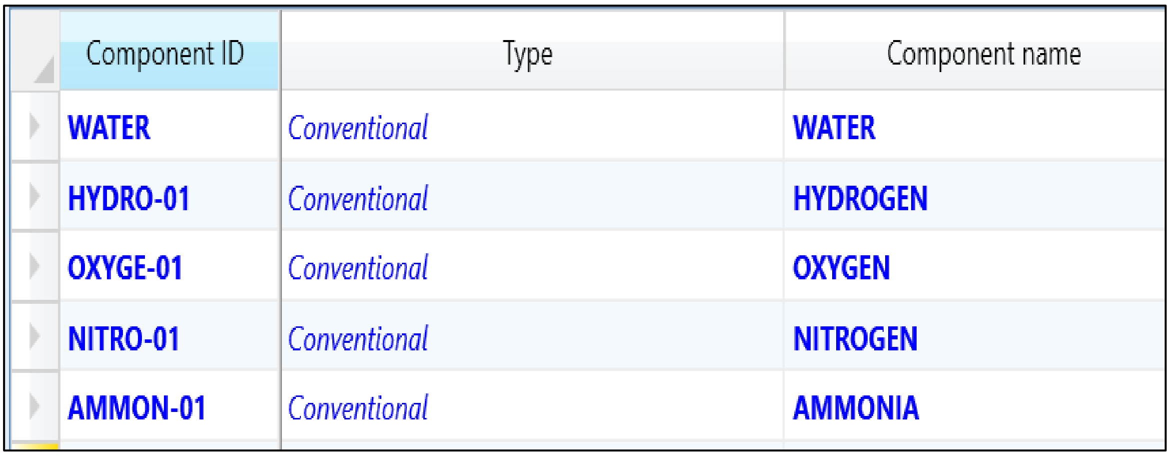
7.1 Simulation tool

Aspen Plus has been used for simulation of this this project.

Aspen Plus is a powerful process simulation software widely used in the chemical engineering field for designing, optimizing, and analyzing chemical processes. Developed by Aspen Technology, this software provides a comprehensive environment for modeling a wide range of chemical processes, from simple unit operations to complex, integrated systems. Aspen Plus enables engineers to simulate the behavior of chemical processes using detailed thermodynamic and kinetic data, facilitating the accurate prediction of process performance. Its robust capabilities in process simulation, combined with a user-friendly interface, make it an essential tool for both academic research and industrial applications.

7.2 Components

The raw material for this process includes air (O2 and N2) and water and the major products are H2, N2 and Ammonia. List of components used for simulation are given below:



Component ID	Type	Component name
WATER	Conventional	WATER
HYDRO-01	Conventional	HYDROGEN
OXYGE-01	Conventional	OXYGEN
NITRO-01	Conventional	NITROGEN
AMMON-01	Conventional	AMMONIA

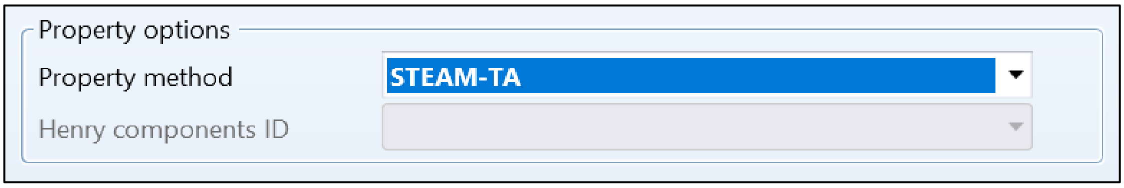
Figure 7.1 List of components

7.3 Fluid Package

Two property packages are used for this simulation:

7.3.1 STEAM-TA

This is used only for water system (water electrolysis).



Property options

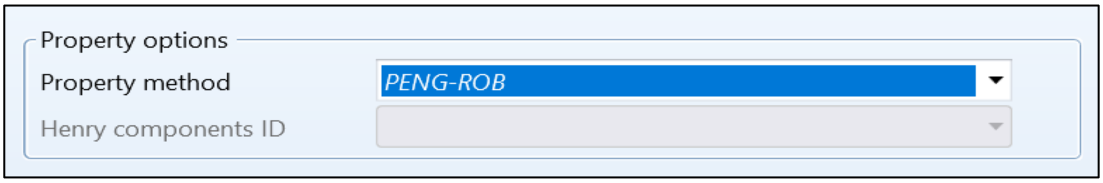
Property method: STEAM-TA

Henry components ID:

Figure 7.2 Fluid Package- 1

7.3.2 PENG-ROB

This property package is used for the rest of the system.



Property options

Property method: PENG-ROB

Henry components ID:

Figure 7.3 Fluid Package-2

7.4 Overall Process Flow Sheet

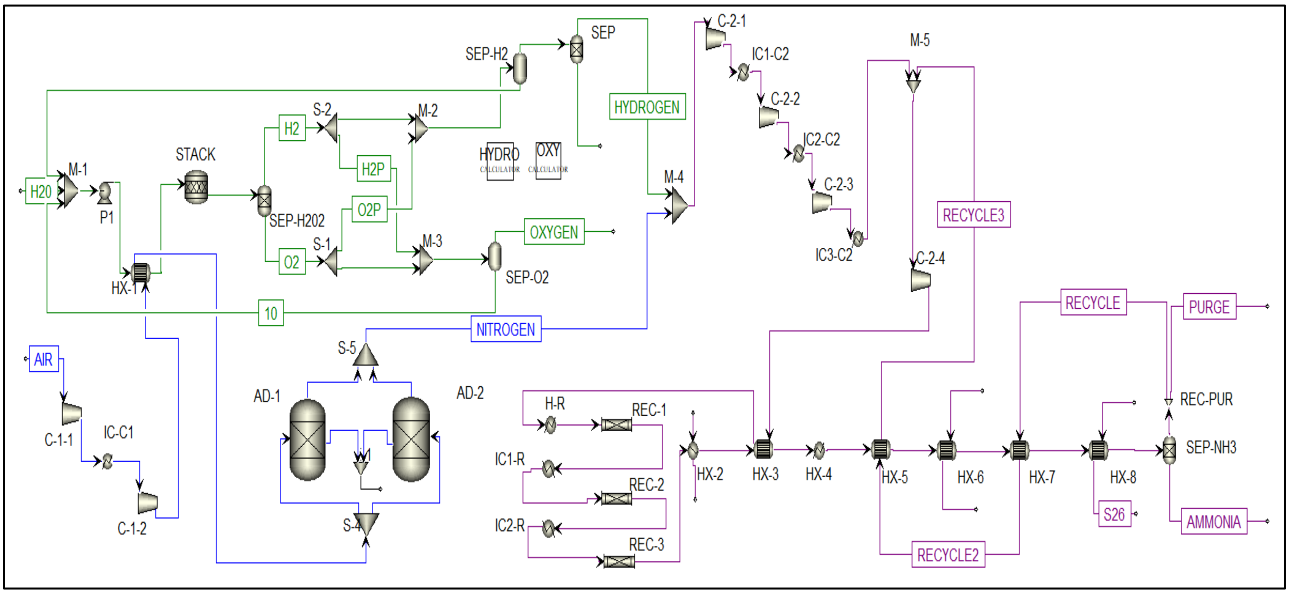


Figure 7.4 Overall Process flow diagram

7.5 Hydrogen Production Unit

7.5.1 Process Flow Sheet

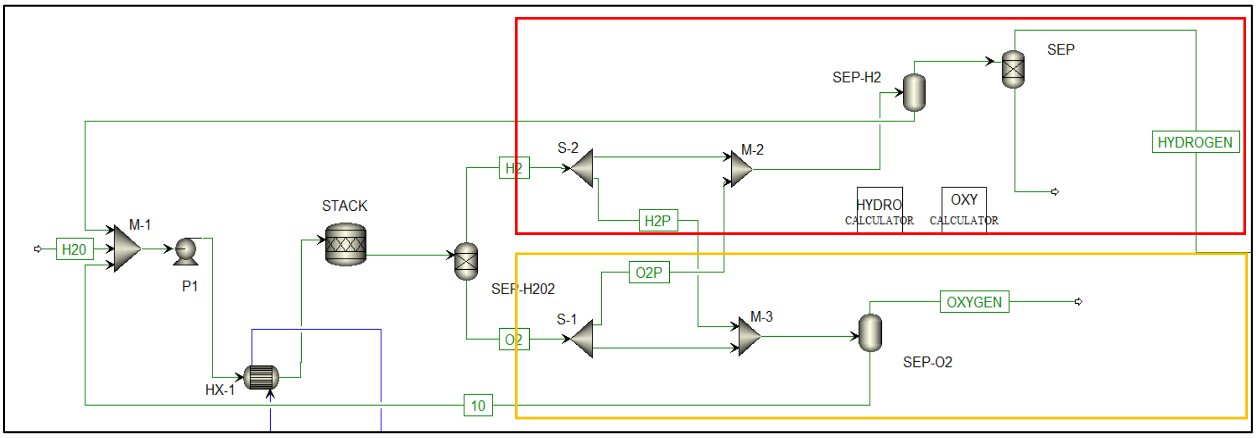
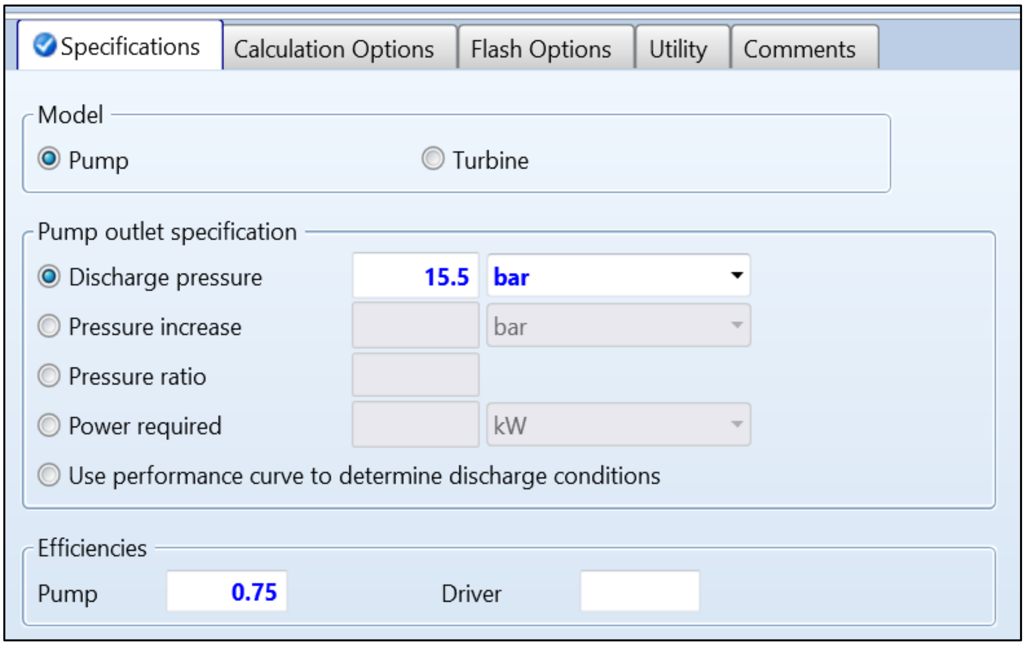


Figure 7.5 Process Flow Diagram for Water Electrolysis

7.5.2 Pump P-1

Pump intakes water at room temperature and discharges it at a pressure of about 15 bar



Model

● Pump ○ Turbine

Pump outlet specification

● Discharge pressure 15.5 bar

○ Pressure increase bar

○ Pressure ratio

○ Power required kW

○ Use performance curve to determine discharge conditions

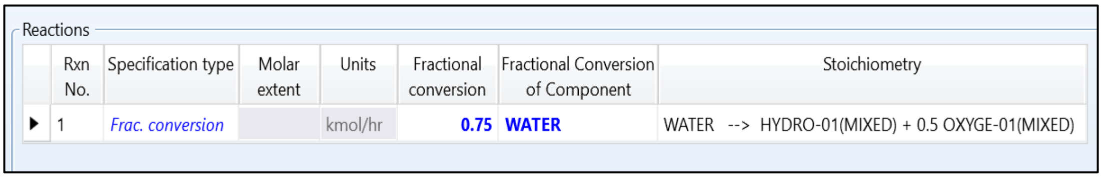
Efficiencies

Pump 0.75 Driver

Figure 7.6 Specifications for P-1

7.5.3 Stack

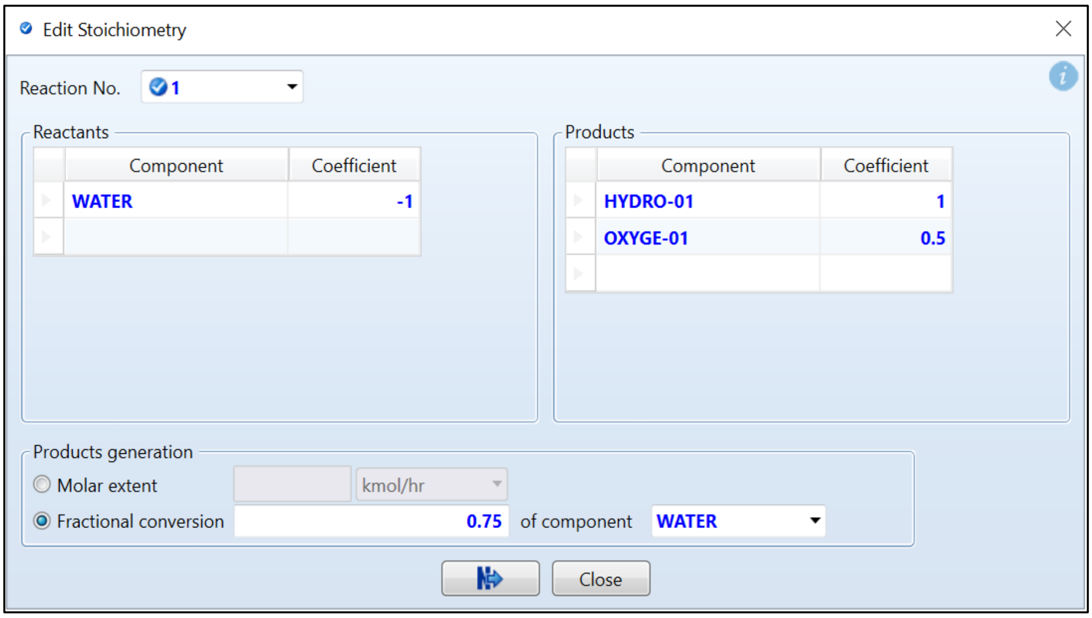
This is a conversion reactor that splits water into hydrogen and oxygen (water electrolysis). Some of the major specifications and the reaction used in the reactor are shown below.



Reactions

Rxn No.	Specification type	Molar extent	Units	Fractional conversion	Fractional Conversion of Component	Stoichiometry
1	Frac. conversion		kmol/hr	0.75	WATER	WATER --> HYDRO-01(MIXED) + 0.5 OXYGE-01(MIXED)

Figure 7.7 Reaction for Stack



Edit Stoichiometry

Reaction No. 1

Reactants

Component	Coefficient
WATER	-1

Products

Component	Coefficient
HYDRO-01	1
OXYGE-01	0.5

Products generation

○ Molar extent kmol/hr

● Fractional conversion 0.75 of component WATER

Figure 7.8 Reaction stoichiometry for Stack

7.5.4 Membrane

A combination of splits is used to demonstrate the membrane present between anode and cathode. Two calculator blocks are used to calculate the permeation of hydrogen from cathode section to anode and permeation of oxygen from anode section to cathode section. (Zaccara et al., 2020)

Hydrogen permeation calculator block uses the following equation.

$$H_2{}^{perm} = (0.0009.e^{0.025T}).\Delta P.A$$

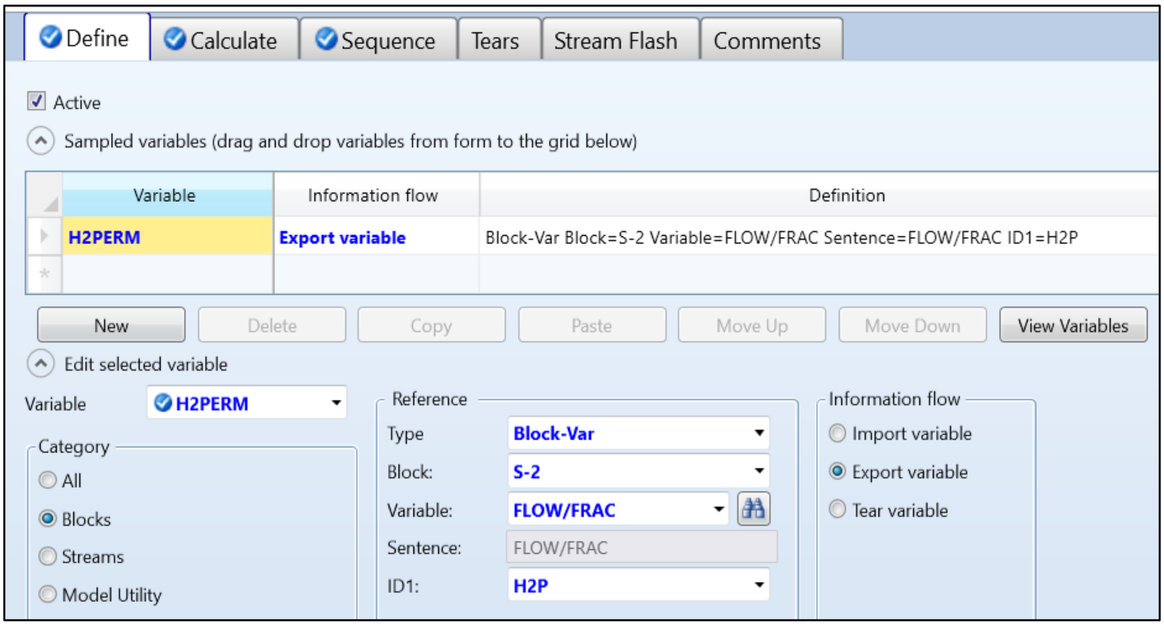
Where,

T = Temperature

ΔP = Pressure difference between cathode and anode

A = active area

Specification used in the hydrogen calculator block are shown below



☑ Active

Sampled variables (drag and drop variables from form to the grid below)

Variable	Information flow	Definition
H2PERM	**Export variable**	Block-Var Block=S-2 Variable=FLOW/FRAC Sentence=FLOW/FRAC ID1=H2P

Edit selected variable

Variable: **H2PERM**

Category

○ All
● Blocks
○ Streams
○ Model Utility

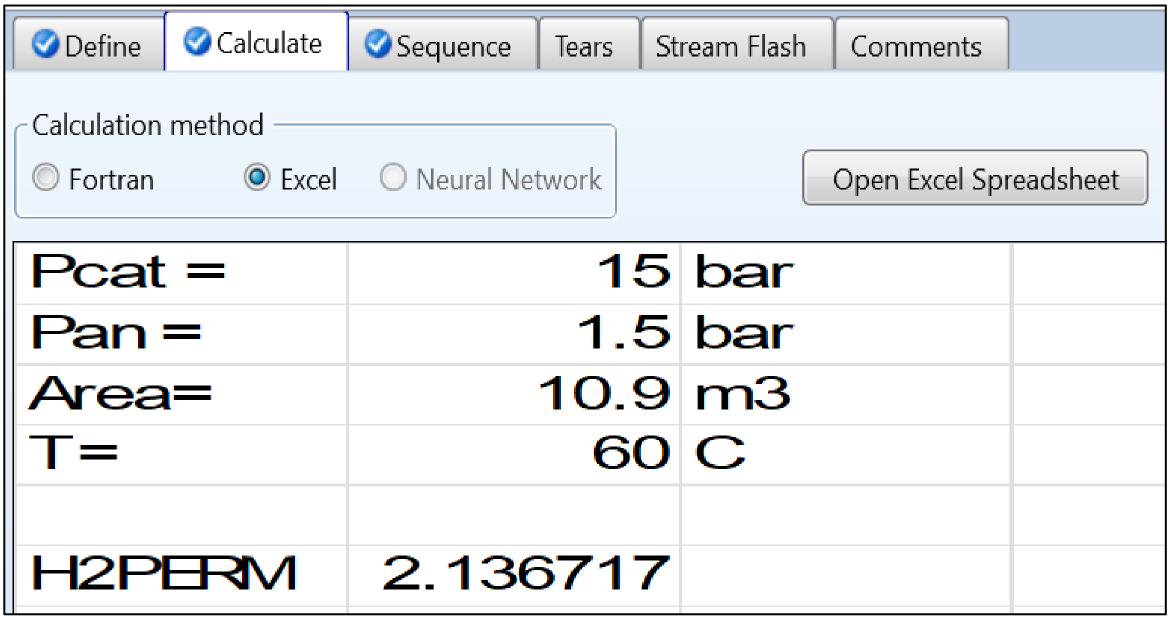
Reference

Type: **Block-Var**
Block: **S-2**
Variable: **FLOW/FRAC**
Sentence: FLOW/FRAC
ID1: **H2P**

Information flow

○ Import variable
● Export variable
○ Tear variable

Figure 7.9 Hydro calculator block specification



Calculation method

○ Fortran ● Excel ○ Neural Network

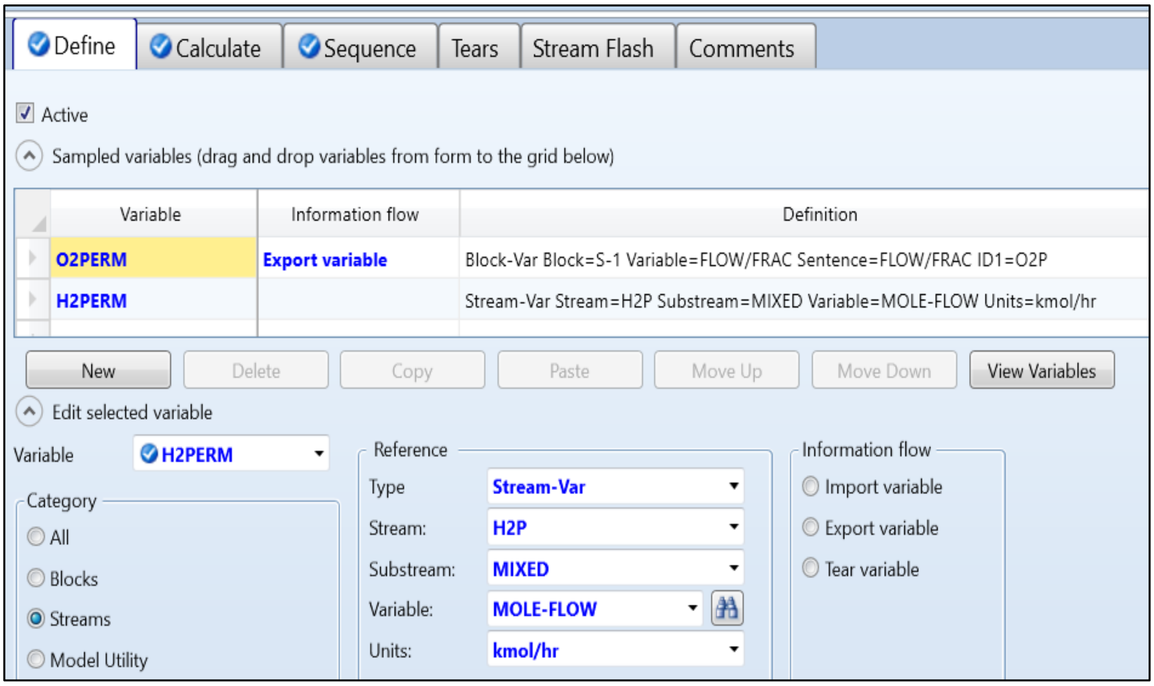
Pcat =	15	bar
Pan =	1.5	bar
Area=	10.9	m3
T=	60	C
H2PERM	2.136717	

Figure 7.10 Hydro calculator block equation

For permeation of oxygen following relation is used

$$O_2^{perm} = 0.5H_2^{perm}$$

Specification used in the hydrogen calculator block are shown below



☑ Active

Sampled variables (drag and drop variables from form to the grid below)

Variable	Information flow	Definition
O2PERM	**Export variable**	Block-Var Block=S-1 Variable=FLOW/FRAC Sentence=FLOW/FRAC ID1=O2P
H2PERM		Stream-Var Stream=H2P Substream=MIXED Variable=MOLE-FLOW Units=kmol/hr

Edit selected variable

Variable: **H2PERM**

Category

○ All
○ Blocks
● Streams
○ Model Utility

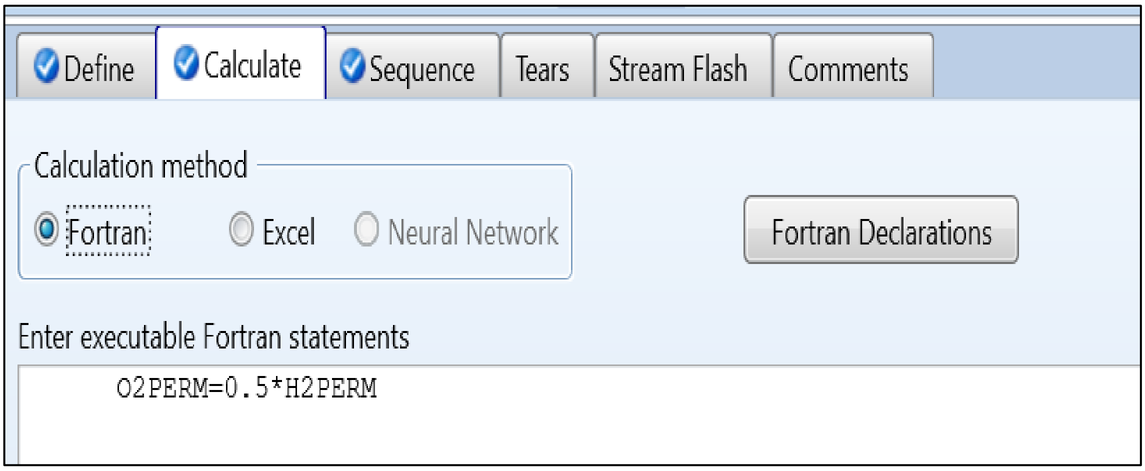
Reference

Type: **Stream-Var**
Stream: **H2P**
Substream: **MIXED**
Variable: **MOLE-FLOW**
Units: **kmol/hr**

Information flow

○ Import variable
○ Export variable
○ Tear variable

Figure 7.11 Oxy Calculator block Specification



Calculation method

● Fortran ○ Excel ○ Neural Network

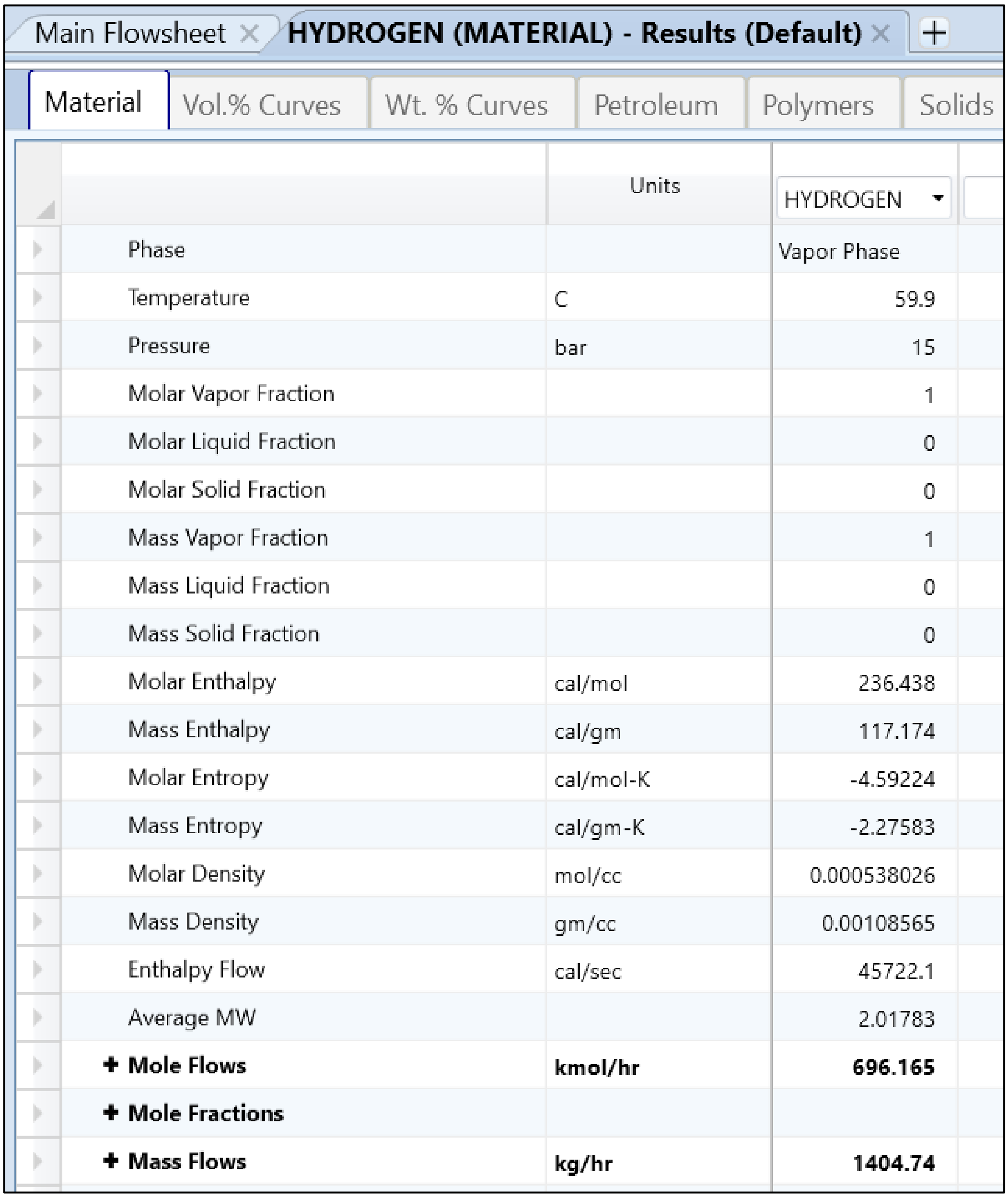
Enter executable Fortran statements

```
      O2PERM=0.5*H2PERM
```

Figure 7.12 Oxy calculator block equation

7.5.5 Product stream

The amount of hydrogen produced by this simulation is equivalent to the one calculated in material balance. The results are shown below.



	Units	HYDROGEN
Phase		Vapor Phase
Temperature	C	59.9
Pressure	bar	15
Molar Vapor Fraction		1
Molar Liquid Fraction		0
Molar Solid Fraction		0
Mass Vapor Fraction		1
Mass Liquid Fraction		0
Mass Solid Fraction		0
Molar Enthalpy	cal/mol	236.438
Mass Enthalpy	cal/gm	117.174
Molar Entropy	cal/mol-K	-4.59224
Mass Entropy	cal/gm-K	-2.27583
Molar Density	mol/cc	0.000538026
Mass Density	gm/cc	0.00108565
Enthalpy Flow	cal/sec	45722.1
Average MW		2.01783
+ Mole Flows	**kmol/hr**	**696.165**
+ Mole Fractions		
+ Mass Flows	**kg/hr**	**1404.74**

Figure 7.13 Stream results for Hydrogen

7.6 Nitrogen Separation Unit

7.6.1 Process Flow Sheet

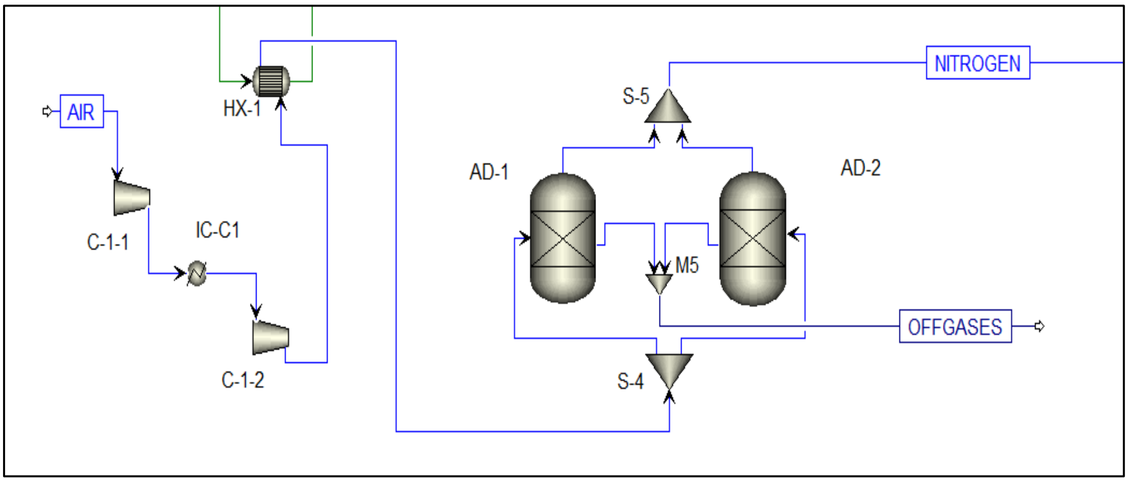
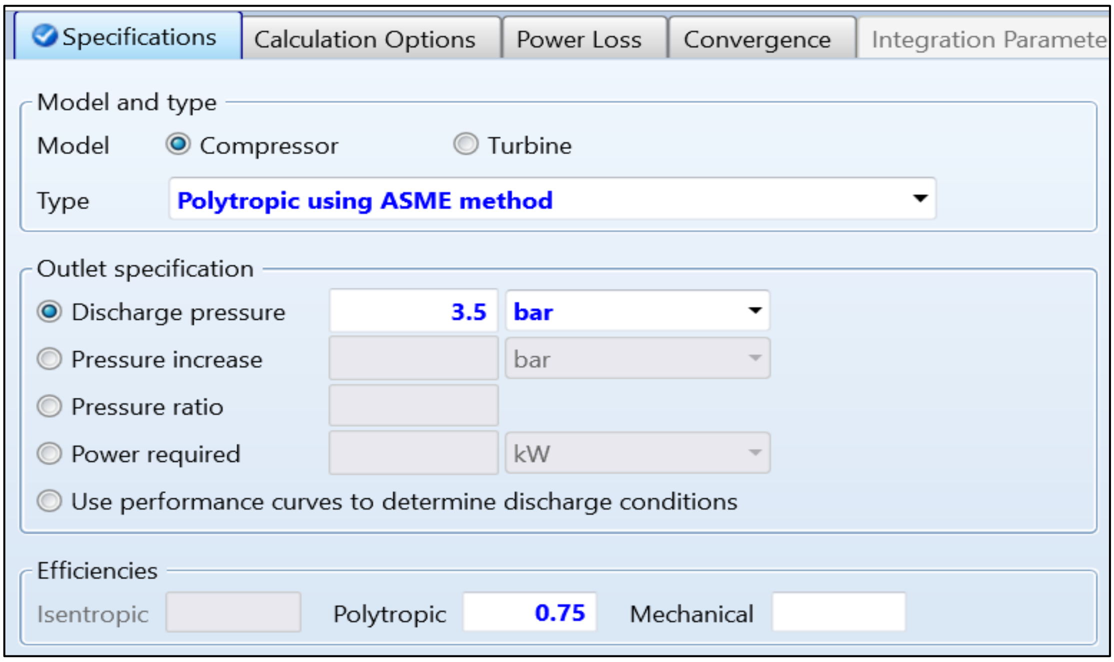


Figure 7.14 Process Flow Sheet for PSA

7.6.2 Air Compressor

This is 2 stage compressor (C-1-1 and C-1-2) with an inter cooler to compress the incoming air up to 12 bar.

Specification used for compressor simulation are shown below



Model and type

Model ● Compressor ○ Turbine

Type Polytropic using ASME method

Outlet specification

● Discharge pressure 3.5 bar

○ Pressure increase bar

○ Pressure ratio

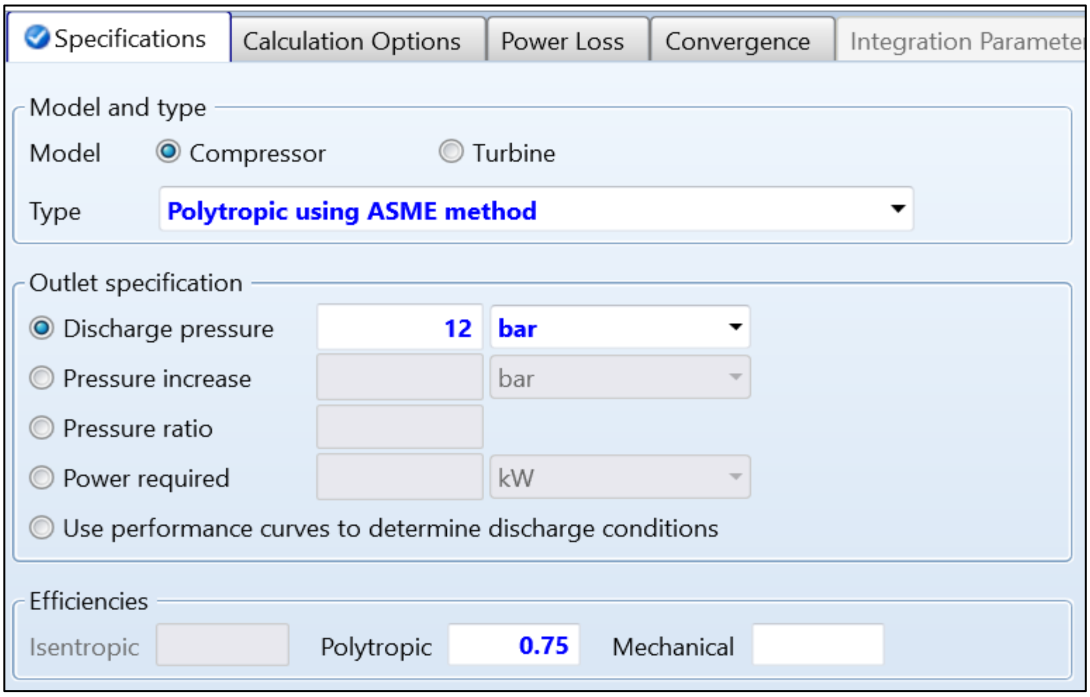
○ Power required kW

○ Use performance curves to determine discharge conditions

Efficiencies

Isentropic Polytropic 0.75 Mechanical

Figure 7.15 Specification for C-1-1



Model and type

Model ● Compressor ○ Turbine

Type: Polytropic using ASME method

Outlet specification

● Discharge pressure 12 bar

○ Pressure increase bar

○ Pressure ratio

○ Power required kW

○ Use performance curves to determine discharge conditions

Efficiencies

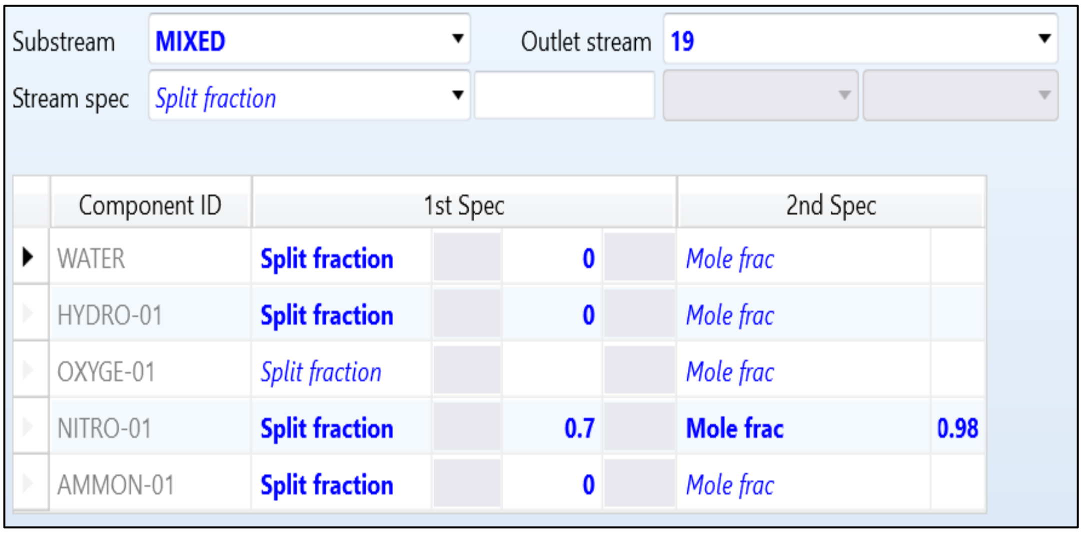
Isentropic | Polytropic 0.75 | Mechanical

Figure 7.16 Specification for C-1-2

7.6.3 Adsorption column (AD-1 and AD-2)

Combination of mixer, tee and separators are used to demonstrate the adsorption column with the nitrogen purity of about 98% and recovery of 70 %. (Sutradhar et al., 2019)

The separations used in the separator are shown below.



Substream: MIXED

Outlet stream: 19

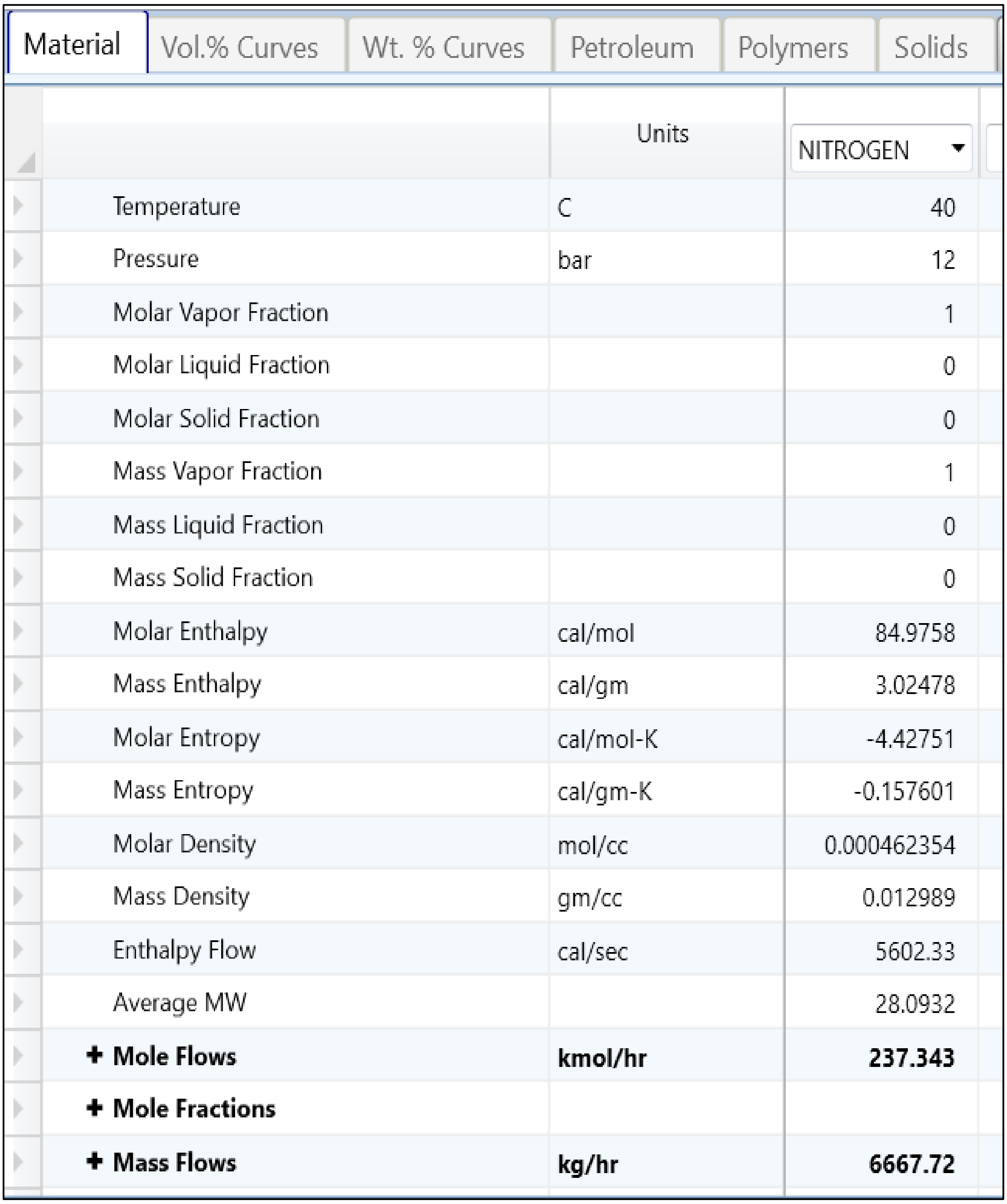
Stream spec: Split fraction

Component ID	1st Spec				2nd Spec	
WATER	Split fraction		0		Mole frac	
HYDRO-01	Split fraction		0		Mole frac	
OXYGE-01	Split fraction				Mole frac	
NITRO-01	Split fraction		0.7		Mole frac	0.98
AMMON-01	Split fraction		0		Mole frac	

Figure 7.17 Specification for Separator AD-1

7.6.4 Product stream (Nitrogen)

The amount of nitrogen produced in this simulation is equivalent to the one calculated in material balance. The results for the stream are given below.



	Units	NITROGEN
Temperature	C	40
Pressure	bar	12
Molar Vapor Fraction		1
Molar Liquid Fraction		0
Molar Solid Fraction		0
Mass Vapor Fraction		1
Mass Liquid Fraction		0
Mass Solid Fraction		0
Molar Enthalpy	cal/mol	84.9758
Mass Enthalpy	cal/gm	3.02478
Molar Entropy	cal/mol-K	-4.42751
Mass Entropy	cal/gm-K	-0.157601
Molar Density	mol/cc	0.000462354
Mass Density	gm/cc	0.012989
Enthalpy Flow	cal/sec	5602.33
Average MW		28.0932
+ Mole Flows	**kmol/hr**	**237.343**
+ Mole Fractions		
+ Mass Flows	**kg/hr**	**6667.72**

Figure 7.18 Stream results for Nitrogen

7.7 Ammonia Synthesis

7.7.1 Process Flow Diagram

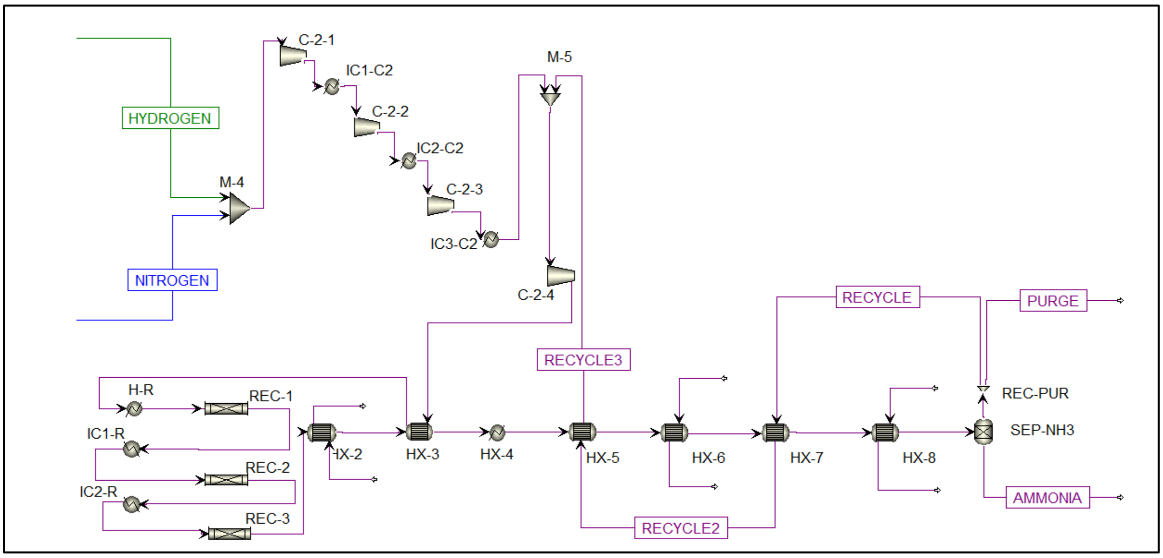
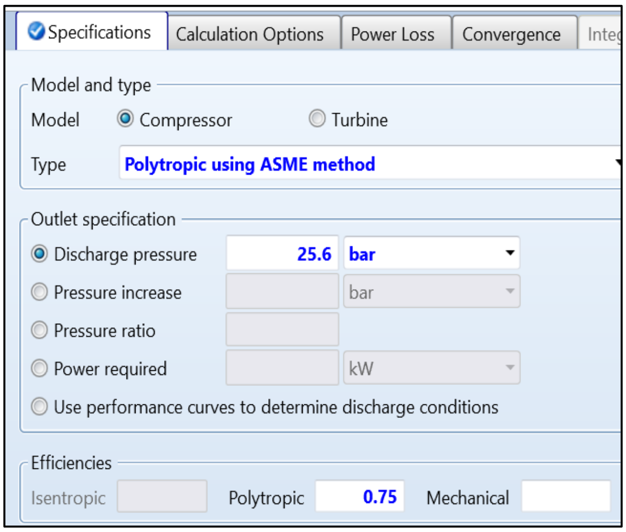


Figure 7.19 Process Flow Sheet- Ammonia Synthesis

7.7.2 Reactor Feed Compressor

This is 4 stage compressor (C-2-1 to C-2-4) with inter coolers to compress the incoming air up to 142 bar.

The specification used for each stage of compressor are shown below.



Model and type

Model ● Compressor ○ Turbine

Type Polytropic using ASME method

Outlet specification

● Discharge pressure 25.6 bar

○ Pressure increase bar

○ Pressure ratio

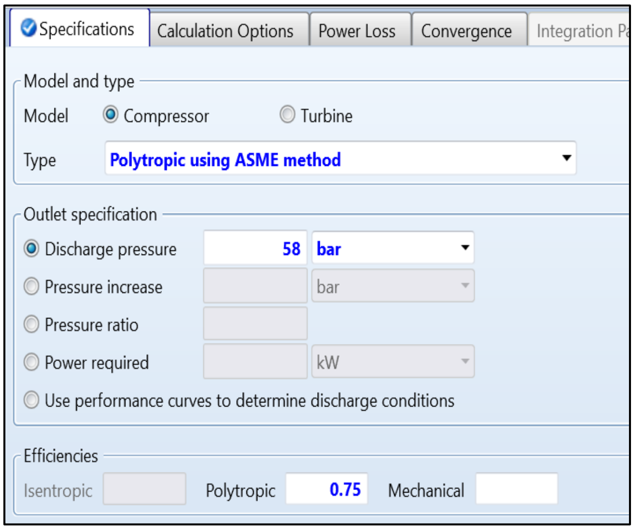
○ Power required kW

○ Use performance curves to determine discharge conditions

Efficiencies

Isentropic Polytropic 0.75 Mechanical

Figure 7.20 Specifications for C-2-1



Model and type

Model ● Compressor ○ Turbine

Type **Polytropic using ASME method**

Outlet specification

● Discharge pressure **58** **bar**

○ Pressure increase bar

○ Pressure ratio

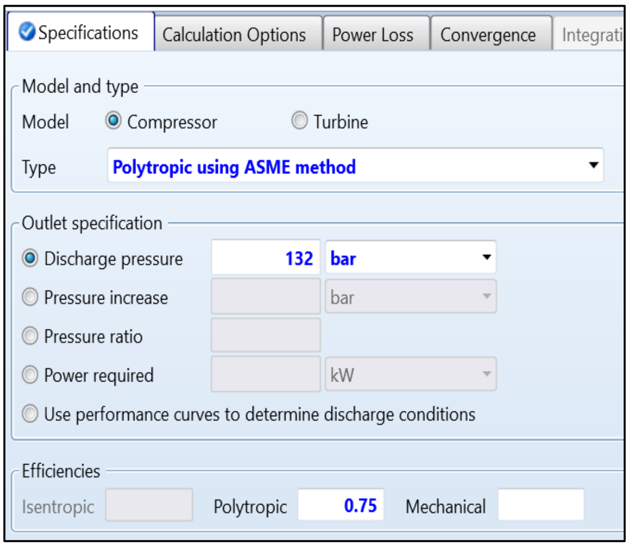
○ Power required kW

○ Use performance curves to determine discharge conditions

Efficiencies

Isentropic Polytropic **0.75** Mechanical

Figure 7.21 Specifications for C-2-2



Model and type

Model ● Compressor ○ Turbine

Type **Polytropic using ASME method**

Outlet specification

● Discharge pressure **132** **bar**

○ Pressure increase bar

○ Pressure ratio

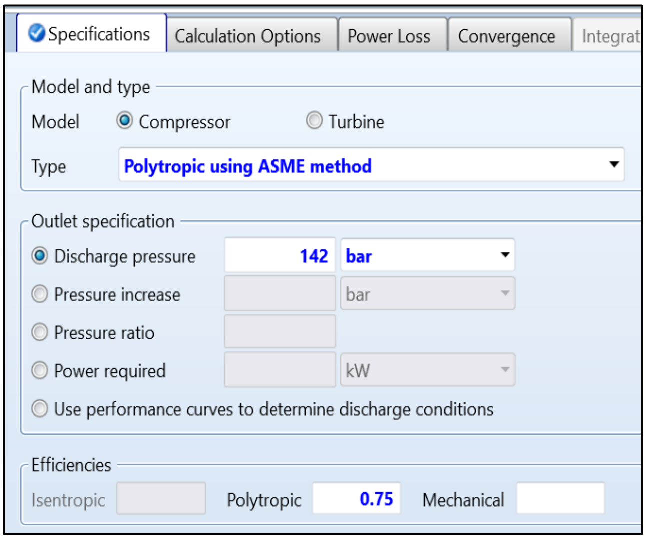
○ Power required kW

○ Use performance curves to determine discharge conditions

Efficiencies

Isentropic Polytropic **0.75** Mechanical

Figure 7.22 Specifications for C-2-3



Model and type

Model ● Compressor ○ Turbine

Type **Polytropic using ASME method**

Outlet specification

● Discharge pressure **142** **bar**

○ Pressure increase bar

○ Pressure ratio

○ Power required kW

○ Use performance curves to determine discharge conditions

Efficiencies

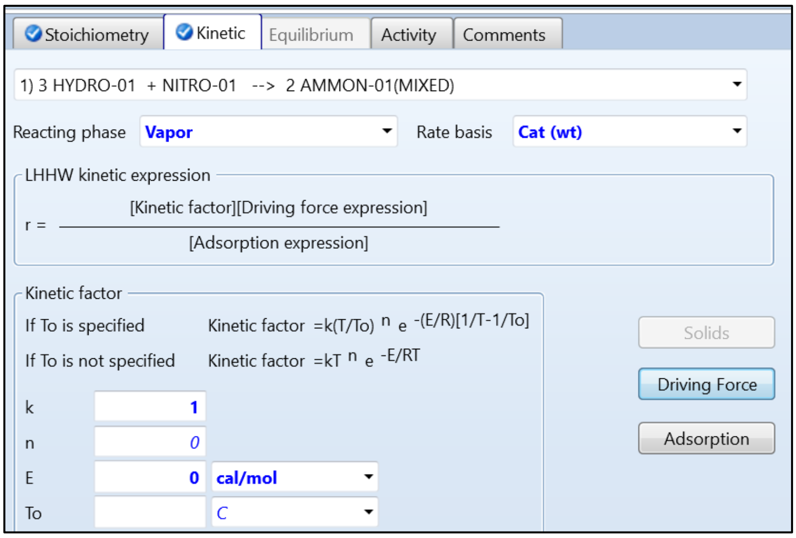
Isentropic Polytropic **0.75** Mechanical

Figure 7.23 Specifications for C-2-4

7.7.3 Ammonia Reactor

Three plug flow reactors are used to demonstrate the three beds of ammonia reactor. The same kinetics and reaction set is used for each reactor. Inter coolers are placed between each bed to maintain the temperature.

Reaction kinetics for one of the reactors is shown below:



1) 3 HYDRO-01 + NITRO-01 --> 2 AMMON-01(MIXED)

Reacting phase: Vapor

Rate basis: Cat (wt)

LHHW kinetic expression

r = [Kinetic factor][Driving force expression] / [Adsorption expression]

Kinetic factor

If To is specified: Kinetic factor $=k(T/To)^{n} e^{-(E/R)[1/T-1/To]}$

If To is not specified: Kinetic factor $=kT^{n} e^{-E/RT}$

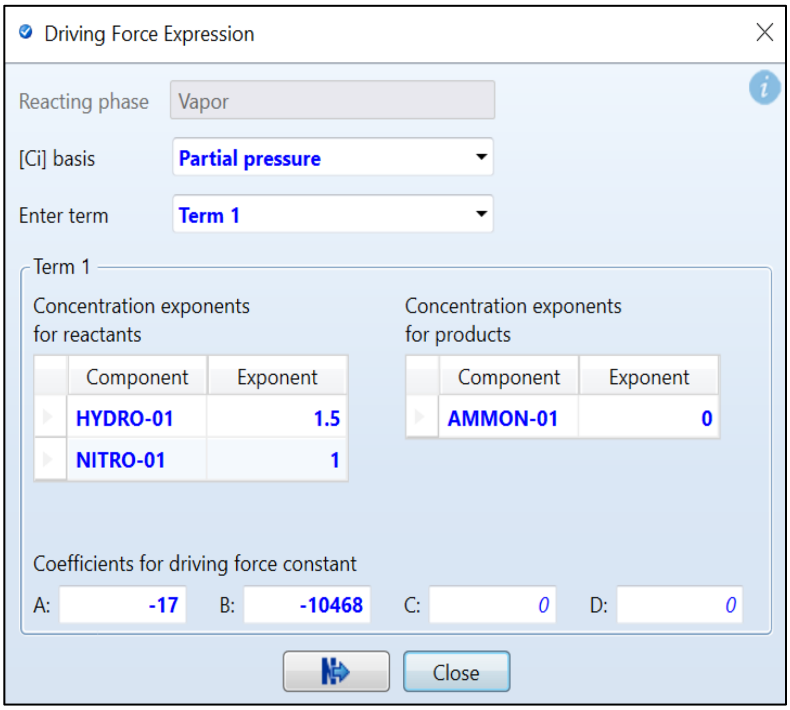
k: 1

n: 0

E: 0 cal/mol

To: C

Figure 7.24 Reaction kinetics



Reacting phase: Vapor

[Ci] basis: Partial pressure

Enter term: Term 1

Term 1

Concentration exponents for reactants

Component	Exponent
HYDRO-01	1.5
NITRO-01	1

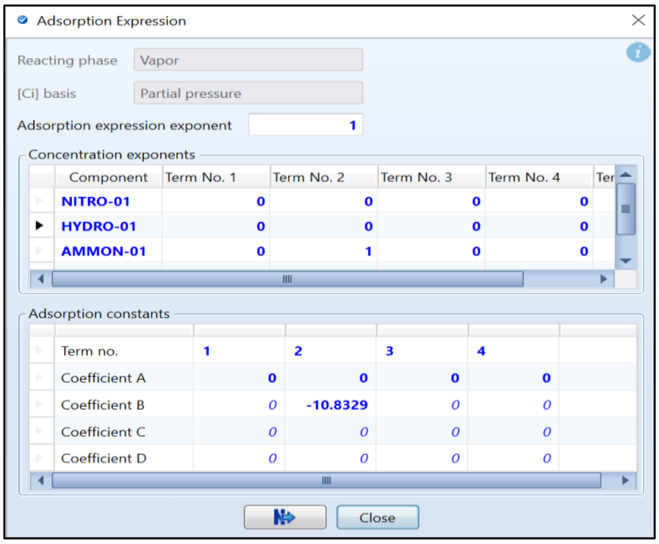
Concentration exponents for products

Component	Exponent
AMMON-01	0

Coefficients for driving force constant

A: -17 B: -10468 C: 0 D: 0

Figure 7.25 Driving Force for reaction kinetics



Reacting phase: Vapor

[Ci] basis: Partial pressure

Adsorption expression exponent: 1

Concentration exponents

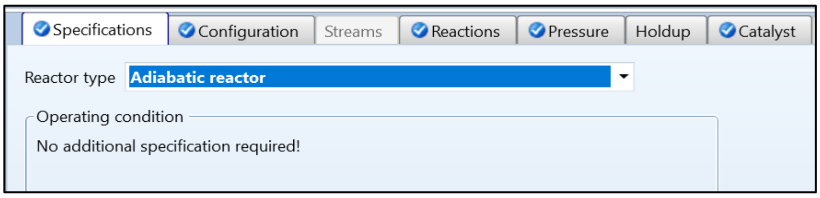
Component	Term No. 1	Term No. 2	Term No. 3	Term No. 4
NITRO-01	0	0	0	0
HYDRO-01	0	0	0	0
AMMON-01	0	1	0	0

Adsorption constants

Term no.	1	2	3	4
Coefficient A	0	0	0	0
Coefficient B	0	-10.8329	0	0
Coefficient C	0	0	0	0
Coefficient D	0	0	0	0

Figure 7.26 Adsorption term for reaction kinetics

Specification used in each bed is according to the reactor design. Specifications of the 1st reactor are shown below.

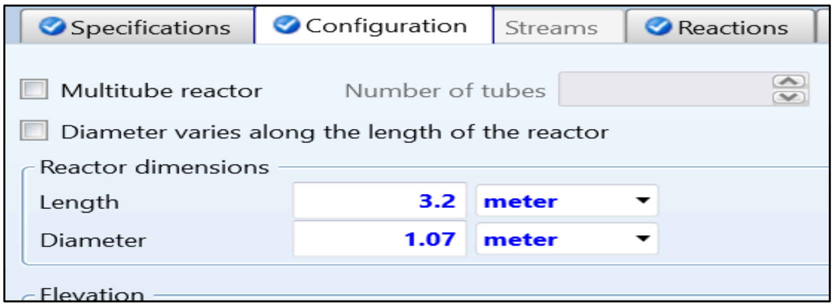


Reactor type: Adiabatic reactor

Operating condition

No additional specification required!

Figure 7.27 Reactor Specifications



☐ Multitube reactor   Number of tubes

☐ Diameter varies along the length of the reactor

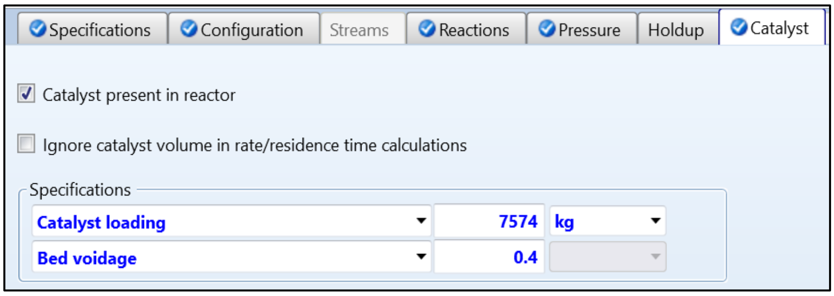
Reactor dimensions

Length: 3.2 meter

Diameter: 1.07 meter

Elevation

Figure 7.28 Reactor configuration



☑ Catalyst present in reactor

☐ Ignore catalyst volume in rate/residence time calculations

Specifications

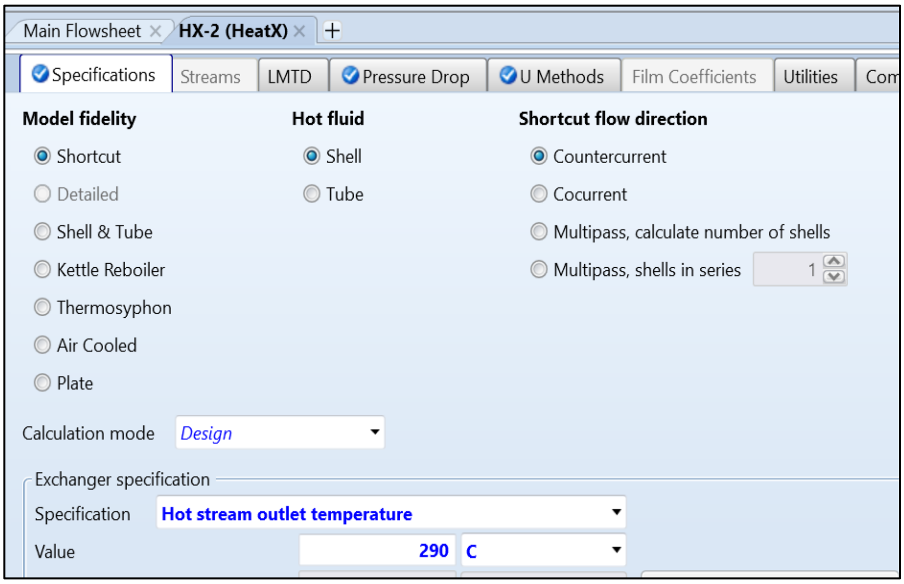
Catalyst loading: 7574 kg

Bed voidage: 0.4

Figure 7.29 Reactor catalyst data

7.7.4 Heat Exchangers

Series of heat exchangers are used to condense ammonia. Short model is used for each shell and tube exchanger with counter current flow. Details of a few of them are shown below.



Model fidelity
- ● Shortcut
- ○ Detailed
- ○ Shell & Tube
- ○ Kettle Reboiler
- ○ Thermosyphon
- ○ Air Cooled
- ○ Plate

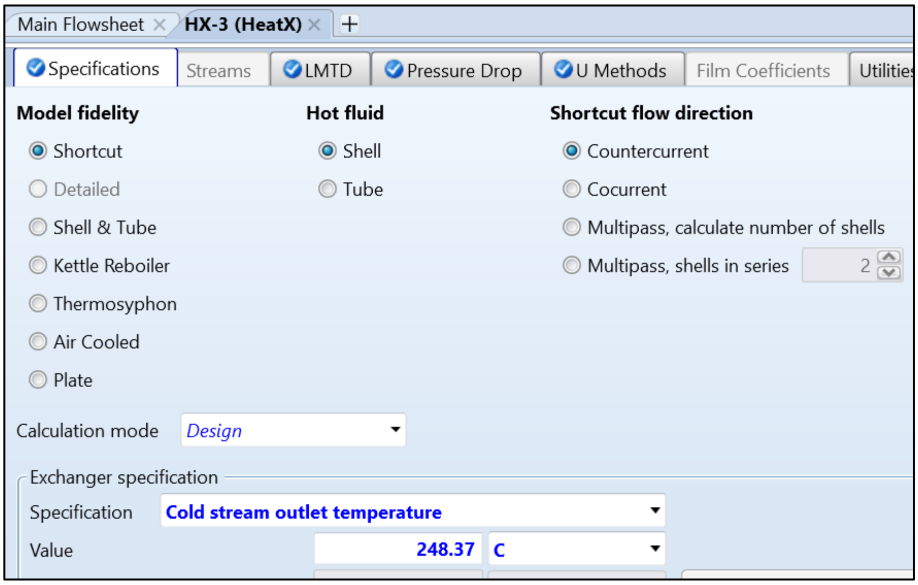
Hot fluid
- ● Shell
- ○ Tube

Shortcut flow direction
- ● Countercurrent
- ○ Cocurrent
- ○ Multipass, calculate number of shells
- ○ Multipass, shells in series 1

Calculation mode: Design

Exchanger specification
Specification: Hot stream outlet temperature
Value: 290 C

Figure 7.30 Input Specification of HX-2



Model fidelity
- ● Shortcut
- ○ Detailed
- ○ Shell & Tube
- ○ Kettle Reboiler
- ○ Thermosyphon
- ○ Air Cooled
- ○ Plate

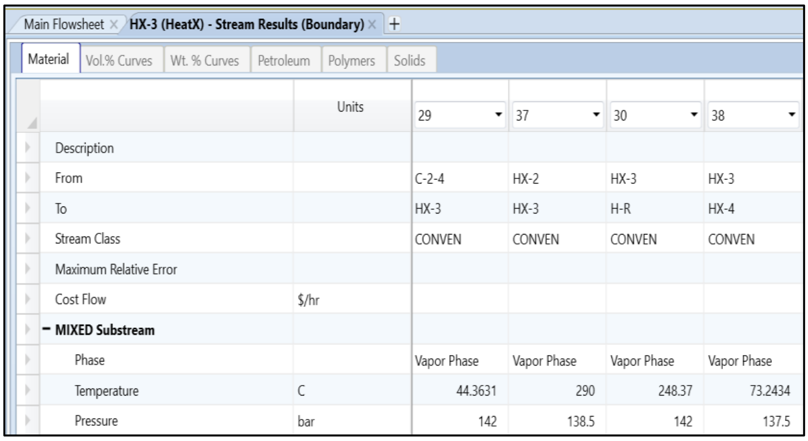
Hot fluid
- ● Shell
- ○ Tube

Shortcut flow direction
- ● Countercurrent
- ○ Cocurrent
- ○ Multipass, calculate number of shells
- ○ Multipass, shells in series 2

Calculation mode: Design

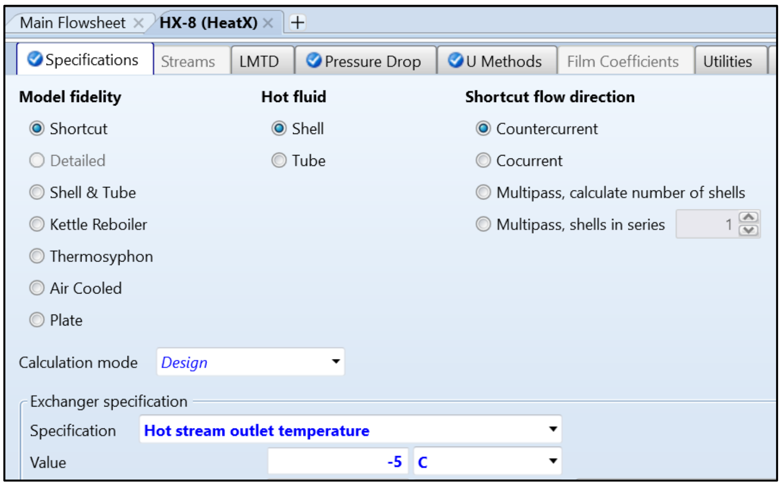
Exchanger specification
Specification: Cold stream outlet temperature
Value: 248.37 C

Figure 7.31 Input Specification of HX-3



	Units	29	37	30	38
Description					
From		C-2-4	HX-2	HX-3	HX-3
To		HX-3	HX-3	H-R	HX-4
Stream Class		CONVEN	CONVEN	CONVEN	CONVEN
Maximum Relative Error					
Cost Flow	$/hr				
MIXED Substream					
Phase		Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase
Temperature	C	44.3631	290	248.37	73.2434
Pressure	bar	142	138.5	142	137.5

Figure 7.32 Steam results for HX-3



Model fidelity

- ● Shortcut
- ○ Detailed
- ○ Shell & Tube
- ○ Kettle Reboiler
- ○ Thermosyphon
- ○ Air Cooled
- ○ Plate

Hot fluid

- ● Shell
- ○ Tube

Shortcut flow direction

- ● Countercurrent
- ○ Cocurrent
- ○ Multipass, calculate number of shells
- ○ Multipass, shells in series 1

Calculation mode: *Design*

Exchanger specification

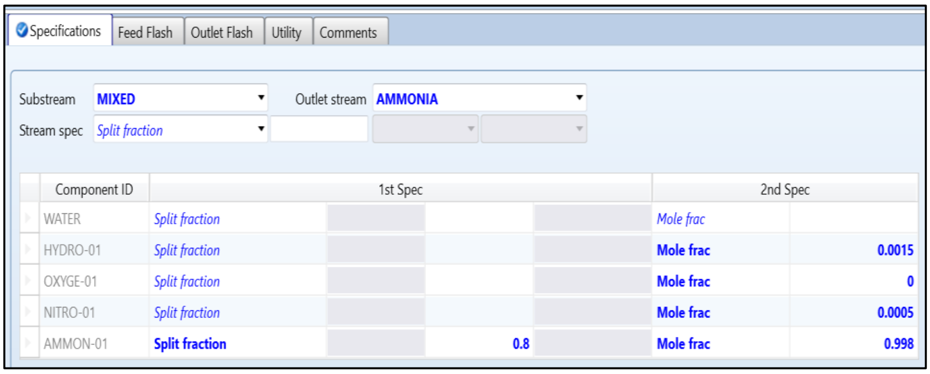
Specification: **Hot stream outlet temperature**

Value: **-5 C**

Figure 7.33 Input Specification of HX-4

7.7.5 Ammonia Separator

The is a two-phase separator that separates liquid ammonia from unreacted gases. It is simulated for 80% ammonia recovery and 99.8% purity. Specifications of ammonia separator are shown below.



Substream: **MIXED**   Outlet stream: **AMMONIA**

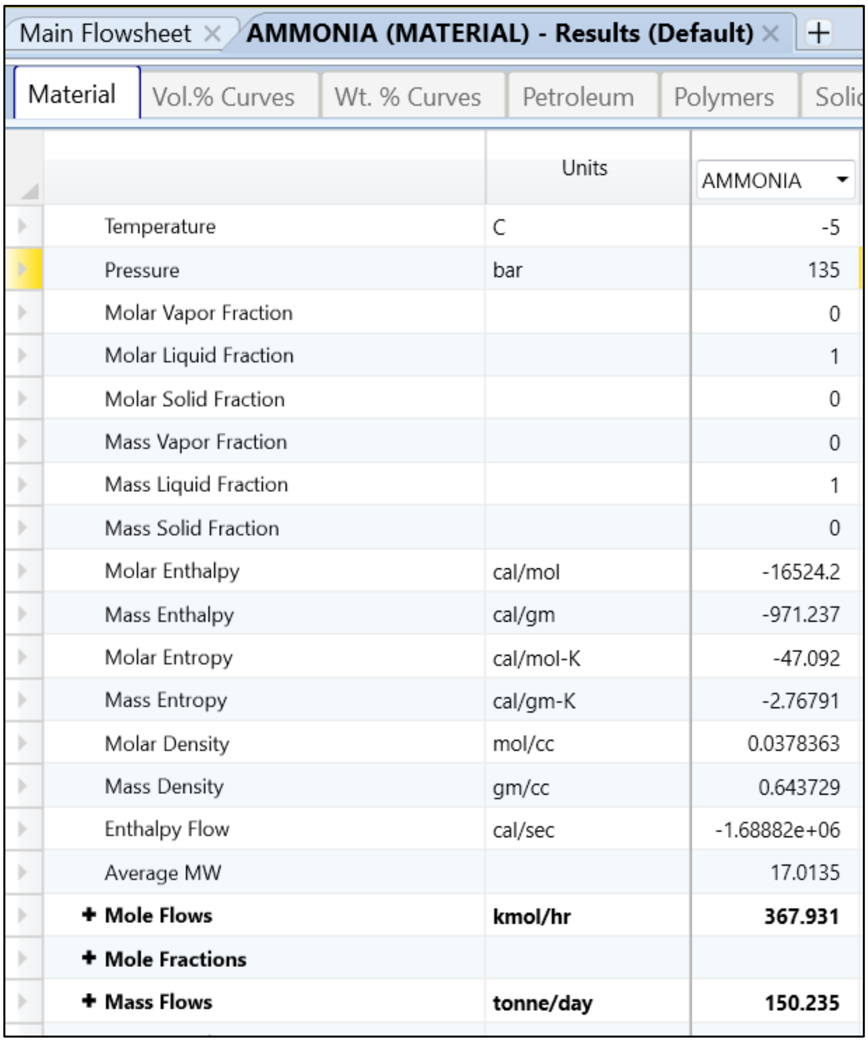
Stream spec: *Split fraction*

Component ID	1st Spec			2nd Spec	
WATER	*Split fraction*			*Mole frac*	
HYDRO-01	*Split fraction*			**Mole frac**	0.0015
OXYGE-01	*Split fraction*			**Mole frac**	0
NITRO-01	*Split fraction*			**Mole frac**	0.0005
AMMON-01	**Split fraction**		0.8	**Mole frac**	0.998

Figure 7.34 Specification of Ammonia Separator

7.7.6 Product Stream (Ammonia)

The amount of ammonia produced in this simulation is equivalent to the one calculated in material balance. The results for the stream are given below.



	Units	AMMONIA
Temperature	C	-5
Pressure	bar	135
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	-16524.2
Mass Enthalpy	cal/gm	-971.237
Molar Entropy	cal/mol-K	-47.092
Mass Entropy	cal/gm-K	-2.76791
Molar Density	mol/cc	0.0378363
Mass Density	gm/cc	0.643729
Enthalpy Flow	cal/sec	-1.68882e+06
Average MW		17.0135
+ Mole Flows	**kmol/hr**	**367.931**
+ Mole Fractions		
+ Mass Flows	**tonne/day**	**150.235**

Figure 7.35 Stream results for Ammonia

CHAPTER 8

PROCESS CONTROL AND INSTRUMENTATION

8.1 Introduction

Instrumentation and process control is an essential part of any chemical plant. It refers to the evaluation, measurement and control of different process parameters using different instruments and softwares. It helps minimize/mitigate the effect of any external disturbance, ensure the stability and safety of an operation, and optimize the performance of an industrial process.

Two major type of control loops are discussed below:

- Feed Forward control loops.
- Feed Backward control loops.

8.2 Feed Forward Control Loop

Feed forward control measures one or more input variables and takes preventive actions accordingly. In this type of control, the disturbance is eliminated before it enters the system, and the system works smoothly.

8.2.1 Ratio Control Loop

H2 and N2 are required in a specific ratio for ammonia synthesis. The ratio can be maintained by applying a simple ratio control loop. For the loop shown below the flowrate of N2 stream is measured and transmitted by the Flow Transmitter. The measured value is multiplied by a user defined number (k) according to the ratio to be adjusted in Ratio station. For example, if the N2:H2 = 1:3, the k should be 3. The output of ratio station becomes the set point for Flow Controller. The controller then calculates the required H2 flowrate accordingly. A transducer then converts the electric signal into pneumatic signal to operate the pneumatic valve and adjust the H2 flowrate.

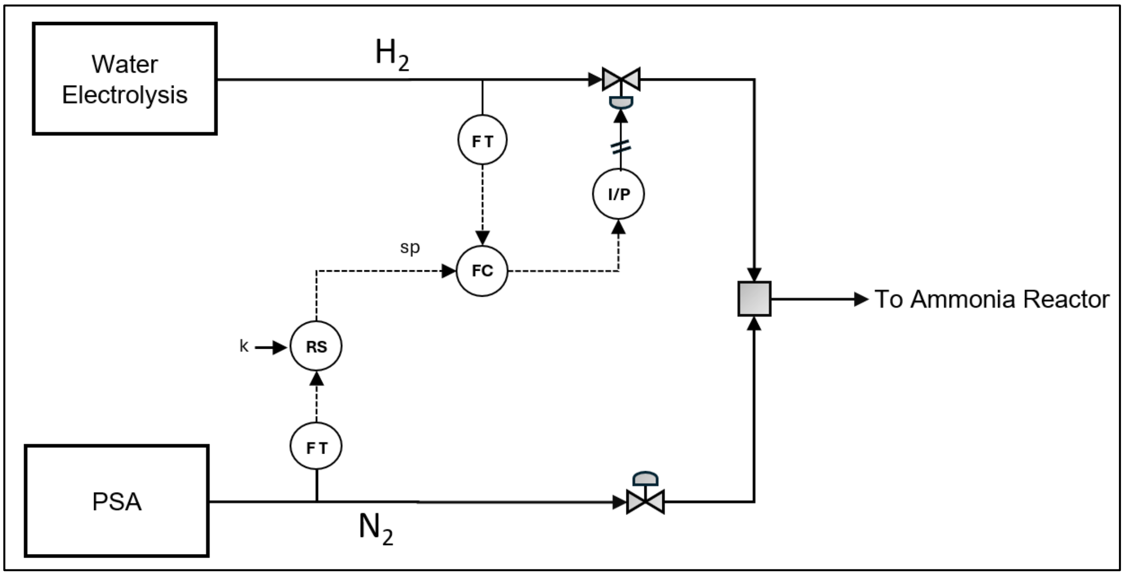


Figure 8.1 Ratio Control Loop

8.3 Feed Backward Control Loop

Feedback control measures one or more output variables and then takes the corrective actions. It waits until the disturbance occurs and then mitigates the effect of the disturbance bringing the system back to stable condition.

8.3.1 Temperature Control Loop

The temperature at the inlet of each bed of ammonia reactor should be maintained properly as the ammonia synthesis reactor is only carried out within a specific temperature range. An intercooler is installed at the outlet of each bed to reduce temperature so that it is within the reaction temperature range. A temperature control loop is applied to control this temperature. Temperature transmitter measures the temperature of the outlet of 1st intercooler (bed 2 inlet) and transmits it to the controller. The controller sets the temperature according to the step point. The electric signal is sent to the transducer which converts it into pneumatic signal. This signal then operates the pneumatic valve installed at the coolant supply of heat exchanger to set the flowrate accordingly.

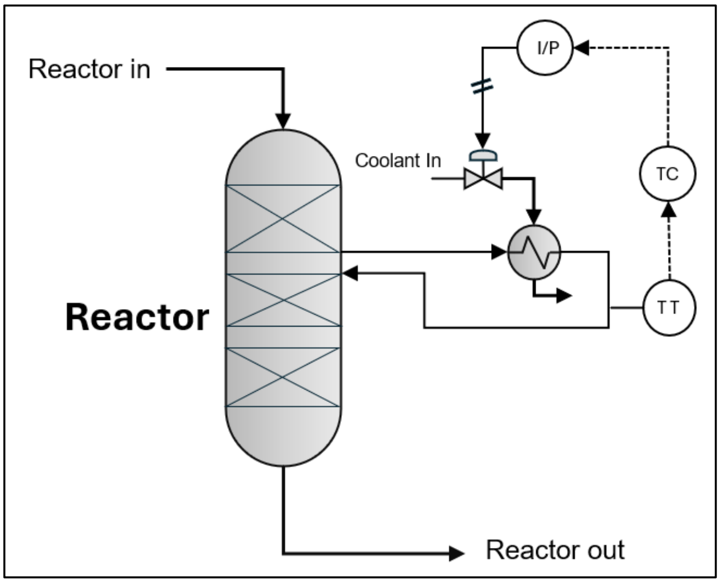


Figure 8.2 Temperature Control Loop

8.3.2 Pressure Control Loop

Pressure of air should be maintained at the inlet of adsorber for proper adsorption and desorption. A compressor is installed at the inlet to get the desired pressure. Pressure control loop is applied here. A pressure transmitter measures the pressure at compressor outlet and transmits it to the controller. Controller performs the necessary calculation using the setpoint. The outlet of the controller is converted into pneumatic signal by transducer. The air in stream is then throttled accordingly by throttling valve to adjust the pressure.

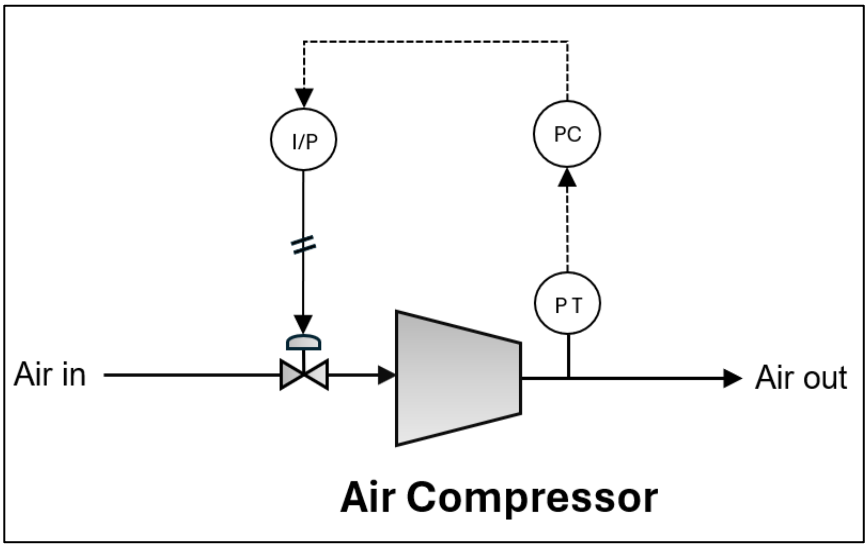


Figure 8.3 Pressure Control Loop

8.3.3 Level control Loop

The liquid level of ammonia in the separator should be maintained for proper separation. A level control loop is installed for this purpose. Level transmitter measures the level of liquid in the separator and sends the signal to the controller. Controller according to the setpoint calculates the required output. The output of controller is converted by transducer from electrical signals into pneumatic signals. The valve is then operated to remove the ammonia from the separator accordingly.

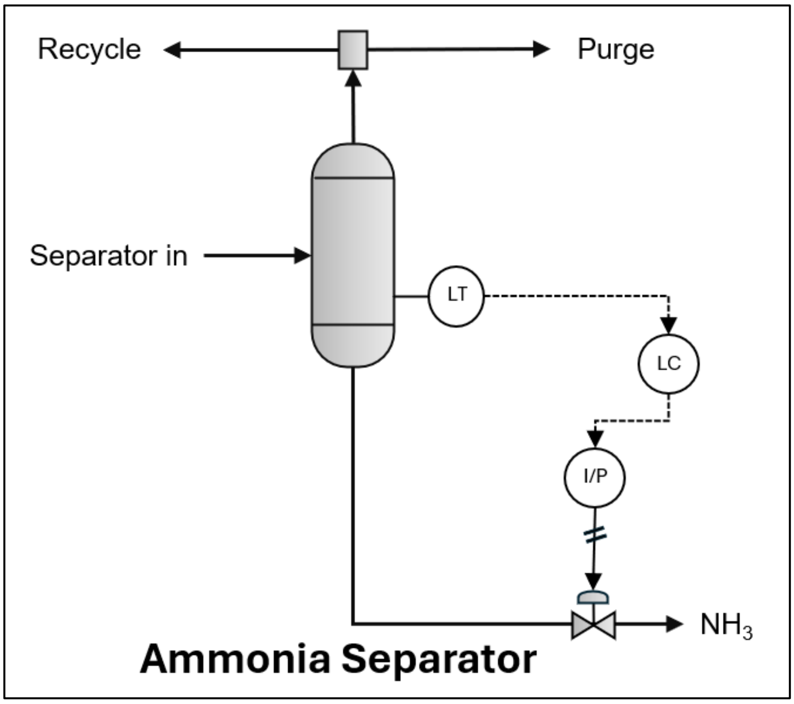


Figure 8.4 Level Control Loop

CHAPTER 9

ECONOMIC ANALYSIS

9.1 Introduction

The economic analysis of a chemical plant is a crucial step that determines its success and financial viability. It is critical in maintaining high standards by ensuring that the primary objective of generating revenue is met without compromising on production's quality or quantity. While economic analysis is a specialized field, a design engineer should be able to make rough cost estimates. This helps choose between different design options and ensure overall feasibility of the process.

It involves determining initial capital investment, including costs for land, equipment purchase and installation and plant construction. Operating cost, such as the cost for raw material, utilities, labors, and maintenance is estimated according to production capacity and efficiency. Revenue projections are made based on market demand and pricing strategies. Cost estimation helps stakeholders in making informed decisions and maximizes the economic return ensuring the business is sustainable and profitable.

Two major books are used for costing purposes. 'Chemical Engineering Design by R. K. Sinnott, J. M. Coulson and J. F. Richardson' & 'Chemical Engineering Design by G. Towler and R. Sinnott'.

9.2 Purchased Equipment Cost

Purchased of each equipment is discussed in detail below:

9.2.1 Water Pump P-1

Type: single stage centrifugal

Flow rate = S = 4.74 l/s

$$Formula\ used : Purchased\ Cost = a + b(S)^n$$

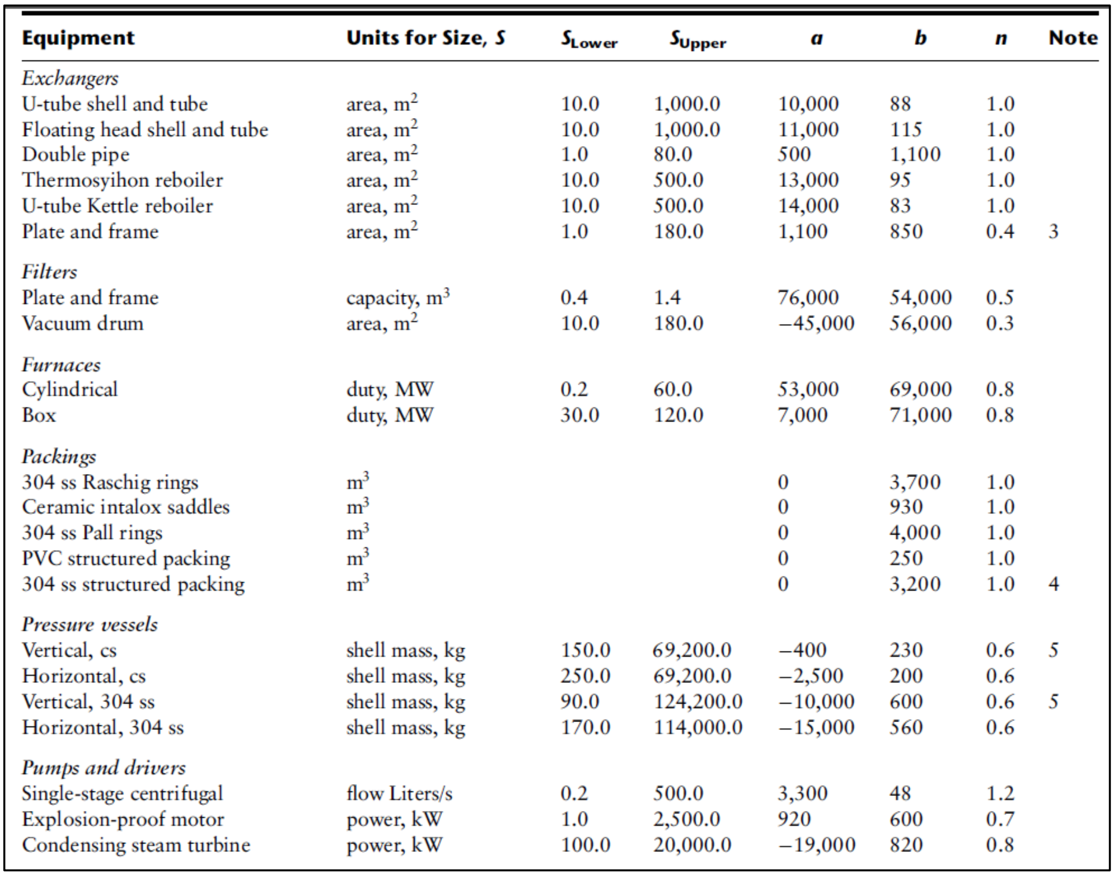
Using the values from Figure 9.1

a = 3300

b = 48

n = 1.2

Cost of Pump (2006) = 3600 $



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 9.1 Purchased equipment cost (Towler & Sinnott, 2007)

9.2.2 Electrolyzer

Estimated cost of PEM Electrolyzer is determined as follows:

Capacity of Electrolyzer = 33600 kg H2/day

Power of Electrolyzer = 73000 kW

Cost in 2019 = 324 $/kW

Cost of 2035 = 143 $/kW

Expected cost in 2024 = 265 $/kW

Cost of Electrolyzer (2024) = 19345000 $

9.2.3 Hydrogen Separator

Length of vessel = 3.42 m

Diameter of vessel = 0.49 m

Formula used: Cost = (bare cost from figure × material factor × Pressure factor)

Using values from Figure 9.2

Bare cost of vessel = 5900 $

Material factor (CS) = 1

Pressure factor (15 bar) = 1.2

Cost of Hydrogen Separator (2004) = 7080 $

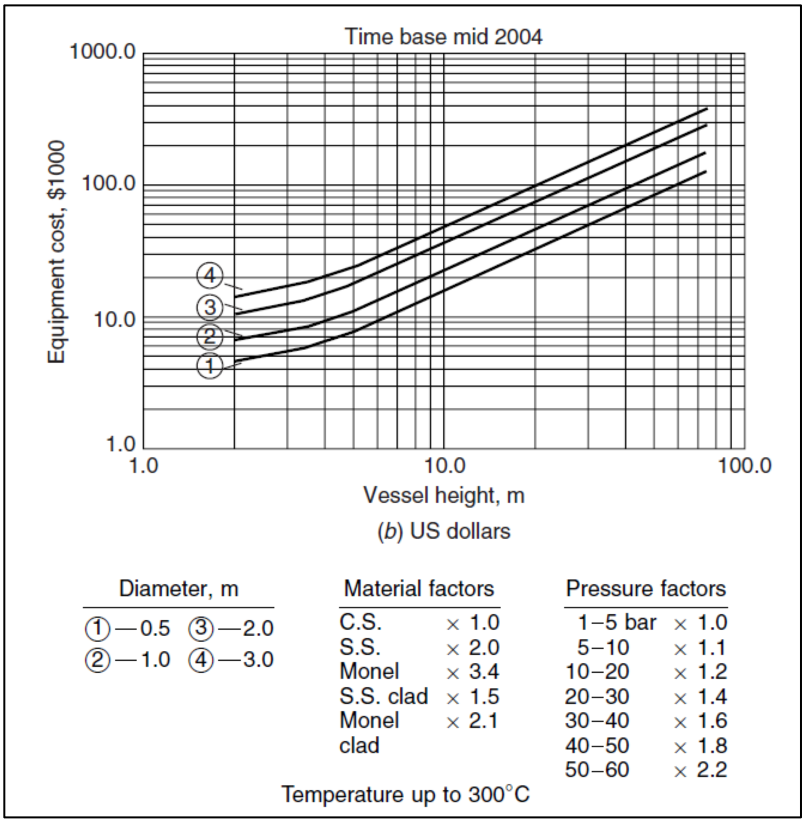


Figure 9.2 Cost for vertical pressure vessel (Sinnott et al., 2005)

9.2.4 Oxygen Separator

Length of vessel = 2.85 m

Diameter of vessel = 0.73 m

Formula used: Cost = (bare cost from figure × material factor × Pressure factor)

Using values from Figure 9.2

Bare cost of vessel = 7500 $

Material factor (CS) = 1

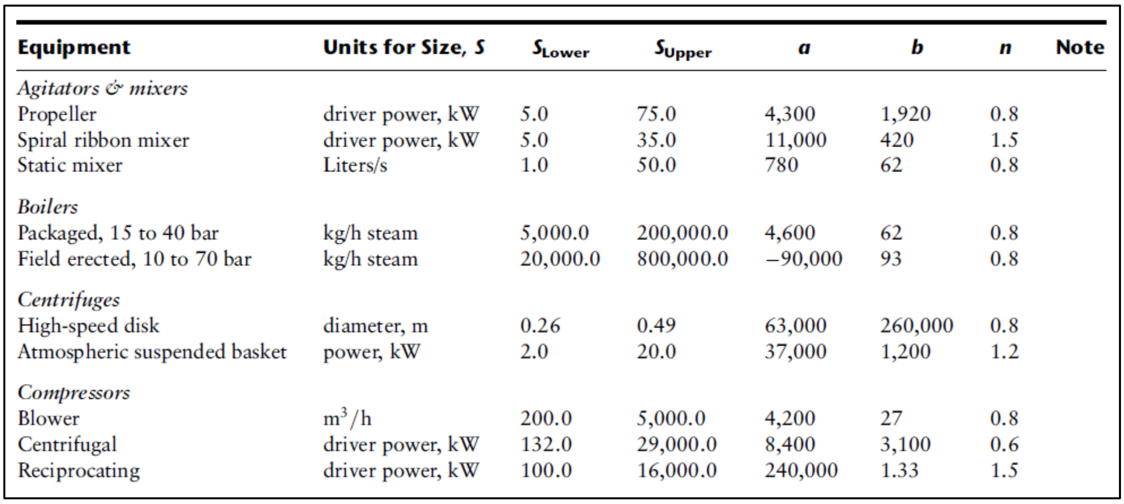
Pressure factor (15 bar) = 1

Cost of Hydrogen Separator (2004) = 7500 $

9.2.5 Air compressor C-1

It is a 2-stage compressor with an inter cooler . The cost of each unit is calculated separated below.

$$\text{Formula used : } Purchased\ Cost = a + b(S)^n$$



Equipment	**Units for Size, *S***	***S***					

Equipment	**Units for Size, S**	**S_{Lower}**	**S_{Upper}**	**a**	**b**	**n**	**Note**
Agitators & mixers							
Propeller	driver power, kW	5.0	75.0	4,300	1,920	0.8	
Spiral ribbon mixer	driver power, kW	5.0	35.0	11,000	420	1.5	
Static mixer	Liters/s	1.0	50.0	780	62	0.8	
Boilers							
Packaged, 15 to 40 bar	kg/h steam	5,000.0	200,000.0	4,600	62	0.8	
Field erected, 10 to 70 bar	kg/h steam	20,000.0	800,000.0	−90,000	93	0.8	
Centrifuges							
High-speed disk	diameter, m	0.26	0.49	63,000	260,000	0.8	
Atmospheric suspended basket	power, kW	2.0	20.0	37,000	1,200	1.2	
Compressors							
Blower	m^3/h	200.0	5,000.0	4,200	27	0.8	
Centrifugal	driver power, kW	132.0	29,000.0	8,400	3,100	0.6	
Reciprocating	driver power, kW	100.0	16,000.0	240,000	1.33	1.5	

Figure 9.3 Purchased equipment cost (Towler & Sinnott, 2007)

Compressor Stages

Type: Centrifugal compressor

Using the values from Figure 9.3

a = 8400

b = 3100

n = 0.6

- **Stage 1**

  Power = S = 634.3 kW

  Cost of stage 1 (2006) = 157200$

- **Stage 2**

  Power = S = 597.6 kW

  Cost of stage 2 (2006) = 152000$

Inter Cooler

- **Inter Cooler 1**

  Type: Floating head Shell and tube

  Heat transfer Area = S = 72.3 m2

  Using the values from Figure 9.1

  a = 11000

  b = 115

  n = 1

  Cost of IC (2006) = 19300 $

Total Cost of Air Compressor C-1 (2006) = 328500 $

9.2.6 Adsorption Column

Two adsorption columns are used. Cost of each includes the cost of vessel and the adsorbent used.

- **Cost of vessel**

Length of vessel = 11.7 m

Diameter of vessel = 3.7 m

Formula used: Cost = (bare cost from figure × material factor × Pressure factor)

Using values from Figure 9.2

Bare cost of vessel = 150000 $

Material factor (CS) = 1

Pressure factor (12 bar) = 1.2

Cost of vessel (2004) = 202400 $

- **Cost of Adsorbent**

Type: Carbon Molecular sieve

Mass of Adsorbent = 44614 kg

Market price in 2004 = 2.8 $/kg

Cost of Adsorbent (2004) = 124600 $

Cost of Adsorption column = Cost of vessel + Cost of Adsorbent

Cost of 1 column (2004) = 304600 $

Cost of 2 columns (2004) = 609200 $

9.2.7 Reactor Feed compressor C-2

It is a 4-stage compressor with inter coolers between each stage. The cost of each unit is calculated separated below.

$$\textit{Formula used}: \textit{Purchased Cost} = a + b(S)^n$$

Compressor Stages

Type: Centrifugal compressor

Using the values from Figure 9.3

a = 8400

b = 3100

n = 0.6

- **Stage 1**

  Power = S = 978 kW

  Cost of Pump (2006) = 201400$

- **Stage 2**

  Power = S = 958.3 kW

  Cost of Pump (2006) = 199000$

- **Stage 3**

  Power = S = 979 kW

  Cost of Pump (2006) = 201500$

- **Stage 4**

  Power = S = 202.5 kW

Cost of Pump (2006) = 83400$

Inter Coolers

Type: Floating head Shell and tube

Using values from Figure 9.1

a = 11000

b = 115

n = 1

- **Inter Cooler 1**

  Heat transfer Area = S = 38.9 m2

  Cost of IC (2006) = 15480$

- **Inter Cooler 1**

  Heat transfer Area = S = 38.8 m2

  Cost of IC (2006) = 15470$

- **Inter Cooler 1**

  Heat transfer Area = S = 39.7 m2

  Cost of IC (2006) = 15560$

Total cost of compressor is sum of each unit discussed above.

Cost of Reactor Feed Compressor (2006) = 731800 $

9.2.8 Ammonia Reactor

- **Vessel**

  Shell mass of vessel = 28600 kg

$$Formula\ used : Purchased\ Cost = a + \ b(S)^n$$

Using the values from Figure 9.1

a = -400

b = 230

n = 0.6

Cost of vessel (2006) = 108100$

- **Catalyst**

  Mass of Catalyst = 25400 kg
  Cost of catalyst (2006) = 0.76 $/kg
  Cost of Catalyst (2006) = 19350 $

- **Inter Coolers**

$$Formula\ used : Purchased\ Cost = a + \ b(S)^n$$

Type: Floating head Shell and tube

Using values from Figure 9.1

a = 11000

b = 115

n = 1

- **Inter Cooler 1**

  Heat transfer Area = S = 9.7 m2

  Cost of IC (2006) = 12100$

- **Inter Cooler 1**

  Heat transfer Area = S = 9.5 m2

  Cost of IC (2006) = 12000$

Cost of Ammonia Reactor +IC (2006) = 151600 $

9.2.9 Ammonia separator

Shell mass of vessel = 3118 kg

$$Formula\ used : Purchased\ Cost = a + b(S)^n$$

Using the values from Figure 9.1

a = -400

b = 230

n = 0.6

Cost of vessel (2006) = 28300$

9.2.9 Heat Exchangers

Type: Floating head Shell and tube

Using Values from figure 9.1

a = 11000

b = 115

n = 1

Heat Exchange area of each exchanger is obtained from Aspen Plus

- **HX-1**

  Heat transfer Area = S = 45.3 m2

  Cost of IC (2006) = 16200$

- **HX-2**

  Heat transfer Area = S = 19.8 m2

  Cost of IC (2006) = 13300$

- **HX-3**

    Heat transfer Area = S = 153.1 m2

    Cost of IC (2006) = 28600 $

- **HX-4**

    Heat transfer Area = S = 60.8 m2

    Cost of IC (2006) = 18000$

- **HX-5**

    Heat transfer Area = S = 38.6 m2

    Cost of IC (2006) = 15400$

- **HX-6**

    Heat transfer Area = S = 39.5 m2

    Cost of IC (2006) = 15500$

- **HX-7**

    Heat transfer Area = S = 17.1 m2

    Cost of IC (2006) = 12900 $

- **HX-8**

    Heat transfer Area = S = 118.2 m2

    Cost of IC (2006) = 24600$

Total cost of Heat exchangers = 144500

9.2.10 Summary

Given of is the cost of all equipments calculated in different years.

Table 9.1 Purchased cost of equipment

Equipment	**Year**	**Equipment Cost ($)**	**Equipment**	**Year**	**Equipment Cost ($)**
Pump P-1	2006	3600	**HX-1**	2006	16200
Electrolyzer	2024	19345000	**HX-2**	2006	13300
H2 Separator	2004	7080	**HX-3**	2006	28600
O2 Separator	2004	7500	**HX-4**	2006	18000
Air Compressor C-1	2006	328500	**HX-5**	2006	15400
Adsorption Columns	2004	609200	**HX-6**	2006	15500
Reactor Feed Compressor C-2	2006	731800	**HX-7**	2006	12900
Reactor +IC	2006	151600	**HX-8**	2006	24600
NH3 Separator	2006	28300			

Cost of each unit is converted in year 2024 using the chemical engineering plant cost index (CEPCI) published in *Chemical Engineering* magazine. The indices are given in the following table.

Table 9.2 CEPCI

Year	**Indices**
2004	444.2
2006	499.6
2024	800.3

Sum of all equipment cost in 2024 given the purchased cost of equipment (PCE)

PURCHASED COST OF EQUIPMENT (PEC) = $22694000 = $22.6M

9.3 Total Investment

9.3.1 Fixed Capital

Factors for estimating the fixes capital cost of any project are given below:

Table 9.3 Typical factors for estimating Fixed Capital cost (Sinnott et al., 2005)

f1 (Equipment erection)	0.4
f2 (Piping)	0.7
f3 (Instrumentation)	0.2
f4 (Electrical)	0.1
f5 (Buildings, process)	-
f6 (Utilities)	-
f7 (Storages)	0.15
f8 (Site development)	-
f9 (Ancillary buildings)	-
f10 (Design and Engineering)	0.3
f11 (Contractor's fee)	0.05
f12 (Contingency)	-

Total Physical Plant Cost(PPC) = PCE (1+f1+…….+f9)

PPC = $ 57.8M

(Fixed Capital) FC = PPC (1+f10+f11+f12)

Fixed Capital Cost = FC = $ 78.0M

9.3.2 Working Capital

Working capital id generally 10 to 15% of the fixed Capital

Working Capital = 0.1 (FC)

Working Capital = $ 7.8M

9.3.3 Total Investment

Total investment is the sum of fixed and working capital.

Total Investment = $ 85.8M

9.4 Annual Operating Cost

Plant attainment = 97%

No of operation days per year = 347

9.4.1 Fixed operating Cost

Table 9.4 Fixed Operating Cost (Sinnott et al., 2005)

Maintenance	3% of FC	$ 2203000
Operating Labor OL	1300$ annually (30 workers)	$ 39000
Laboratory	20% of OL	$ 7800
Supervision	20% of OL	$ 7800
Plant Overheads	40% of OL	$ 19400
Capital Charges	2% of FC	$ 7344000
Insurance (1% of FC)	1% of FC	$734400

Fixed operating Cost = $ 10.9M

9.4.2 Variable Operating Cost

- **Utilities**

Electricity (annual)

Mass of H2 = 116650000 kg

Cost of electricity per kWh = 0.036 $/kWh

Total Electricity Cost = $20.9M

Cooling water (Annual)

Mass of water = 63.24×10^{8} kg

Cost of water per kg = 1.1×10^{-5} $/kg

Total cost of water = $ 0.12M

- **Miscellaneous Material (5% of Maintenance Cost) =** $ 0.23 M

Total Variable Cost = $ 21.3 M

9.4.3 Annual Production Cost

Annual Production Cost = Total Variable Cost + Fixed Operating Cost

Annual Production Cost = $32.3M

9.5 Annual Revenue

Market price of ammonia = 0.8 $/kg

Production capacity = 54.57×10^{8} kg

Annual Revenue = $ 43.8M

9.6 Annual Profit

Annual Profit = Annual revenue – Annual production cost

Annual Proft = $ 11.5M

9.7 Payback Period

Pay Back Period = Total Investment / Annual profit

Payback Period = 7.4 years

Detailed calculation for payback period is given below:

Table 9.5 Payback period calculations

No. of Years	Cash Inflow ($)	Cash Outflow ($)	Net Cash Flow ($)	Cumulative Present Worth ($)
0	0	85.8M	-85.8M	-85.8M
1	43.8M	32.3M	11.5M	-74.3M
2	43.8M	32.3M	11.5M	-62.8M
3	43.8M	32.3M	11.5M	-51.4M
4	43.8M	32.3M	11.5M	-39.9M
5	43.8M	32.3M	11.5M	-28.4M
6	43.8M	32.3M	11.5M	-17.0M
7	43.8M	32.3M	11.5M	-5.53M
8	43.8M	32.3M	11.5M	5.95M
Pay Back Period is between 7th and 8th year.				

CHAPTER 10

HAZOP ANALYSIS

10.1 Introduction

Hazard and Operability analysis is a standard tool used in risk assessment to identify the potential hazards and operability issues in chemical processes.

It consists of following steps. (Crowl & Louvar, 2011)

1. Breaking down the flow sheet into several units and selecting one unit for study.
2. Choose a study node.
3. Describe the design intent of study node.
4. Choose a process parameter (Flow, temperature, pressure etc.)
5. Apply guide words.
6. Identify possible causes.
7. Look for possible consequences.
8. Recommend action.

10.2 Electrolyzer

Table 10.1Hazop Analysis for Electrolyzer

Study Node	Process Parameter	Guide Word	Possible Causes	Possible Consequences	Action Required
Water inlet line	Flow	No/Low	Possible blockage/ leakage in the line, RO system failure, Inlet valve malfunctioning	Incomplete reaction, reduced production rate	Install strainer in the lines, check and repair/replace faulty valves.

		High	Inlet valve malfunctioning, (Fail Open)	Accumulation of unreacted reactant, compressor duty increased, over pressurization	check and repair/ replace faulty valves, install pressure release valves.
	Temperature	Higher	Faulty heat exchanger, failure of Temperature control system	Overheating, membrane degradation, catalyst deactivation	Repair/ relace faulty components of temp control system, install additional temp sensors
		Lower	Faulty heat exchanger, fouling.	Decreased rate of reaction, reduced production	Proper cleaning of exchangers
Voltage supply	Electricity (voltage)	High	Faulty wiring, lightening	Overheating, possibility of blast	Voltage regulator, Interlocks
		Low	Faulty wiring	Shut down of Electrolyzer	Proper monitoring. Repair/replace faulty wiring
Cell	Pressure	High	Outlet valves fail closed, outlet line blockage	Pressure built up leading to blast	Proper maintenance of valves, installing pressure sensors
		Low	Leakage in cell or lines	Reaction rate can be affected	Proper checking of cell and lines, installing pressure sensors

10.3 Heat Exchanger

Table 10.2 Hazop Analysis for Heat Exchanger

Study Node	Process Parameter	Guide Word	Possible Causes	Possible Consequences	Actions Required
Heat Exchanger	**Flow**	**Less**	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
		More	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
	Pressure	**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

		Low	Leakage in the shell Leakage in tubes	Improper Heat Exchange	Install low-pressure indicator, Check for leakages.
	Temperature	**High**	high heating supply Temp	Required outlet temp is not achieved	Install high flow temperature and flow alarm
		Low	low heating supply Temp	Improper heat exchange	Install controllers

CONCLUSION

The Haber-Bosch process has improved global food production to a great extent. But at the same time, it has posed serious threats to our environment. Now is the best time to look for alternatives as fossil fuels consumed in this process are rapidly depleting and a significant amount of damage has already been done to the environment. This project has presented a great alternative to the conventional ammonia production process in the form of green ammonia. It focuses on using technologies that are sustainable in the long run. The versatility of green ammonia, serving various industries and applications positions it as a crucial element in decarbonizing sectors and can play a great role in achieving the goal of net-zero carbon emission by 2050.

The successful application of green ammonia technology can help transform various sectors. In agriculture, it provides an environmentally friendly alternative for fertilizer production, mitigating the environmental footprint of food production. In the energy sector, green ammonia serves as a versatile energy carrier and a potential fuel for power generation and transportation.

With further research and development, the technical and economic challenges associated with this technology can be overcome and green ammonia can emerge as an effective method for large scale ammonia worldwide.

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