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(Ammonia production plant)

A project submitted to the Chemical & Petrochemical Engineering
Department University of Salahaddin-Erbil

In the partial fulfillment of the requirement for the degree of bachelor of
science in Chemical and Petrochemical Engineering Department

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Chapter 1

Introduction

3.1.1 General overview

3.1.2 What is Ammonia?

Ammonia (NH_3) is an essential compound of nitrogen and hydrogen. It is created by the regular decay of vegetable and animal bodies. The demise and rot of animals and plants cause the nitrogen compounds exhibit in them to get deteriorated, producing ammonia. Ammonia, likewise, is present in the soil as ammonium salts.

Ammonia is a colorless highly irritating gas with a sharp suffocating odor. It dissolves easily in water to form ammonium hydroxide solution which can cause irritation and burns. Ammonia gas is easily compressed and forms a clear, colorless liquid under pressure. It is usually shipped as a compressed liquid in steel cylinders. Ammonia is not highly flammable, but containers of ammonia may explode when exposed to high heat.

In the textile industry, ammonia is used in the manufacture of synthetic fibers, such as nylon and rayon. In addition, it is employed in the dyeing and scouring of cotton, wool, and silk. Ammonia serves as a catalyst in the production of some synthetic resins. More important, it neutralizes acidic by-products of petroleum refining, and in the rubber industry it prevents the coagulation of raw latex during transportation from plantation to factory. Ammonia also finds application in both the ammonia-soda process (also called the Solvay process), a widely used method for producing soda ash, and the Ostwald process, a method for converting ammonia into nitric acid.

About 80% of the ammonia produced in industry is used in agriculture as fertilizer. Ammonia is also used as a refrigerant gas, to purify water supplies, and in the manufacture of plastics, explosives, fabrics, pesticides, dyes and other chemicals. It is found in many household and industrial-strength cleaning solutions. Cleaning solutions for industrial use contain higher concentrations of ammonia and can quickly cause irritation and burns. [1]

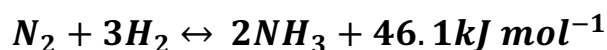
3.1.3 History:

The production of ammonia over the last century has been fundamental in supporting the increase in population due to its use as a fertilizer. The use of ammonia in fertilizers, which provide a fixed nitrogen source, has supported 27% of the world's population over the last century. To facilitate the massive increase in demand, German chemist Fritz Haber in 1908 developed a method for ammonia synthesis from H_2 and N_2 under high pressure and temperature using recycling. This process was industrialized by Carl Bosch, with the first ammonia synthesis plant being built in 1911. Due to this the process of producing ammonia from H_2 and N_2 at high temperature and pressure is known as the Haber–Bosch process.

Fritz Haber and Carl Bosch won the Nobel Prize in Chemistry in 1918 and 1931 respectively for their work on this process. In 2007, Gerhard Ertl won the Nobel Prize in Chemistry for his great contribution on the surface chemistry of iron catalysts. Today most ammonia synthesis plants use fused-iron catalysts that use a variety of carefully designed promoter materials. As will become evident, these plants require high pressure and temperature to achieve the desired conversion and as such require a significant energy input. It is therefore the goal of any new ammonia synthesis catalyst to ease these conditions by achieving high catalytic activity at reduced temperatures and pressures, enabling a more energy-efficient process.

In the conventional Haber–Bosch process, fossil fuels such as natural gas and coal are normally used as the energy sources for ammonia synthesis, releasing millions of tonnes of CO_2 to the atmosphere, which is about 1–2% of the global CO_2 emission. The use of low-carbon renewable energy sources has been proposed to produce green ammonia. According to the roadmap for ammonia economy, in the foreseeable future, the Haber–Bosch process is still the dominant ammonia synthesis technology, although other emerging technologies such as electrochemical and photocatalytic synthesis of ammonia are also promising. Green ammonia production can alleviate the pressure on renewable electricity storage if the “surplus” electricity from wind and solar energy is used as the energy source for ammonia synthesis.

The reaction of hydrogen and nitrogen to produce ammonia is as follows



This reaction requires the use of a catalyst, high pressure (100–1,000 atmospheres), and elevated temperature (400–550 °C). Actually, the equilibrium between the elements and ammonia favours the formation of ammonia at low temperature,

but high temperature is required to achieve a satisfactory rate of ammonia formation. Several different catalysts can be used. Normally the catalyst is iron containing iron oxide. [2]

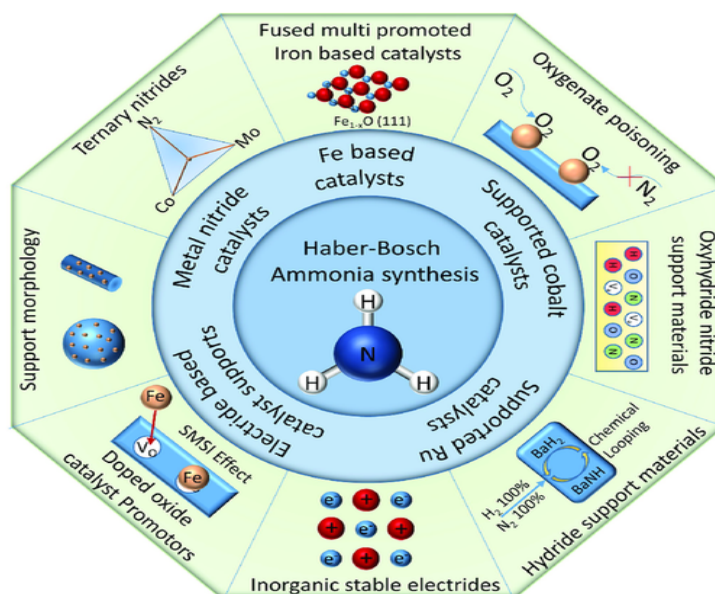


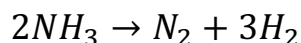
Figure 1 Graphical overview of strategies to improve Haber–Bosch ammonia synthesis

3.1.4 Chemical and Physical Properties:

3.1.5 Chemical properties:

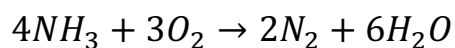
1) Thermal Stability

Ammonia is exceptionally inert. In any case, we can disintegrate it into hydrogen and nitrogen by advancing over metallic impetuses that have been heated.[3]



2) Combustibility

It is flammable in air.



3.1.6 Physical properties:

The physical properties of ammonia. [4]

Appearance	Colorless liquefied gas.
Odour	Pungent, suffocating.
pH water solution (1%)	11.7
Melting point (triple point)	-77.7°C
Boiling point	-33.4°C at 101.3 kPa
Explosive limits	16-27% NH₃ by vol. in air at 0 °C
Auto-ignition temperature	651°C
Vapour pressure	1013kPa at 25°C
Relative vapour density	0.6 (air =1)
Solubility in water	529g/l⁻¹ at 20 °C
Solubility in organic solvents	Soluble in alcohol, acetone, chloroform
Liquid density	0.6386g/cm⁻³(at 0°C, 101.3kPa)
Gas density	0.7714g/l⁻¹ (at 0°C, 101.3kPa)

3.1.7 Plant processes improvements:

Several changes have been made in ammonia plant technology during the first few years of the 21st century, enabling current plants to raise output volumes and to construct new plants with greater and greater capacities. The market is currently dominated by three technology licensors – KBR (Kellogg Brown and Root), Haldor Topsøe, and ThyssenKrupp Industrial Solutions (TKIS).[5]

We have some method of producing ammonia plant design:

3.1.8 1. KBR (Kellogg Brown and Root) plant design

Most of KBR's newly built ammonia plants use its Purifier method, which incorporates the main reformer, an upstream liquid nitrogen wash purifier to eliminate impurities and change the H₂: N₂ ratio, a patented thermal energy boiler system, unitized coolers, and a horizontal ammonia synthesis converter.[5]

3.1.9 2. Haldor Topsøe designed plant

Except for its patented side-fired visionary, which utilizes radiant burners to provide fuel for the transforming reaction, it is very conventional. Haldor Topsøe also sells a patented iron-based synthesis catalyst, one-, two- or three-bed radial-flow adapters, and a patented bayonet-tube waste-heat burner.[5]

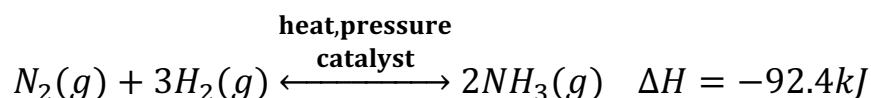
Uhde now known as tkIS (ThyssenKrupp Industrial Solutions) is another company with a long innovative history in the ammonia industry with its first ammonia plant built-in 1928. Uhde developed its dual-pressure process for large-scale plants in late 2001.[5]

3.2 Haber Bosch Process:

We discussed some ammonia production plant method in brief but here we focused on one process and described in detail and it is Haber bosch process. Haber bosch was the first industrial chemical process to use high pressure for a chemical reaction. It is directly combines nitrogen from the air with hydrogen under extremely high pressure and moderately high temperature.[6]

There are some point that describe Haber process:

- In this Haber-Bosch process, we take hydrogen atom and combine it with nitrogen gas taken from air, and these are in ratio of 1:3 by its volume.
- For maintaining the constant equilibrium condition, the gases are passed from the four beds of the catalyst.
- Cooling is also maintained in every bed of catalyst.
- Unreacted gases are also recycled while passing through different levels.
- The catalyst used here is iron maintaining its temperature at 400°-450°C and pressure of about 150-200 atm.
- In the last stage of the process the produced ammonia is cooled down in liquid solution, which is further collected and stored.
- **The materials that are used in the Haber process are:** Air, which helps in supplying the nitrogen. Iron works as a catalyst. Natural gas and water which helps in the requirement of energy to produce the reactants and also supplying the hydrogen.
- The reaction between nitrogen gas and hydrogen gas to produce ammonia gas is **exothermic**, releasing 92.4kJ/mol of energy at 298K (25°C).



3.2.1 PID diagram of Haber process by using hysys simulation :

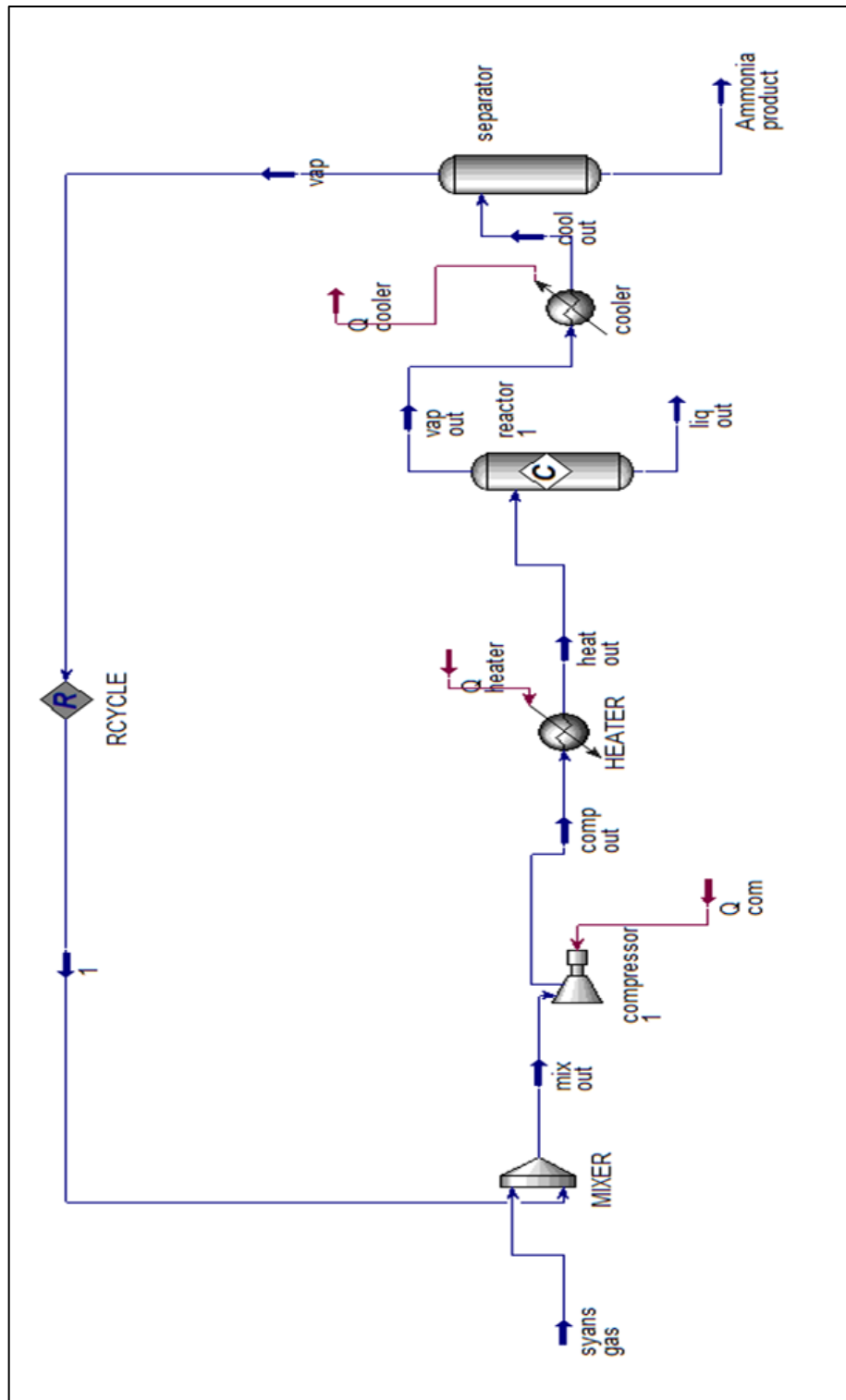


Figure 2 Ammonia production from Natural Gas (methane).

3.2.2 Operating variable by using hysys simulation :

	Unit	syans gas	comp out	mix out	heat out	vap out	liq out	cool out
Vapour Fraction		1	1	1	1	1	0	0.971688129
Temperature	C	280	299.595165	164.5716748	500	530.3105451	530.310545	10
Pressure	kPa	2550	2799.5	2799.5	2789.5	2789.5	2789.5	2689.5
Liquid Volume Flow	M³/h	3.49248317	3.49248317	82.46021302	82.46021302	80.60737029	0	80.60737029
Heat Flow	kJ/h	731374.248	798124.902	-10184198.4	-72107738.6	-72107267.1	0	-11738785.8

Table 2 hysys simulation readings 1

	Unit	vap	liq	purge	s 10	s11	compressed out 2
Vapour Fraction		1	0	1	1	1	1
Temperature	C	10	10	10	10	10	183.0265386
Pressure	kPa	2689.5	2689.5	2689.5	2689.5	2689.5	12699.5
Liquid Volume Flow	m3/h	79.00931387	1.598056428	0.790093139	78.21922073	78.96772985	78.96772985
Heat Flow	kJ/h	-113471416.9	-3867368.86	-1134714.17	-112336702.8	-113404954.2	-102639323.3

Table 1 hysys simulation readings 2

Chapter 2

Material balance

2.1 MATERIAL BALANCE

Our target is using 1000kg/hr (1ton/hr)

And producing ammonia with 90% conversion

M.B without recycle

Over reactor

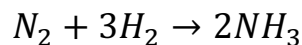
Fresh feed we have 1000kg/hr of N₂ and H₂ with mole fraction 0.25 of N₂ and 0.75 H₂

$$0.25 \times 1000 \frac{kg}{hr} = 250 \frac{kg}{hr} N_2$$

$$0.75 \times \frac{1000kg}{hr} = 750kg/hr H_2$$

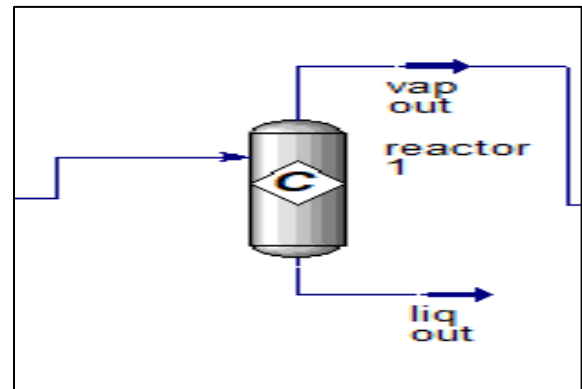
2.2 M.B over reactor without recycle

Reaction in the reactor



Input = output

$$\frac{250kg}{hr} + \frac{750kg}{hr} = 1000 \frac{kg}{hr}$$



1000 kg/hr (Synthesis gas) = (Conversion × feed mass rate) + unreacted feed mass rate

In the reactor we have conversion with 90%

And in every reactor we have loss in conversion to 5 or 6 percent

Conversion * feed mass rate = reactor product

So, $86\% \times 1000 = 860 \frac{kg}{hr}$ of ammonia is produced

Then remain 14% of unreacted feed

5% of N₂

9% of H₂

So With 2.5% of N₂ and 7.5% of H₂ and 25 kg/hr N₂ and 75 kg/hr H₂

In the reactor we just have top product (vap out) and because the temperature is very high and all product is a vapor

Name of component		N ₂	H ₂	NH ₃
input	composition	25%	75%	0
	Mass rate	250 kg/hr	750 kg/hr	0
Output	Composition	5%	9%	86%
	Mass rate	50kg/hr	90 kg/hr	860 kg/hr

2.3 M.B over separator without recycle

The separator (efficiency) is 80%

In separator we have inlet feed with 50 kg/hr of N₂ and 90 kg/hr of H₂

And 860 kg/hr of NH₃

We have losses in separator efficiency 3%

We have efficiency of separator is 97% liquid produce

We have losses

Input = output

Inlet feed = top (vap) + Ammonia product

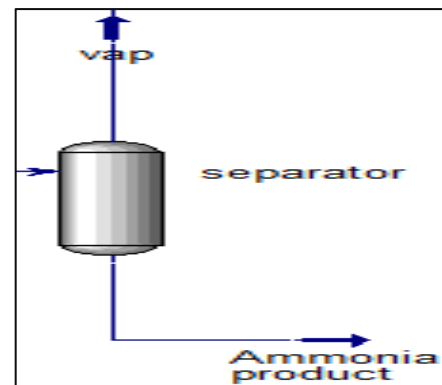
860 kg/hr. NH₃

Ammonia product = eff * ammonia produced in reactor (= 97% * 860=833 kg/hr)

Feed Ammonia - Ammonia product = top Ammonia product

$$860 - 833 = 27 \frac{kg}{hr}$$

And also, we have 90 kg/hr of N₂ and 50 kg/hr of H₂



Name			N ₂	H ₂	NH ₃
input	Composition		5%	9%	86%
	Mass rate		50 kg/hr	90 kg/hr	860kg/hr
output	Bottom product (Ammonia product)	Composition	0	0	100%
		Mass rate	0	0	833 kg/hr
	Top product (vap)	Composition	30%	54%	16%
		Mass rate	50 kg/hr	90 kg/hr	27kg/hr

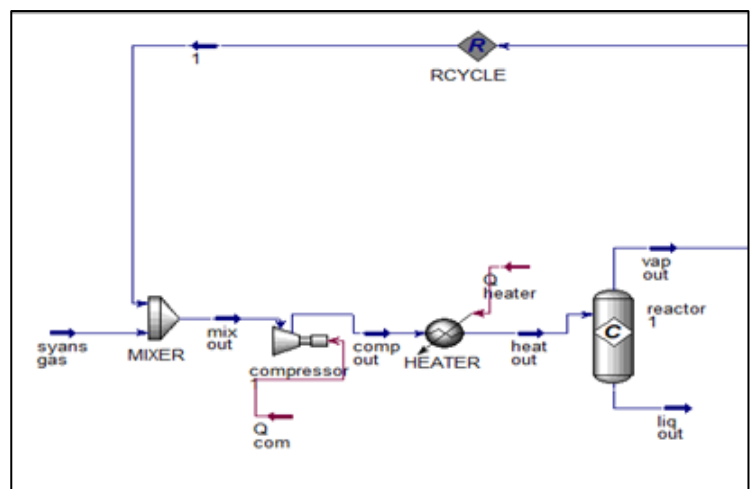
2.4 M.B over reactor with recycle

Synthesis gas (fresh feed) mass rate: 250 kg/hr of N₂, 750 kg/hr of H₂

1 (Recycled) mass rate is: 25 kg/hr N₂ ,75 kg/hr H₂, kg/hr NH₃

The overall feed mass rate to the reactor:

1100 kg/hr of Synthesis gas + 180 kg/hr of NH₃ = 1180 kg/hr



Reactor conversion 86%

Ammonia produced in reactor= conversion * Synthesis gas (mass rate)

$$= 86\% * 1143 \text{ kg/hr} = 941 \text{ kg/hr } \text{NH}_3$$

Output rate of the reactor

Ammonia produced + Recycled Ammonia = Ammonia outlet (mass rate)

$$941 + 40 = 981 \frac{\text{kg}}{\text{hr}} \text{NH}_3$$

Mole fraction = 91.5% NH_3

$$1183 - 983 = 202 \frac{\text{kg}}{\text{hr}} \text{ of unreacted Synthesis gas remain}$$

$$202 \times 0.75(\text{composition of } \text{N}_2) = 151 \frac{\text{kg}}{\text{hr}} \text{ and } 12.7\% \text{ of } \text{H}_2$$

$$202 * 0.25(\text{composition of } \text{N}_2) = 51 \frac{\text{kg}}{\text{hr}} \text{ and } 4.3\% \text{ of } \text{N}_2$$

name		N_2	H_2	NH_3
Input	composition	24.2%	72.5%	3.3%
	Mass flow	286 kg/hr	857 kg/hr	40 kg/hr
Output	composition	4.3%	12.7%	83%
	Mass flow	51 kg/hr	151kg/hr	981 kg/hr

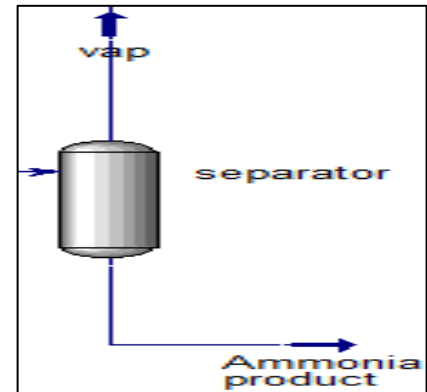
2.5 M.B over the separator with recycle

Input = out put

Input: 981kg/hr NH_3

151kg/hr H_2

51kg/hr N_2



As we said and indicate the efficiency of the separator is 80 % that is mean we can separate 86% off Ammonia that is became liquid :

Bottom Product

Separator Efficiency * Amount produced in reactor = Ammonia product

$$97\% * 981 = 952 \frac{\text{kg}}{\text{hr}} \text{NH}_3$$

So we have 952kg/hr NH_3 As a bottom product and as a liquid

Top product

Total ammonia - Ammonia in bottom product = unseparated Ammonia

$$981 \frac{\text{kg}}{\text{hr}} - 952 \frac{\text{kg}}{\text{hr}} = 29 \frac{\text{kg}}{\text{hr}} \text{ unseparated } \text{NH}_3 \text{ and remain as gas.}$$

And also we have the unreacted Synthesis gas (27.5 kg/hr N_2)and(82.5 kg/hr H_2)

Name			N_2	H_2	NH_3
input	Composition		4.3%	12.7%	83%
	Mass rate		51 kg/hr	151kg/hr	981 kg/hr
output	Bottom product (Ammonia product)	Composition	0	0	100%
		Mass rate	0	0	952 kg/hr
	Top product (vap)	composition	18.9%	55.6%	25.4%
		Mass rate	51 kg/hr	151kg/hr	29 kg/hr

2.6 Overall Martial Balance

We have one reactor and one separate

We have 2 input streams and 2 out put streams

In the input streams we have fresh feed Synthesis gas and recycled from separator that is mixed with fresh feed and compressed and heated and sent to the reactor.

In output stream we have 2 streams one is bottom product that is liquid NH_3 and it is pure product almost by 100% of Ammonia

Another product is vapor product that is mixture of N_2 and H_2 and NH_3 and recycled back to the reactor

Input		fresh feed			Recycle		
	Name	N_2	H_2	NH_3	N_2	H_2	NH_3
	Composition	0.25	0.75	0	18.9%	55.6%	25.4%
	Mass flow	250 kg/hr	750 kg/hr	0	51 kg/hr	151kg/hr	29 kg/hr
Overall input after mixer		name	N_2	H_2	NH_3		
		Composition	24.2%	72.5%	3.3%		
		Mass flow	286 kg/hr	857 kg/hr	40 kg/hr		

Output		Recycle, top product (Vap)			Bottom Product (Ammonia product)
	Name	N_2	H_2	NH_3	Pure NH_3
	composition	18.9%	55.6%	25.4%	100 %
	Mass flow	51 kg/hr	151kg/hr	29 kg/hr	952 kg/hr

2.7 Material Balance by Aspen hysys simulation

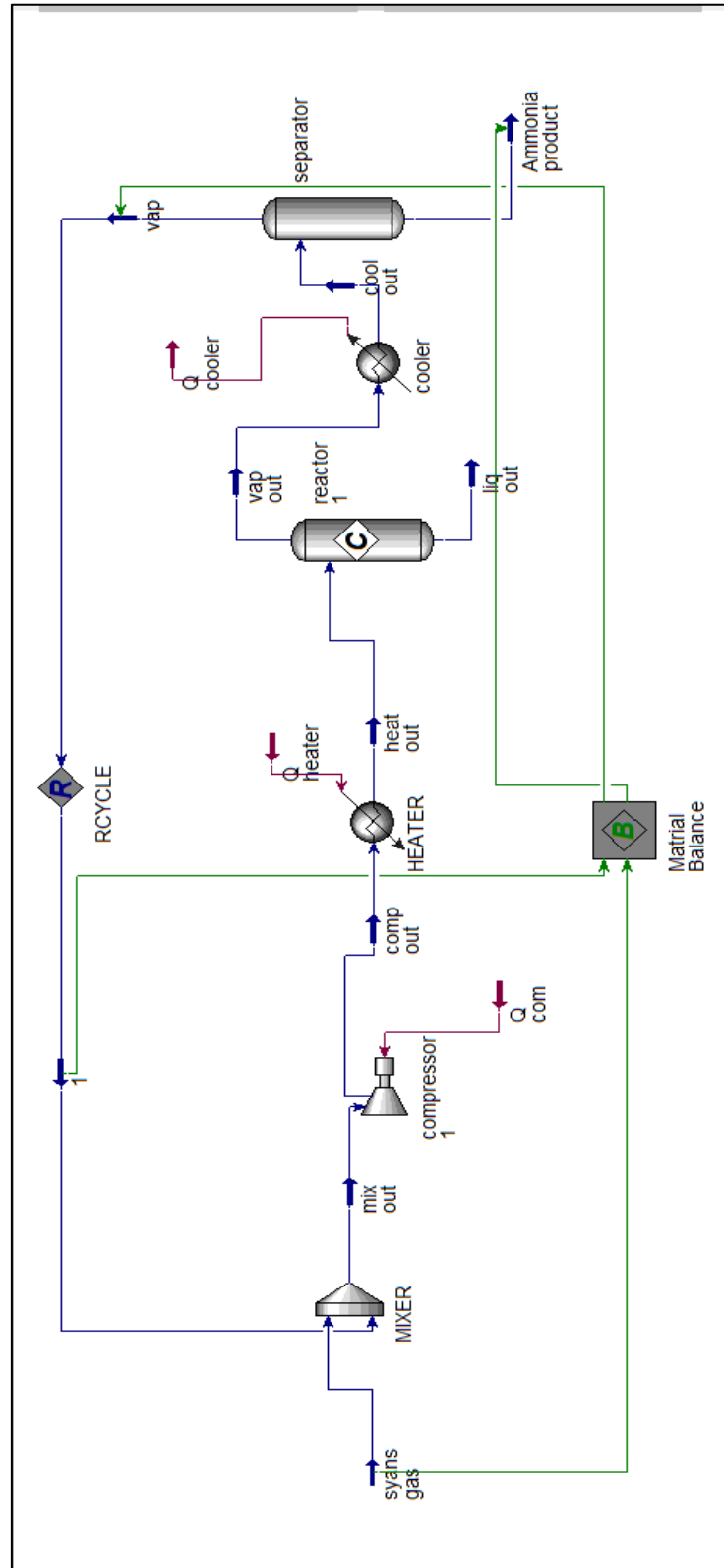


Figure 3 material balance by hysys simulation

Martial stream and condition

Name	synthesis gas	1	Ammonia product	vap
Vapour	1	0.999	0	1
Temperature [C]	240	10.00	10	10
Pressure [kPa]	2550.	2689.5	2689.5	2689.5
Molar Flow [kgmole/h]	117.436	12.57	58.766	12.59
Mass Flow [kg/h]	1000.	158.015	952	158.14
Std Ideal Liq Vol Flow [m3/h]	3.56	0.378	1.62	0.37
Molar Enthalpy [kJ/kgmole]	7412.438	-12628.1	-67944.21	-12620.50
Name	Composition			
	1	synthesis gas	Ammonia product	vap
Nitrogen	0.1887	0.25	0	0.1891
Hydrogen	0.55675	0.75	0	0.5564
Ammonia	0.2544	0	1	0.2544

Table 2 material stream 3

CHAPTER 3

Energy balance

3.3 Energy balance:

Gas heat capacity:

$$C_p = a + bT + cT^2 + dT^3$$

Where: C_p Gas heat capacity $\frac{KJ}{Kg.C}$

T: temperature C

a, b, c and d constants

component	a	b	c	d
N_2	31.15	-1.356×10^{-2}	2.679×10^{-5}	-1.168×10^{-8}
H_2	27.143	9.273×10^{-3}	-1.38×10^{-5}	7.645×10^{-9}
NH_3	27.315	2.383×10^{-2}	1.707×10^{-5}	-1.184×10^{-8}

Table 3 ()

component	$\Delta H_{f_{25^\circ C}} \text{ kJ/kg}$
NH_3	-2689

Table 4 (())

3.4 Energy Balance on compressor:



$$P_1 = 2550 \text{ kpa}$$

$$P_2 = 2800 \text{ kpa}$$

$$T_1 = 240$$

$$T_2 = ?$$

$$\left(\frac{T_2}{T_1}\right) = \left(\frac{P_2}{P_1}\right)^m$$

$$m = \frac{(\gamma-1)}{(eff \times \gamma)}$$

Eff = efficiency of compressor = %80

$$\gamma = \frac{cp}{cv} \cong 1.4$$

$$m = \frac{(1.4 - 1)}{(0.8 \times 1.4)} = 0.35$$

$$\left(\frac{T_2}{240 \text{ } ^\circ\text{C}}\right) = \left(\frac{2800 \text{ kpa}}{255 \text{ kpa}}\right)^{0.35}$$

$$T_2 = 250^\circ\text{C}$$

$$Q \text{ in} + Q \text{ heating} = Q \text{ out}$$

Because Q heating is so small its negligible

So $Q_{in} = Q_{out}$

$Q_{in} = [240^{\circ}\text{C}], [25^{\circ}\text{C}, t_{ref}] \text{ CP in } \Delta T_i$

Cp for N_2 at 240°C is $1.06 \frac{\text{kJ}}{\text{kg} \times \text{C}}$

$$Q_{\text{N}_2} = 286 \times 1.06 \times (340 - 25)$$

$$= 95495 \frac{\text{kJ}}{\text{hr}}$$

Cp for H_2 at 240°C is $14.52 \frac{\text{kJ}}{\text{kg}}$

$$Q_{\text{H}_2} = 857 \times 14.52 \times 225$$

$$= 2799819 \frac{\text{kJ}}{\text{kg}}$$

For NH_3 the Cp = 2.632

$$Q_{\text{NH}_3} = 40 \times 2.63 \times (240 - 25) \times$$

$$= 22618 \frac{\text{kJ}}{\text{hr}}$$

$$Q_{in} = 2799819 + 95495 + 22618$$

$$= 2917.9 \times 10^3 \frac{\text{kJ}}{\text{hr}}$$

$$Q_{in} = Q_{out}$$

$$2917.9 \times 10^3 \frac{\text{kJ}}{\text{hr}}$$

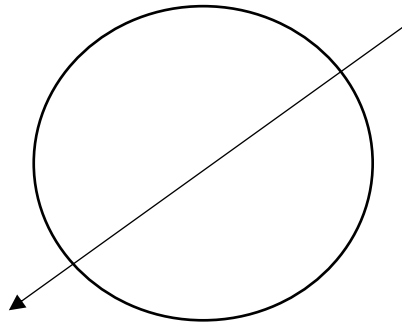
3.5 Energy balance for heater:

$$N_2 = 286 \frac{kg}{hr}$$

$$H_2 = 857 \frac{kg}{hr}$$

$$NH_3 = 40 \frac{kg}{hr}$$

$$T=250^{\circ}C$$



$$286 \frac{kg}{hr} N_2$$

$$857 \frac{kg}{hr} H_2$$

$$40 \frac{kg}{hr} NH_3$$

$$T=500^{\circ}C$$

$$Q_{in} = 2917.9 \times 10^3 \frac{kJ}{hr}$$

$$Q_{out} = \sum_{25}^{500} m_{out} C_{P_{out}} \Delta T$$

$$C_p \text{ of } N_2 \text{ at } 500^{\circ}C \text{ is } 1.18 \frac{kJ}{kg}$$

$$Q_{N_2} = m c_p \Delta T$$

$$286 \times 1.18 \times (500 - 25) = 160303.5 \frac{kJ}{hr}$$

$$C_p \text{ of } H_2 \text{ at } 500^{\circ}C \text{ is } 14.67$$

$$857 \times 14.67 \times (500 - 25)$$

$$= 5971790 \frac{kJ}{hr}$$

Cp NH₃ at 500°C is $3.234 \frac{kJ}{kg}$

$$Q_{NH_3} = 40 \times 3.234 \times (500 - 25)$$

$$= 61446.2 \frac{kJ}{hr}$$

$$Q_{out} = 160303.5 + 5971790 + 61446.2$$

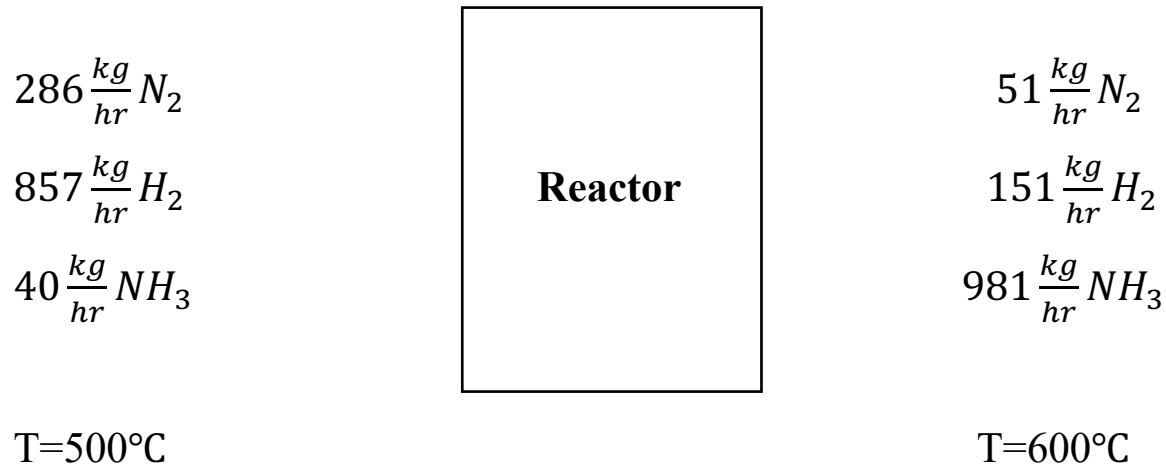
$$= 6193.5 \times 10^3 \frac{kJ}{hr}$$

$$Q_{in} + Q_{heating} = Q_{out}$$

$$Q_{heating} = 6193.5 \times 10^3 - 2917.9 \times 10^3$$

$$= 3275.6 \times 10^3 \frac{kJ}{hr}$$

3.6 Energy balance of reactor:



The reaction is $N_2 + 3H_2 \rightarrow 2NH_3$

$$Q \text{ in} = Q \text{ out} + Q \text{ reaction} + Q \text{ conversion}$$

$$Q \text{ in} = 6193.5 \times 10^3 \frac{kg}{hr}$$

Then reaction with conversion = %86

$$Q \text{ out} = \sum_{25}^{600} m \text{ out } CP_{out} \Delta T_{out}$$

At $600^\circ C$ the CP of $H_2 = 14.7 \frac{kJ}{(kg.c)}$

$$N_2 = 1.21 \frac{kJ}{(kg.c)}$$

$$NH_3 = 3.65 \frac{kJ}{(kg.c)}$$

$$QN_2 = m Cp \Delta T = 51 \times 1.21 \times (600 - 25)$$

$$= 35483.25 \frac{kJ}{hr}$$

$$QH_2 = m Cp \Delta T = 151 \times 14.7 \times (600 - 25)$$

$$= 1276327.5 \frac{kJ}{hr}$$

$$QNH_3 = m Cp \Delta T = 981 \times 3.65 \times (600 - 25)$$

$$= 2058873 \frac{kJ}{hr}$$

$$Q_{out} = 35483 + 1276327.5 + 2058873 = 3370683 \frac{kJ}{hr}$$

Q reaction

$$N_2 \text{ reacted } m = 286 - 51 = 235 \frac{kg}{hr} \text{ of } NH_3$$

$$\Delta H = -2689 \frac{kJ}{kg}$$

$$Q = m \times \Delta H = 235 \times -2689$$

$$= -637293 \frac{kJ}{hr}$$

$$Q_{in} = Q_{out} + Q_{reaction} + Q_{cool}$$

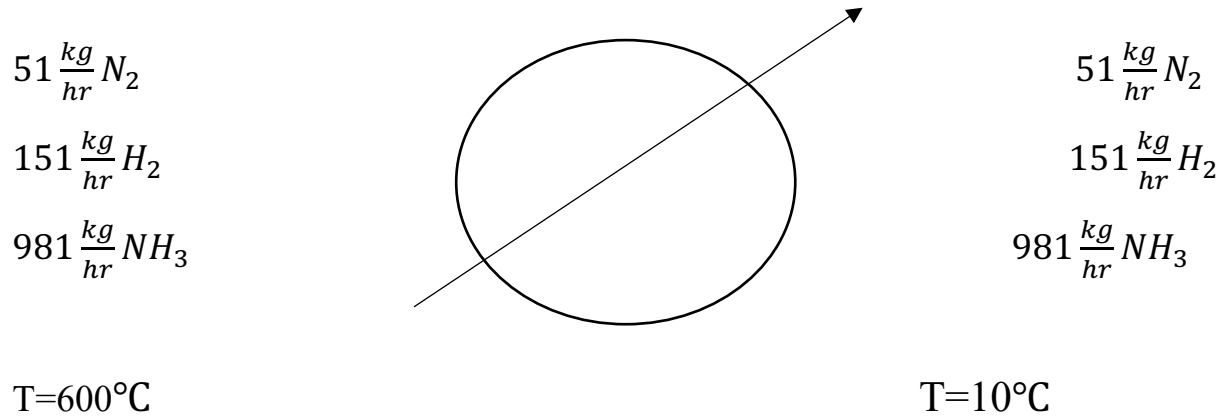
$$Q_{cool} = Q_{in} - Q_{out} - Q_{reaction}$$

$$Q_{cool} = 6193.5 \times 10^3 - 3370.7 \times 10^3 - (-637293)$$

$$Q_{cool} = 3459593 \frac{kJ}{hr}$$

$$= 3459.6 \times 10^3 \frac{kJ}{hr}$$

3.5 Energy balance on cooler:



$$Q_{in} = Q_{out} + Q_{cool}$$

$$Q_{in} = 3370.7 \times 10^3 \frac{\text{kJ}}{\text{hr}}$$

$$\text{At } 10^\circ\text{C} \text{ the CP of } \text{H}_2 = 14.25 \frac{\text{kJ}}{(\text{kg} \cdot ^\circ\text{C})}$$

$$\text{N}_2 = 1.04 \frac{\text{kJ}}{(\text{kg} \cdot ^\circ\text{C})}$$

$$\text{NH}_3 = 2.2 \frac{\text{kJ}}{(\text{kg} \cdot ^\circ\text{C})}$$

$$Q_{\text{N}_2} = m C_p \Delta T$$

$$= 51 \times 1.04 \times (25 - 10)$$

$$= 795 \frac{\text{kJ}}{\text{hr}}$$

$$Q_{\text{H}_2} = m C_p \Delta T = 151 \times 14.25 \times (25 - 10)$$

$$= 32276.25 \frac{\text{kJ}}{\text{hr}}$$

$$Q_{NH_3} = m C_p \Delta T = 981 \times 2.2 \times (25 - 10)$$

$$= 32373 \frac{kJ}{hr}$$

$$Q_{out} = 795 + 32276.25 + 32373$$

$$= 65444 \frac{kJ}{hr}$$

$$Q_{in} = Q_{out} + Q_{cool}$$

$$Q_{cool} = Q_{in} - Q_{out}$$

$$= 3370.7 \times 10^3 \frac{kJ}{hr} - 65444 \frac{kJ}{hr}$$

$$Q_{cool} = 3305.25 \times 10^3 \frac{kJ}{hr}$$

CHAPTER 4

Equipment design

Chemical Industries involve problems in process design, unit operations, equipment design and overall plant design. In design of a chemical plant these problems cannot be segregated. However, these problems may be advantageously segregated for study and development because of different principles involved in it. The course goes deeper into the various aspects of mechanical design in the chemical process plant. It stresses upon the design and analysis of the basic process equipment viz. vessels, distillation column, absorption column, heat exchanger, driers and

evaporators etc, The course emphasizes on the development of design skills to take design related decisions. Whatever be the earlier conception, today a chemical engineer is expected to be able to make complete design of a piece of chemical equipment. A number of problems will be solved to illustrate the concepts clearly.

	m. kg/h	n.kmol/hr
N ₂	285	32.549
H ₂	857	97.51

For N₂

$$m = 32.549 \frac{\text{kmol}}{\text{hr}} \bigg| \frac{\text{hr}}{3600\text{s}} = 0.00904 \frac{\text{kmol}}{\text{s}}$$

P N₂ at 500 °C

$$pv = nRT$$

$$\frac{n}{v} = \frac{p}{RT} = \frac{2740000\text{pa}}{8.314 \times 773\text{k}}$$

$$434.12 \frac{\text{mol}}{\text{m}^3} \times 28 \frac{\text{g}}{\text{mol}} = 12155 \frac{\text{g}}{\text{m}^3}$$

$$12155 \frac{\text{g}}{\text{m}^3} \times 10^3 \frac{\text{kg}}{\text{g}} = 12.155 \frac{\text{kg}}{\text{m}^3}$$

$$Qv = 286 \times \frac{\text{kg}}{\text{hr}} \times \frac{\text{hr}}{3600\text{s}} \times \frac{\text{m}^3}{12.155\text{kg}}$$

$$Qv = 0.0065 \frac{m^3}{s}$$

$$CA_0 = \frac{m}{Qv} = \frac{0.00904}{0.0065} = 1.39 \frac{mol}{l}$$

For H₂

$$m = 97.51 \frac{kmol}{hr} \times \frac{hr}{3600s} = 0.0271 \frac{kmol}{s}$$

$$\frac{m}{v} = \frac{p}{RT} = \frac{2790000pa}{8.314 \times 773k}$$

$$= 434 \frac{mol}{m^3}$$

$$p = \frac{m}{v} = 434 \frac{mol}{m^3} \times \frac{2g}{mol} \times \frac{kg}{1000g} = 0.875 \frac{kg}{m^3}$$

$$Qv = 857 \frac{kg}{hr} \times \frac{hr}{3600s} \times \frac{m^3}{0.857kg} = 0.272 \frac{m^3}{s}$$

$$CA_0 = \frac{m}{Qv} = \frac{0.0271}{0.0272} = 0.1 \frac{mol}{l}$$

K for reactor at 500°C is K= 6.7×10⁻²

The reaction is $3H_2 + N_2 \rightarrow 2NH_3$

So $-ra = k [H_2]^3[N_2]$

$$-ra = 6.7 \times 10^{-2} [0.1]^3 [1.39]$$

$$= 9.3 \times \frac{10^3 mol}{l.s}$$

Reactor conversion X = 0.86

$$v = \frac{F_0 \times X}{-ra}$$

$$F_0 = (32.549 + 97.51)$$

$$130 \frac{\text{kmol}}{\text{hr}} \times \frac{1000 \text{mol}}{\text{kmol}} = 130000 \frac{\text{mol}}{\text{hr}} \times \frac{\text{hr}}{3600 \text{s}} = 36.125 \frac{\text{mol}}{\text{s}}$$

$$v = \frac{F_0 \times X}{-ra} = \frac{36.125 \times 0.86}{9.3 \times 10^{-3}} = 3.34 \text{m}^3$$

Since we know the volume we can calculate the D and L

$$\text{We can use the volume} = \pi r^2 h + \frac{2}{3} \pi r^3$$

And also we can use the rule of thumb

$$L = 2D = 4r$$

$$v = \pi r^2 \times 4r + \frac{2}{3} \pi r^3$$

$$= 4\pi r^3 + \frac{2}{3} \pi r^3 = 3.34 \text{m}^3$$

$$r = 0.61 \text{m} \quad D = 2r = 1.22 \text{m}$$

$$L = 2D = 2 \times 1.22 = 2.44 \text{m}$$

We use ASTM A516 grade 70 , high strength carbonate steel

$$r = 0.61 \text{ m}$$

$$\text{joint efficiency} = 0.9$$

$$(\tau_c) \text{ corrosion allowance} = 2.79 \text{mm} = 2.79 \times 10^{-3} \text{m}$$

$$p = 2790 \text{kpa} \times \frac{0.145 \text{psia}}{\text{kpa}} = 404.25 \text{psia}$$

$$\text{Maximum allowable stress} = 11037 \text{ psia}$$

$$\text{thickness} = \frac{pr}{SE - 0.6p} + \tau_c$$

$$\frac{404.25 \times 0.61}{11037 - 0.6 \times 404.25} + 2.79 \times 10^{-3} = 0.0282 \text{ m} = 2.82 \text{mm}$$

$$\tau = \frac{v}{v_0} = \frac{3.3}{2.131} = 1.61 \text{hr}$$

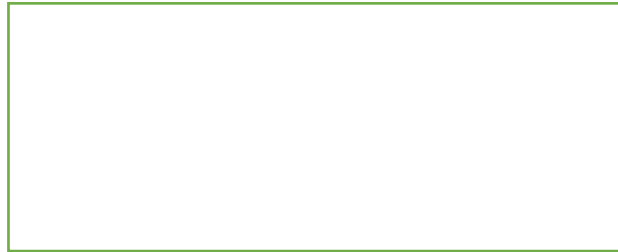
$$\text{space velocity} = \frac{1}{\tau} = 0.625 \frac{1}{h}$$

Compressor

2550 kpa

1183 kg/h

240°C



2800 kpa

260°C

We use centrifugal compressor

Specific heat ratio (γ)

$$\gamma = \frac{c_p}{c_v}$$

$$C_p \text{ for } N_2 = 1.04 \frac{kJ}{kg.k}$$

$$C_v \text{ for } N_2 = 0.743 \frac{kJ}{kg.k}$$

$$C_p \text{ for } H_2 = 14.307 \frac{kJ}{kg.k}$$

$$C_v \text{ for } H_2 = 10.181 \frac{kJ}{kg.k}$$

$$C_p \text{ for } NH_3 = 2.218 \frac{kJ}{kg.k}$$

$$C_v \text{ for } NH_3 = 1.524 \frac{kJ}{kg.k}$$

$$(\gamma) \text{ average} = 1.4$$

$$T_s = T_{\text{inlet}} = 240^\circ\text{C} = 513 \text{ K}$$

$$CR = \frac{\text{discharge pressure}}{\text{section pressure}}$$

$$CR = \frac{2800}{2550} = 1.1$$

$$m = 1183 \frac{kg}{hr} = 0.329 \frac{kg}{s}$$

$$h_1 = \frac{X}{m} = \frac{6.6 \times 10^5}{1183} = 557.9 \frac{kJ}{kg}$$

$$h_2 = \frac{7.34 \times 10^5}{1183} = 620.4 \frac{kJ}{kg}$$

$$h_{2s} = h_1 \left(v_1 \times \frac{p_2}{p_1} \right)^{\left(\left(\frac{\gamma-1}{\gamma} \right) \times \left(\frac{\gamma}{\gamma-1} \right) \right)}$$

$$V = \frac{v}{m} = \frac{M_w R T}{P} = 78.6 \frac{m^3}{kg}$$

$$\text{So } h_{2s} = 792 \frac{kJ}{kg}$$

Actual work

$$w = m(h_2 - h_1)$$

$$w = 0.329(620 - 557.9) = 63.91 kJ$$

Adiabatic work

$$w_{ad} = m(h_{2s} - h_1)$$

$$w_{ad} = 0.329(792 - 557.9) = 77 kJ$$

$$\eta_{ads} = \frac{63.91}{77} = 0.83$$

$$\eta_c = \frac{w}{w_{ads}} = 0.789$$

$$power = \frac{m \gamma T_s (CR)^{\left(\frac{\gamma-1}{\gamma}-1\right)}}{\eta_{ad} \times \eta_{yc}}$$

$$power = \frac{0.329 \times 1.4 \times 513 \times \frac{2800}{2550}^{\left(\frac{1.4-1}{1}-1\right)}}{0.729 \times 0.83}$$

$$power = 365.27 \frac{kJ}{s} = 365.27 kW$$

Heater

$$1183 \frac{kg}{hr}$$

$$260^{\circ}C$$

$$2800 \text{ kpa}$$



$$500^{\circ}C$$

$$Q_{heater} = 3308 \times 10^3$$

$$power = \frac{Q_{heater}}{m \Delta T}$$

$$m = 1183$$

$$average \text{ } CP = 1.36 \frac{kJ}{kg \cdot K}$$

$$\Delta T = 500 - 260 = 240 \text{ K}$$

$$m \cdot cp \cdot \Delta T = 3308000$$

$$m = \frac{3308000}{1.38 \times 250} = 9366 \frac{kg}{hr}$$

$$p = \frac{cp}{m \cdot \Delta T} = \frac{3308000}{9366.9 \times 240} = 140.3 \text{ kW}$$

Finding surface area

$$A = \frac{Q}{h \times \Delta T}$$

h = heat transfer coefficient

we selected silicon carbide (SiC) for the tube

$$h \text{ for (SiC) is } 179 \frac{W}{m^2 \cdot K}$$

$$A = \frac{1919.44 \times 10^3}{179 \times 250} = 18.6 \text{ m}^2$$

$$A = 2\pi r^2 + 2\pi rL$$

$$L = 20r$$

$$A = 2\pi r^2 + 40\pi r^2$$

$$42\pi r^2 = 16.6 \text{ m}^2$$

$$r = 0.369 \text{ m}$$

$$L = 7.38 \text{ m}$$

Electrical power of heater

We have $Q = 919.44 \text{ kw}$

And for (SiC) η heater element efficiency = 0.85

$$\text{so } p = \frac{Q}{\eta} = \frac{919.44}{0.85} = 1081.7 \text{ kw}$$

Electrical resistance

$$R = \frac{p}{\frac{L}{A}}$$

$$p \text{ for (SiC) } = 2.2 \times 10^{-3} \frac{\text{ohm}}{\text{m}}$$

$$R = 5 \times 10^{-2} \text{ ohm}$$

CHAPTER 5

Economy

Economy and installation cost

This chapter will provide the economic analysis of the adipic acid synthesis chemical process. The primary purpose of economic analysis is to determine the profitability of a process,

This will determine the method is economically profitable or not. Costing and project evaluation: To choose between different designs and evaluate projects, the design engineer must be able to create quick, rough cost estimates.

Chemical plants are developed to earn a profit, so an estimate of the required investment and the cost of output is required before a project's viability can be determined. This chapter will go through the economics of the adipic acid production chemical process,

the primary purpose of economic analysis is to determine the profitability of a process, which will determine whether or not the method is economically viable.

Capital Cost Estimates: Accuracy and Purpose The amount of design detail available determines the accuracy of an estimate.

The time spent preparing the estimate and the accuracy of the cost data provided

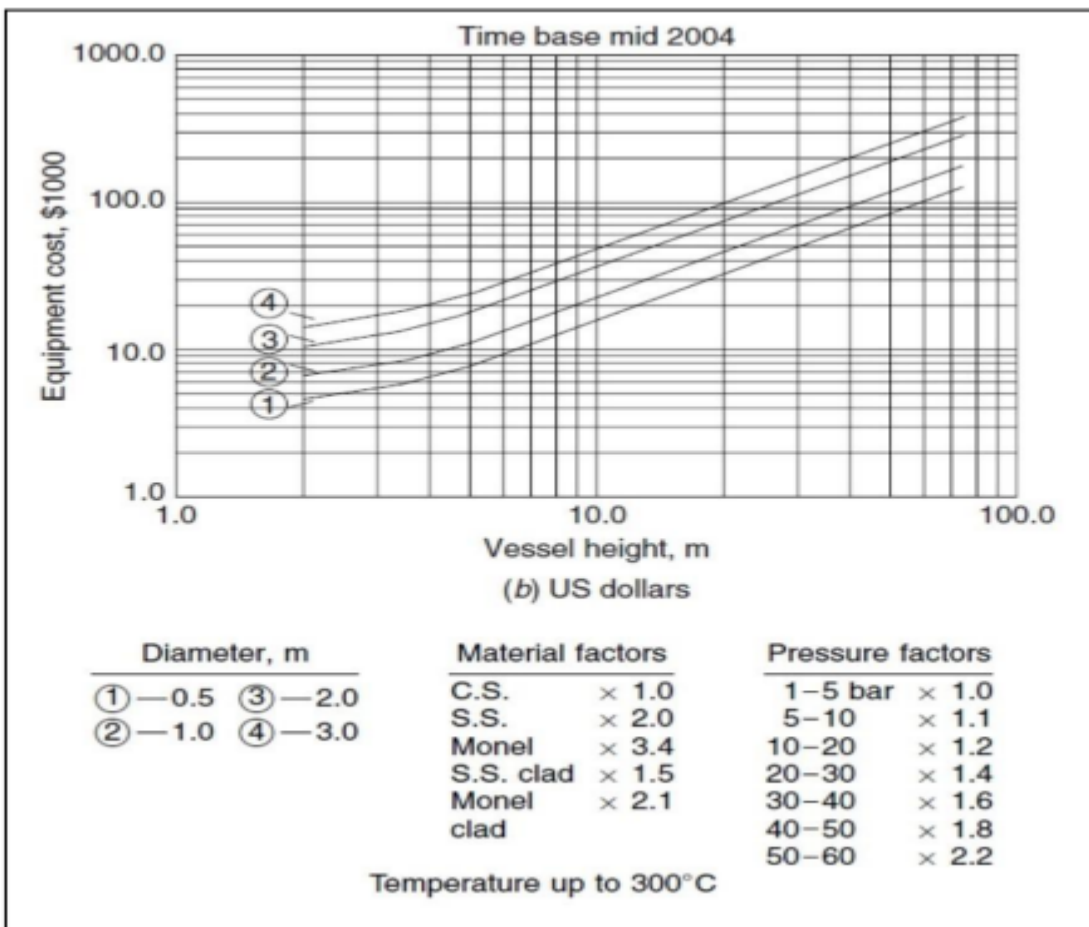


Figure: Vertical Pressure Vessels. Time Base Mid-2004

Purchased Cost = (Bare Cost of the Figure) × Material Factor × Pressure Factor

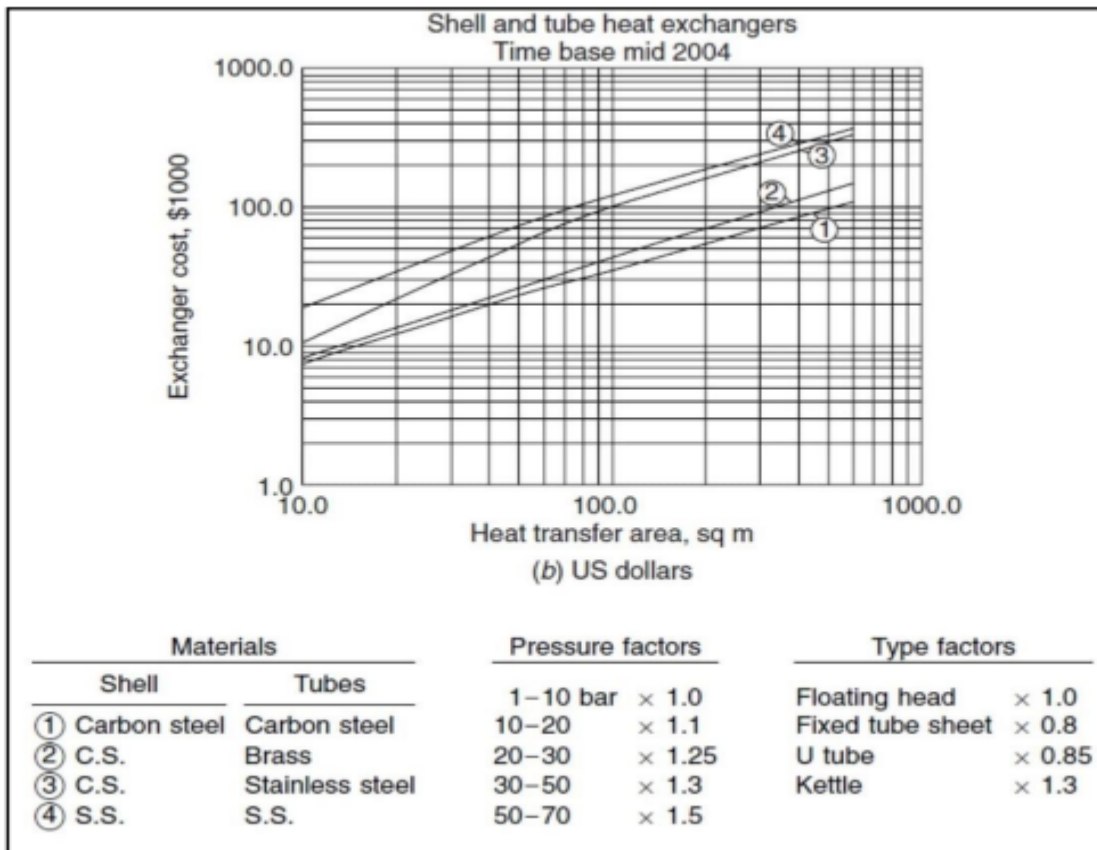


Figure: Shell and tube heat exchangers. Time base mid-2004

Purchased cost = (bare cost of the figure) × Type factor × Pressure factor

5.2 Cost of Reactor:

H = 2.44m D = 1.22 m Material used = stainless steel P = 27.9 bar

Vertical Column, Cost from Figure 5-2

Purchased cost = bare cost of the figure × Material factor × Pressure factor

Purchased cost = 5000 × 1 × 1.4

Purchased cost = 7000\$ (Time base mid 2004)

Total cost = 7000 × 1.45

Total cost = 10150\$ (Cost in year 2023)

5.3 Cost of Condenser

Area heat transfer = 4.3 m^2

Carbon steel shell and tube

Pressure= 26.9bar

Fixed tube sheet

From Figure 5-1 Exchanger

Cost= $2 \times 1000\$ = 2000\$$

Pressure factor= 1.25

Type factor=0.8

Purchased cost = (bare cost of the figure) \times Type factor \times Pressure factor

Total cost of exchanger = $2000 \times 1.25 \times 0.8 = 200\$$ (cost in 2004)

Total cost of exchanger = $1.45 \times 2000 = 2900\$$ (cost in 2023)

Equipment	Unit Cost	NO.Unit	Total Cost
Compressor	2500\$	1	2500\$
Heater	5500\$	1	5500\$
Reactor	10150\$	1	10150\$
Cooler	2900\$	1	2900\$
Separator	1100\$	1	1100\$

Total Equipment cost =23000\$

Direct cost

a-Installation cost = (20-30% of TEC) Assume 25%

Installation cost = $25\% \times 23000 = 5750\$$

b-Piping installation Cost =(6-30 of TEC)Assume 25%

Piping installation Cost = $23000 \times 10\% = 5750\$$

c-Electrical installation cost = (10-40% of TEC) assume 30%

Electrical installation cost= $23000 \times 30\% = 6900\$$

d-Service facilities: (30-80% of TEC) Assume 35%

Service facilities= $23000 \times 35\% = 8050\$$

e-Yard improvement: (10-15% of TEC) Assume 12%

Yard improvement= $23000 \times 12\% = 2760\$$

f-Land improvement: (4-8% of TEC) Assume 5%

Land= $23000 \times 5\% = 1150\$$

Total Direct Cost = $30000\$$

Indirect cost

a-Engineering and supervision=15% of Direct Cost

Engineering and supervision= $15\% \times 21000 = 3150\$$

b-Constriction fee:(2-7% of DC) 5%

Contraction fee= $5\% \times 2100 = 1050\$$

Total indirect cost = $1050 + 3150 = 4200\$$

Fixed Capital Investment

Fixed Capital Investment=(DC+IC)= 34000

Total capital Investment

a-Local taxes:((2-8% of FCI) assume 5%

Local taxes = $0.05 \times 34000 = 1700\$$

b-Insurance:(0.4-5% of FCI) assume 4%

Insurance = $4\% \times 34000 = 1360\$$

Total Capital investment = $3000\$$

Direct production

Raw material:(5-10% of TEC) assume 10%

Raw material = $10\% \times 23000 = 2300\$$

Maintenance:2-10% of TEC assume 5%

Maintenance = $5\% \times 23000 = 1150\$$

Operating labor : (10-20 % of TEC) assume 10%

Operating labor = $10\% \times 23000 = 2300\$$

Laboratory charges :(92-5% of TEC) assume 3%

Laboratory charges = $3\% \times 23000 = 690\$$

Total Direct production = 6300\$

Other unmentioned costs = 100000\$

Investment

Total income = produce day rate *number production day in year *price per unit

Ammonia production = $952\text{kg/hr} \times 24\text{hr/day} = 22848\text{kg/day}$

Total income = $22848\text{kg/day} \times 300\text{day} \times 1\$ = 6854400\$$

Total invest for first year = income -total costs = 4750000\$

Chapter 6

Safety

What are the potential health effects of ammonia?

Main Routes of Exposure: Inhalation. Skin contact. Eye contact.

Inhalation	VERY TOXIC, can cause death. Can cause severe irritation of the nose and throat. Can cause life-threatening accumulation of fluid in the lungs (pulmonary edema). Symptoms may include coughing, shortness of breath, difficult breathing and tightness in the chest. Symptoms may develop hours after exposure and are made worse by physical effort. Long-term damage may result from a severe short-term exposure.
Skin Contact	CORROSIVE. The gas irritates or burns the skin. Permanent scarring can result. Direct contact with the liquefied gas can chill or freeze the skin (frostbite). Symptoms of more severe frostbite include a burning sensation and stiffness. The skin may become waxy white or yellow. Blistering, tissue death and infection may develop in severe cases.
Eye Contact	CORROSIVE. The gas irritates or burns the eyes. Permanent damage including blindness can result. Direct contact with the liquefied gas can freeze the eye. Permanent eye damage or blindness can result.
Ingestion	Not a relevant route of exposure (gas).
Effects of Long-Term (Chronic) Exposure	May harm the respiratory system. Can irritate and inflame the airways.

FIREFIGHTING MEASURES

EXTINGUISHING MEDIA

-Water spray or fog. - Foam.

FIRE FIGHTING

- Alert Emergency Responders and tell them location and nature of hazard.
- Wear breathing apparatus plus protective gloves.

GENERAL FIRE HAZARDS/COMBUSTIBLE PRODUCTS: Combustible

solid which burns but propagates flame with difficulty.

Avoid generating dust, particularly clouds of dust in a confined or unventilated space as dusts may form an explosive mixture with air, and any source of ignition, i.e. flame or spark, will cause fire or explosion. Dust clouds generated by the fine grinding of the solid are a particular hazard; accumulations of fine dust may burn rapidly and fiercely if ignited, combustion products include: carbon monoxide, carbon dioxide, other pyrolysis products typical of burning organic material, May emit poisonous fumes, may emit corrosive fumes.

FIRE INCOMPATIBILITY: Avoid contamination with oxidizing agents i.e. nitrates, oxidizing acids, chlorine bleaches, pool chlorine as ignition may result.

PERSONAL PROTECTION: Glasses, Safety Glasses, Chemical goggles, Gloves (dependent on usage), Respirator, Particulate.

ACCIDENTAL RELEASE MEASURES

▪ **MINOR SPILLS:** Remove all ignition sources, Clean up all spills immediately, Avoid contact with skin and eyes, Control personal contact by using protective equipment, Use dry clean up procedures and avoid

generating dust, Place in a suitable, labelled container for waste disposal.

- **MAJOR SPILLS:** Moderate hazard, caution: Advise personnel in area, Alert Emergency Responders and tell them location and nature of hazard.

HANDLING AND STORAGE

- **PROCEDURE FOR HANDLING:** Avoid all personal contact including inhalation, Wear protective clothing when risk of exposure occurs, and Empty containers may contain residual dust which has the potential to accumulate following settling. Such dusts may explode in the presence of an appropriate ignition source, do not cut, drill, grind or weld such containers. In addition ensure such activity is not performed near full, partially empty or empty containers without appropriate workplace safety authorization or permit.

- **RECOMMENDED STORAGE METHODS:** Glass container, Polyethylene or polypropylene container, Check containers are clearly labeled and free from leaks.

- **STORAGE REQUIREMENTS:** adipic acid is stable, non-toxic, and not easy to deliquesce, be careful of water-proof, rain-proof when transportation. When the content is higher than 14%, it is easy to have static to cause fire, store in original containers and keep containers securely sealed.

Health hazard

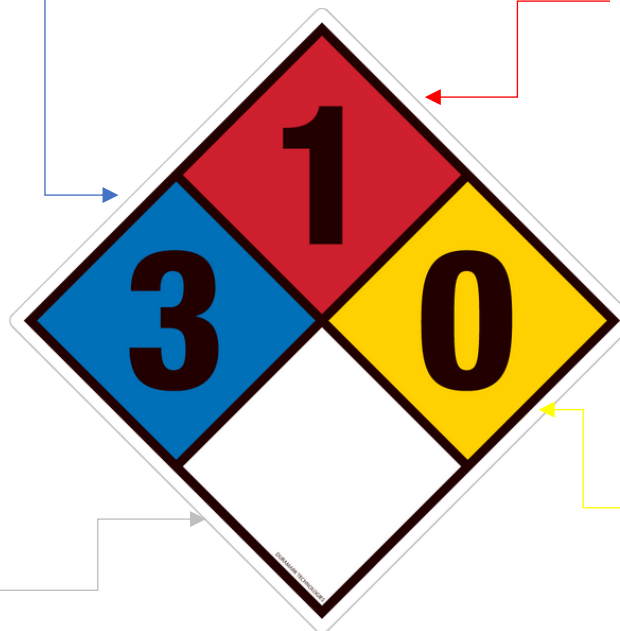
4 deadly
3 extreme danger
2 hazardous
1 slightly hazardous
0 normal material

Fire hazard flash point

4 below 73 F
3 below 100 F
2 below 200 F
1 above 200 F
0 will not burn

Specific hazard

OX oxidizer
ALK alkaline
W use no water
SA simple asphyxiate
ACID acid
COR corrosive




Instability

4 may detonate
3 stock + may detonate
2 violent chemical change
1 unstable if heated
0 stable



Hazard symbol meaning : physical , chemical and environmental hazard:

GHS pictogram	Danger
	Explosive substances or mixtures and article containing explosive
	Flammable gases, aerosols, liquid and/or solids ; self reactive substances and mixtures; pyrophoric liquids and /or solids; substances and mixtures capable of self heating; substances and mixtures which, in contact with water, emit flammable gases; organic peroxides
	Oxidizing gases, liquids and/or solids
	Gases under pressure; compressed, liquefied, dissolved and/or cryogenic liquefied gas
	Corrosive; corrosive to metals
	Acutely hazardous to the aquatic environment; chronically hazardous to the aquatic environment; harmful to the ozone layer

3.6 Conclusion:

3.6.1 Why did we choose Haber-Bosch process?

We chose this process because it was starting of developing the modern ammonia plant and also it is typical ammonia production flow sheet.

In this process we get a good amount of ammonia with better conversion than the other ancient ammonia plants with less economy cost and high-quality ammonia also with less pollution to environment.

The Haber-Bosch process is extremely important because it was the first of processes developed that allowed people to mass-produce plant fertilizers due to the production of ammonia. It was also one of the first industrial processes developed to use high pressure to create a chemical reaction

In our project the results **supported by aspen hysys**

an ammonia production plant is a complex and significant industrial facility that plays a crucial role in meeting the global demand for ammonia, a key ingredient in various industries such as agriculture, chemical manufacturing, and energy production. The production of ammonia involves a multi-step process that requires careful design, engineering, and operational considerations.

Ammonia production plants employ advanced technologies and processes to ensure efficient and sustainable production. The plant typically includes units such as reforming, synthesis, purification, and compression, which work together to convert feedstock, such as natural gas or nitrogen, into ammonia through the Haber-Bosch process.

The design and operation of an ammonia production plant require a comprehensive understanding of chemical engineering principles, process optimization, safety protocols, and environmental considerations. Factors such as feedstock selection, reaction kinetics, temperature, pressure, catalysts, and energy efficiency are carefully optimized to maximize production while minimizing costs and environmental impact.

Safety is of utmost importance in an ammonia production plant due to the hazardous nature of ammonia, which requires strict adherence to safety protocols, risk assessment, and robust safety systems to protect both the workers and the surrounding environment.

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