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Original Research Article

Design of a Four Bed Reactor Converter for Ammonia Synthesis

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Abstract: Ammonia is widely used for production of many chemicals such as urea, and also as refrigerant in industrial systems. Ammonia is produced via the Haber process, in which nitrogen reacts with hydrogen in the presence of iron catalyst. The hydrogen is form by reacting natural gas and steam at high temperature. Ammonia synthesis is a reversible, thus temperature gradient occurs as the reaction progresses. The inlet temperature is usually high. To achieve this progressive temperature reduction a suitable packed bed reactor is required. A good configuration of a packed bed would help in reducing the complexities in the heat transfer equipment while ensuring a progressive reduction in temperature from the first to the fourth bed. Subsequently there is a decrease in the composition of hydrogen and nitrogen from bed to bed and a corresponding increase in ammonia conversion. This forms the bases of this design. To actualize the design, inlet operating conditions for the reactor were assumed to be $15m^3$/sec flow rate, pressure of 2.896×10^7Pa and temperature of 720k the diameter was calculated to be 1.5m. A gas velocity of 0.439m/s, reactor height 5.23m, mass of catalyst =14178.5kg, and volume of reactor zone/catalyst $=4.051m^3$ were obtained.

Keywords: Haber process, Ammonia, synthesis, Reactor design.

1. INTRODUCTION

It is estimated that about 150 million tons of ammonia is produced annual with yearly proposed increase of 2.3 tons (Ahmed, *et al.*, 2024). Ammonia is very essential in the agricultural sub-sector. On the global perspectives, it is estimated that 50% food production depends heavily on availability of ammonia and as the world population continued to increase exponential it is imperative to harness efficient method for the production of ammonia which would reduce environmental impact (carbon emission).

Ammonia synthesis is very crucial for developing countries like Nigeria where agriculture has long been a cornerstone of Nigeria's economy, providing livelihoods for millions of people and contributing significantly to the nation's GDP. According to (ACTIONAID NIGERIA, 2023), in the first quarter (Q1) of 2023, agriculture accounted for about 19.5% of GDP, compared to trade (15.97%), telecommunication and information service (14.13%), oil and gas (6.21%), food, beverage and tobacco (5.31%), and trade (15.97%).

Ammonia is produced via a process known as Haber process, in which nitrogen from the air react with hydrogen in the presence of iron catalyst to form ammonia. The hydrogen used for the process is form by reacting natural gas and steam at high temperature.

Ammonia (NH_3) is very important chemical; it is widely used as industrial feedstock for production of many chemicals such as fertilizer, urea and also as refrigerant in industrial systems. In addition, a great number of nitrogen compounds such as; pharmaceuticals products, nitric acid, explosives, polymers and coolants can be produced from ammonia (Suhan, *et al.*, 2023).

As earlier said, ammonia synthesis is regarded as the core of the fertilizer plant where ammonia synthesis reactor is the primary component of this section. Therefore, optimum production of urea greatly, depends on the effective method of ammonia production. It is produced following the Haber-Bosch process by the reaction between gaseous nitrogen (collected from air) and hydrogen (from natural gas) combined in the ratio of 1:3 respectively. Amongst these two raw materials, hydrogen has the highest cost implication on the entire production process (Panahandeh *et al.,* 2003; Gunorubon and Raphael, 2014; Almallahi, *et al.,* 2023). This is due to the source in which it is been generated from (Natural gas).

A conventional ammonia production process consists of production of the synthesis gas, compression of the gas to the required pressure and synthesis loop of ammonia conversion in a reactor (Baddour et al., 1965 as cited in Suhan *et al.,* 2023). The reaction is highly exothermic (Khademi and Sabbaghi, 2017).

Several methods have been adopted to enhance ammonia production, aside from generating the hydrogen from natural gas source which created serious environmental problem. These methods include electrochemical synthesis, photochemical ammonia synthesis and electrolysis of water to generate green hydrogen, although these processes are still under development, the need of these methods arises in order to achieve zero emission of carbon during ammonia production (Katie, 2022).

Several reactors are in used for ammonia production, it include continuous stirrer tank reactor, fluidize bed reactor, fixed bed reactor etc. these reactors are complemented by other unit operation equipment like separators, heat exchangers, pumps etc. the focus of this work is to design FIXED bed reactor with four chambers which is capable of enhancing ammonia production. FIXED bed reactor has the merit of good catalyst distribution, better temperature control during reaction, efficient mixing and longer catalyst lifespan. With these unique characteristics a FIXED bed with four chambers has the potential of given high yield of ammonia (Suleiman *et al.,* 2013).

According to Coulson and Richardson's Chemical Engineering Design, (Coulson, *et al.,* 2005) the methodology of the design is initiated by a specific objective in mind. Consequently, the objective of this article is to improve the scholarly understanding of ammonia synthesis by undertaking a simple academic design of a four bed reactor for ammonia production. A step-by-step full computation, along with their respective results are included to give the scholars a full comprehension of the design process. Consequently, this study is solely focused on the reactor design aspect of the ammonia synthesis process. Gas velocity reactor height 5.23m, catalyst height and mass were calculated based on data from literature.

2. The Chemical Engineering Design of the Ammonia Reactor

The process involves the use of a continuous process, as it is a lot more appropriate when a high scale productions is required, with a lower production cost (Suhan, *et al.,* 2023). According to (Coulson, *et al.,* 2005), the lower flexibility of the reactor is not as much needed to raise issue for this reactor design. The reaction is heterogeneous exothermic as the ammonia homogenous reaction is too ineffective (Levenspiel, 1999). A fixed bed reactors is chosen in placed of a fluidized reactor mainly because of; its Widespread application, lower operating costs, greater control over product quality, Improved temperature control (Abbas and G, 2015), absence of severe fouling, Good catalyst life, and Proven processes design. Figure 2 shows a schematic diagram of a 4 bed ammonia reactor converter.

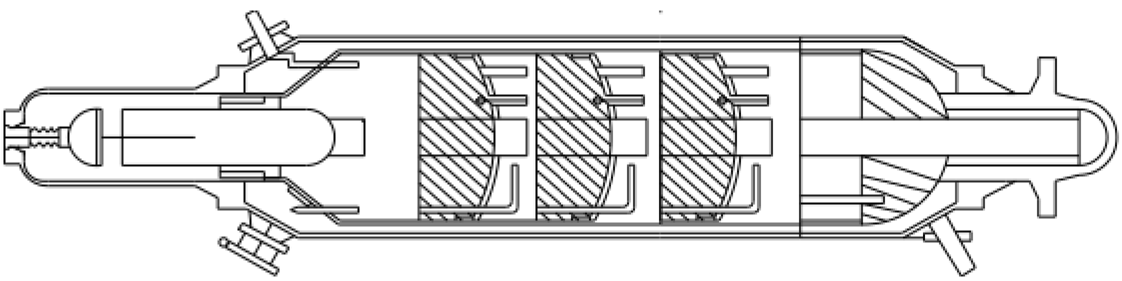

Figure 1: Typical four Bed Ammonia Reactor Converter

1. Design Algorithm

a) Select the mole percentage of feedstock composition into the inlet of the converter.
b) Calculate the composition of each feedstock component in each individual beds together with the total volume of feedstock component in each bed
c) Obtain the volumetric flow rate of each component in each individual bed
d) Compute the fractional conversion in each bed
e) Determine the mole fraction of NH_3, N_2 and H_2 for each bed
f) Obtain the partial pressure of each components in their respective beds
g) Evaluate the volume of the reactor
h) Compute the mass of catalyst in each bed
i) Calculate the cross sectional area occupied by each catalyst

j) Obtain the height of the reactor
k) Compute the gas velocity in the reactor

2.1 Mathematical Design Development

The following assumptions have been made for this design.

A. The model is one-dimensional, with temperature and molar gradients varying only axially.
B. The compartments of the discretized reactor volume are well mixed.
C. The system contains no heat or mass diffusion.
D. Individual gases and gas mixtures exhibit ideal gas behavior.
E. The activity of the catalyst is consistent throughout the reactor.
F. The coefficient of heat transfer, the heat of reaction, and the heat capacities are constants. (Glemmestad, *et al.*, 2018).
G. The reactor's pressure is precisely controlled.
H. The reactor arrives to steady state at 720K

Inlet Operating Conditions

1. Temperature = 720K
2. Pressure = 2.898×10^7Pa
3. Volumetric flow rate of the gas mixture = 20m^3/sec
4. Flow rate = 15m^3/sec
5. Number of moles of the gas mixture = 15kmoles
   But 1kmole of any gas at S.T.P occupies 22.4m^3
   :. 15kmol of a gas at S.T.P occupies 15 * 22.4 = 336m^3

3. COMPUTATIONS AND RESULTS

3.1. Material balance

Data: The reactor consist of 4 catalytic beds i.e. N = 4

Table 3.1 gives the feedstock composition (Model %).

Table 3.1: Feedstock composition (Mole and volume %)

Compound	Mole %	% by volume
N_2	21.75	21.75m^2
H_2	65.25	65.25m^3
NH_3	5.0	5.0m^3
CH_4	4.00	4.00m_3
A_r	4.00	4.00m_3

Note: that the outlet from each bed becomes the inlet of the next bed

Total volume of feedstock charge into the reactor

:. Volume of $H_2 + N_2$ = 100-(CH_4+ A_r + NH_3)
= mole ratio of $H_2 : N_2$
= 3: 1

Sum of mole $H_2 + N_2$ = 4

:. % of Nitrogen by volume = $\frac{1}{4}$ * 100-(CH_4+ A_r + NH_3)

Table 3.2 below gives the volume of Ammonia produced from the individual beds.

Table 3.2: Below gives the volume of Ammonia produced from the individual beds

Compound	Bed 1	Bed II	Bed III	Bed IV
Volume of Ammonia produced (m^3)	10.0m^3	13.0m^3	16.0m^3	19.0m^3

3.2 Composition of the components in the individual beds

Outlet stream of bed I

Initial volume of Ammonia into the reactor = 5m^3

Volume of NH_3 in the outlet stream of bed 1 has increased by; (10-5) m^3 = 5m^3 from the stoichiometric equation, the subsequent decrease in the values of N_2 and $3H_2$ can be calculated.

$N_2 + 3H_2 \rightleftharpoons 2NH_3$
2.5 7.5 5
Volume of CH_4 = $4m^3$
Volume of A_r = $4m^3$
Volume of N_2 at the outlet stream of bed 1 = 21.75-2.5
= $19.25m^3$
Volume of H_2 at the outlet stream of bed 1 = 65.25-7.5
= $57.75m^3$

Total volume of discharge from bed 1 = (10 + 4 + 4 + 4 + 19.25 + 57.75) m^3 = $95m^3$

The above computational steps (for bed I) are used to calculated the volume of discharge from bed 1-4.

The material balance containing the volume flow rate (m^3sec), Volume (m^3), vol. % is equally calculated from and presented in table 3.3.

Table 3.3: The Material Balance

Bed/Shelves Number(n)	stream	Components	Volume flow rate (m^3sec)	Volume (m^3)	Vol. %
ONE	INLET	CH_4	0.6	4.00	4
		A_{Rs}	0.6	4.00	4
		NH_3	0.75	5.00	5
		N_2	3.3625	21.75	21.75
		H_2	9.7875	65.25	65.25
		TOTAL (∑)	**15.00**	**100.00**	**100.00**
ONE	OUTLET	CH_4	0.63158	4.00	4.2106
		A_R	0.63158	4.00	4.2106
		NH_3	1.57895	10.00	10.526
		N_2	3.0395	19.25	20.26
		H_2	9.11842	57.75	60.789
		TOTAL (∑)	**15.00**	**95.00**	**100.00**
TWO	OUTLET	CH_4	0.652	4.00	4.348
		A_R	0.652	4.00	4.348
		NH_3	2.12	13.00	14.1304
		N_2	2.89	17.75	19.29347
		H_2	8.68	53.25	57.88
		TOTAL (∑)	**15.00**	**92.00**	**100.00**
THREE	OUTLET	CH_4	0.674	4.00	4.494
		A_R	0.674	4.00	4.494
		NH_3	2.696	16.00	17.977
		N_2	2.739	16.25	18.2584
		H_2	8.216	48.75	54.775
		TOTAL (∑)	**15.00**	**89.00**	**100.00**
FOUR	OUTLET	CH_4	0.6976	4.00	4.651
		A_R	0.6976	4.00	4.651
		NH_3	3.3140	19.00	22.093
		N_2	2.572	14.75	17. 151
		H_2	7.718	44.25	51.45
		TOTAL (∑)	**15.00**	**86.00**	**100.00**

3.3. Calculation of the Mole Fraction, Partial Pressure and Fractional Conversion of Each Bed

Calculation of the Mole Fraction in Each Bed

Given the stoichiometric equation

$N_2 + 3H_2 \rightleftharpoons 2NH_3$

Since X_1 =Volume of component i that have reacted it follows the volume of component i that is remaining is given by $1-X_i$

Similarly,
The volume of N_2 reaming is given by $1 - X_A$
Where X_A = Fractional conversion of N_2

In accordance with Avogadro's law the volumes of the various reactants can be converted to relative number of moles

:. $1 - X_A$ represents the number of moles of Nitrogen

:. $N_2 + 3H_2 \rightleftharpoons 2NH_3$

$1 - X_A \quad 3(1 - X_A) \qquad 2(X_A)$

The above stoichiometric equation is in accordance with GAY LUSSAC's Law which states that when gases react, they do so in volumes which are in simple ratios with one another and to the volumes of the products if gaseous provided that the temperature and pressure remain constant. The total number of moles is given by;

$(1 - X_A) + 3(1 - X_A) + 2(X_A)$

$1 - X_A + 3 - 3X_A + 2X_A$

$1 - X_A + 3 - 3X_A + 2X_A$

Total no of moles = $4 - 2X_A$

3.4 Calculation of the Partial Pressure in Each Bed

Total Pressure	=	286Psia
Total Pressure in paschal	=	2.898×10^7Pa
But partial pressure	=	$P_l = Y_l P$
Where P	=	total pressure in the reactor
P_l	=	partial pressure of the various components in each bed
Y_l	=	mole fraction of the various components

3.5 Calculation of the Fractional Conversion in each bed

The fractional conversion X_A of a given reactant A can be defined as the fraction of reactant converted into product as

$X_A = \frac{N_{AO} - N_A}{N_{AO}}$

Where

N_{AO} = Initial volume of reactant A

N_A = Final volume of reactant A

Similarly, let

N_{AO} = Final volume obtained from the various outlet beds

$X_A = \frac{1 - N_A}{N_{AO}}$

The length of a reaction is determined by the limiting reagent in the reaction. In the synthesis of Ammonia, the limiting reagent is Nitrogen since the initial volume of Nitrogen charged into the reactor is $21.75m^3$ as compared to $65.25m^3$ of Hydrogen it is the limiting reagent.

:. N_{AO} = Initial volume of Nitrogen = $21.75m^3$

N_A = Volume obtained from the various outlets

3.6. Calculation of the Equilibrium Composition

To calculate the equilibrium composition of Ammonia we must calculate the equilibrium constant K_p for Ammonia

For what we make use of the formula

$\text{Log}(kp)^{1/2} = \frac{2078.8}{T} + 2.4943\log T + \beta_T - 1.8564 * 10^{-7}{}_{T2} + 1$ 1

Where

T = Temperature =720k

β = a constant = $1.256 * 10^{-4}$

I = -2.206

$Kp = \frac{P_{NH3}}{P_{H2}^{3/2} \times P_{N2}^{1/2}}$ 2

Where,

P_{NH3} = Partial pressure of NH_3

P_{H2} = Partial pressure of H_2

P_{N2} = Partial pressure of N_2

$P_{NH3} = \frac{X_e}{100} P$ 3

Where,

$\frac{X_e}{100}$ = ratio of composition of NH_3 at equilibrium

$\frac{1 - X_e}{100}$ = composition of N_2 and H_2

P = total pressure of the reactor

Using the stoichiometric equation

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

$$\frac{1}{4}\left(1-\frac{X_e}{100}\right)+\frac{3}{4}\left(1-\frac{X_e}{100}\right)=\frac{X_e}{100}\,4$$

Ratio of Nitrogen at equilibrium = $\frac{1}{4}\left(1-\frac{X_e}{100}\right)$

Ratio of Hydrogen at equilibrium = $\frac{3}{4}\left(1-\frac{X_e}{100}\right)$

∴ $P_{N2} = \frac{1}{4}\left(1-\frac{X_e}{100}\right)P$

$P_{N2} = \frac{3}{4}\left(1-\frac{X_e}{100}\right)P$

$P_{NH3} = \frac{X_e}{100}P$

$$1.0750 \text{ X } 10^4 \frac{\frac{X_e}{100}P}{\left[\frac{1}{4}\left[\frac{1-X_e}{100}\right]^{1/2}p\right]\left[\frac{3}{4}\left[\frac{1-X_e}{100}\right]^{3/2}P\right]} \quad 5$$

3.7. Reactor Sizing

3.7.1. Calculation of the Volume of the Reactor

To calculate the volume of the reactor we recall

$$\frac{V}{F_o}=\frac{\tau}{C_{Ao}} \quad 6$$

Where F_o = the feed rate

C_{Ao} = the initial concentration

But $\frac{C_{Ao}}{F_o}=\frac{1}{V_o}$: $\tau=\frac{V}{V_o}=C_{Ao}\int_o^{XAF}\frac{dx_A}{R}$ 7

But $R_A=\frac{dP_{NH3}}{d\tau}=\left\{K_1P_{N2}\left[\frac{P_{H2}^3}{P_{NH3}^2}\right]^{\alpha}-K_2\left[\frac{P_{HN3}^2}{P_{H2}^3}\right]^{1-\alpha}\right\}$ 8

Given that α = 0.5, β = 0.8,

R_A = $(K_1P_{N2})^{0.8}\frac{P_{H2}^{1.2}}{P_{HN3}}-(K_2)^{0.8}\frac{P_{NH3}^{0.8}}{P_{HN3}}$

R_A = $\left[\frac{K_1P_{N2}}{K_2}\right]^{0.8}\frac{P_{H2}{}^{1.2}}{P_{HN3}{}^{0.8}}-\frac{P_{NH3}{}^{0.8}}{P_{H2}{}^{1.2}}$

Where,

k_1 and k_2, based upon the Gibbs free energy approach, are:

$K_1=K_{o,1}\,\mathcal{E}^{--}\frac{E_1}{R_{cat}T_{28}}$ (Levenspiel, 1999)

$K_2=K_{o,2}\,\mathcal{E}^{-}\frac{E_2}{R_{cat}T_{28}}$ (Levenspiel, 1999)

t $\frac{K_1}{K_2}$ = Kp, Gillespie and Beattie (1930)

Therefore,

R_A = $(K_pP_{N2})^{0.8}\frac{P_{H2}{}^{1.2}}{P_{NH3}{}^{0.8}}-\frac{P_{NH3}{}^{0.8}}{P_{H2}{}^{1.2}}$

K_1 = $3.455 \text{ X } 10^{19}\frac{1}{T}\beta e^{-e/RT}$ 9

Where

Temperature of the reactor = 720k

Activation energy E = 170kj/gmol

β = 0.8,

R = 8.314kJ/k; by substitution

K_1 = $3.485 * 10^{19}\frac{1}{720}\,0.8^{\,e-\frac{170}{8}-314*720}$

K_1 = $3.485 * 10^{19}\frac{1}{720}\,0.8^{\,e-\frac{170}{8}-314*720}$

K_1 = $0.004840 * 10^{19}\,0.8^{\,e-0.02839}$

= $0.004840 * 10^{19} * 0.97200920$

= $3.763 * 10^{16}$

K_1 = $3.763 * 10^{16}$

$\frac{K_1}{K_2} = K_p : K_2 = \frac{K_1}{K_p}$

$R_A = (K_p P_{N2})^{0.8} \frac{P_{H2}^{1.2}}{P_{NH3}^{0.8}} - \frac{P_{NH3}^{0.8}}{P_{H2}^{1.2}}$

$\tau = \frac{V}{V_o} C_{NH30} \int_{XA1}^{XA1} \left[\frac{1}{(K_p P_{N2})^{0.8} \frac{P_{H2}^{0.8}}{P_{NH3}^{1.2}}} \right] dX_A$ 10

$\tau = \frac{V}{V_o} = C_{Ao} \int_{XA1}^{XAN} \frac{P_{H2}^{1.2} P_{NH3}^{0.8}}{(K_p P_{N2})^{0.8}} \frac{dX_{An}}{P_{H2}^{1.44} - P_{NH3}^{0.64}}$ 11

$P_{NH3} = P_{NH30}^{0.8} (1 - X_A)^{0.8} dX_A \frac{P_{H2}^{1.2}}{(K_p - P_{N2})^{0.8}}$ 12

$\tau = \frac{V}{V_o} C_{NH30} \int_{XA1}^{XA1} \frac{P_{NH30}^{0.8} (1-X_A)^{0.8} dX_A}{P_{N2}^{1.44} - P_{NH30}^{0.64} (1-X_A)^{0.64}} \frac{P_{H2}^{1.2}}{(K_P - P_{N2})^{0.8}}$ 13

$\frac{P_{NH30}^{0.8} (1-X_A)^{0.8}}{P_{N2}^{1.44} - P_{NH30}^{0.64} (1-X_A)^{0.64}} = D$ 14

$\tau = \frac{V}{V_o} \frac{P_{H2}^{1.2} C_{NH30}}{(K_p - P_{N2})^{0.8}} \int_{XA1}^{XAN} DdX_A$ 15

The integral $\int_{XA1}^{XAN} DdX_A$ can be evaluated in any one of the three ways; graphically, numerically, or analytically. For this design, trapezoid rule is applied. (Stroud, 2003).

$\int_{XA1}^{XAN} DdX_A \approx \frac{h}{2} [y_0 + 2y_{A1} + 2y_{A2} \dots\dots\dots.. 2y_{n-1} + y_n$ 16

Where,

n is the number of strips

$y_n = f(x_n)$ are the values of $f(x_n)$ at the points x_i where i = 0, 1, 2. . . n.

Note that $x_0 = a$ $x_n = b$

h is the width of each strip and $h = \frac{b-a}{n}$

$x_1 = a + h$, $x_2 = a + 2h$, $x_3 = a + 3h$, and…. so on.

$\frac{P_{H2}^{1.28}}{(K_p - P_{N2})^{0.8}}$ 17

$C_{NH30} = \frac{P_{NH30}}{RT}$ 18

$P_{NH30} = C_{NH30} * R * T$ 19

$V_n = V_o C_{NH30} R\, T \int_{0.1149}^{0.1839} DdX_A * \frac{P_{H2}^{1.2}}{(K_p P_{N2})^{0.8}}$ 20

Where,

V_n = volume of each bed in the reactor.

Note; The function D is evaluated at certain selected values given in the tables below.

3.4.2 Mass of Catalyst in Each Bed

1. Calculation of the Mass of Catalyst in Each Bed

Given,

Density (ρ) = $\frac{\text{Mass}}{\text{Volume}}$ 21

Mass = Density * Volume

Where ρ = Density of iron (the catalyst used is iron)

= $3500 kg/m^3$

Volume of the reactor equals the sum of the catalyst pellets occupies V_R

$V_R = \sum V_1 + V_2 + V_3 + V_4$

3.4.3. Calculation of Cross Sectional Area Occupied by Catalyst

Cross sectional area of the reactor is given by $\frac{\pi}{4} - (D^2 - d^2)$ 22

Where,

D = Diameter of the reactor = 1.5m

D = Annular space = 0.3m

3.4.4 Calculation of the height of the reactor

Calculation of the height is given by

$h_n = \frac{V}{A}$ 23

Where,

h_n = height of n catalyst bed
V = volume occupied by each catalyst bed
A = cross sectional area occupied by each catalyst
Height of reactor =∑ height of bed 1 + bed 11 + bed 111 + bed 1V

3.5. Calculation of the gas velocity in the reactor

The gas velocity is given by; E = $\frac{V_1}{A_C} = \frac{V_o}{\pi d h_s}$ 24

Where E = the gas velocity
A_c = surface area of the inner tube of the reactor
V_o = volumetric flow rate of the gases in the inner tube
π = 3.142
d = inner tube diameter
h_5 = height of the catalytic bed
A_c = $\pi d h_s$ 25

In calculating the gas velocity in the inner tube the compressibility factor must be determined. The compressibility factor of hydrogen is

Given as Z = $\frac{PV}{RT}$ 26

Where P = $3 * 10^7$Pa = 300bar
T = 720k

Using the ideal gas equation, V_1 is obtained

$$\frac{P_l V_l}{T_l} = \frac{P_2 V_2}{T_2} \quad 27$$

Where,
P_l = pressure of gas mixture at s.t.p = $1.10325 * 10^5$Pa
T_2 = 720k
P_2 = $3 * 10^5$Pa

4.0 RESULTS AND EXPLANATIONS

4.1 The Mole Fraction, Partial Pressure and Fractional Conversion

The mole fraction, partial pressure and fractional conversion of the t beds are shown in Table 4.

Table 4: Mole fraction, partial pressure and fractional conversion of the different beds

Bed Number	Component	Moles	Y_l	$P_l * 10^7$	X_A
1	N_2 H_2 NH_3	0.8851 2.6553 0.8161	0.23476 0.7042 0.06095	$0.680 * 10^7$ $2.040 * 10^7$ $0.17663 * 10^7$	0.1149
2	N_2 H_2 NH_3	0.8161 2.4482 0.3678	0.22468 0.67405 0.101026	$0.6511 * 10^7$ $1.9533 * 10^7$ $0.293 * 10^7$	0.1839
3	N_2 H_2 NH_3	0.74713 2.24139 0.5074	0.2138 0.64145 0.1447	$0.6959 * 10^7$ $1.8589 * 10^7$ $0.4193 * 10^7$	0.25287
4	N_2 H_2 NH_3	0.678161 2.03448 0.643678	0.20205 0.60616 0.191978	$0.5855 * 10^7$ $1.7566 * 10^7$ $0.555 * 10^7$	0.32183

4.2 Equilibrium conversion

The equilibrium conversion as calculated from equation 7 gives a value of;
X_e = equilibrium conversion ≅ 99%

4.3 Reactor sizing

Table 5 to 9, gives the generated data for the function D using trapezoidal rule for the reactor sizing.

Table 5: Generated data for the function D using trapezoidal rule for bed I

A	1- X_A	D
0.00000	1.00000	$3.1 * 10^{-6}$
0.028725	0.971275	$3.0 * 10^{-6}$
0.05745	0.943255	$2.9 * 10^{-6}$

A	1- X_A	D
0.086175	0.913825	$2.8 * 10^{-6}$
0.1149	0.8851	$2.7 * 10^{-6}$

Table 6: Generated data for the function D using Trapezoidal rule for bed II

X_A	1-X_A	D
0.1149	0.8851	$4.4 * 10^{-6}$
0.13215	0.86785	$4.3 * 10^{-6}$
0.1494	0.8506	$4.2 * 10^{-6}$
0.16665	0.83335	$4.1 * 10^{-6}$
0.1839	0.8161	$4.0 * 10^{-6}$

Table 7: Generated data for the function D using Trapezoidal rule for bed III

X_A	1-X_A	D
0.1839	0.81610	$5.8 * 10^{-6}$
0.2011425	0.798857	$5.7 * 10^{-6}$
0.218385	0.781615	$5.6 * 10^{-6}$
0.23567	0.764373	$5.5 * 10^{-6}$
0.25287	0.74713	$5.4 * 10^{-6}$

Table 8: Generated data for the function D using Trapezoidal rule for bed IV

X_A	1-X_A	D
0.25287	0.74713	$7.1 * 10^{-6}$
0.27011225	0.72988775	$7.0 * 10^{-6}$
0.287354	0.7126455	$6.9 * 10^{-6}$
0.304596	0.695404	$6.8 * 10^{-6}$
0.321839	0.07811	$6.7 * 10^{-6}$

Table 9: Height of the beds

Bed	Height (m)
Bed 1	0.619
Bed 2	0.579
Bed 3	0.115
Bed 4	1.958
Total height of bed	**4.311**

4.3 Volume of the reactor

Table 10: Tabulation of the volume of the reactor for each bed

Reactor	Volume (m^3)
Bed 1	0.579
Bed 2	0.542
Bed 3	1.08
Bed 4	1.85
Total volume of the reactor V_R	**4.051**

Table 10 shows the volume of the reactor. Considering bed by bed, the total volume of the reactor is = $4.051m^3$

4.4 Mass of Catalyst in each Bed

Table 11: Mass of catalyst in each bed

Bed	Mass (kg)
Bed 1	2026.5
Bed 2	1897
Bed 3	3780
Bed 4	6475
Total	**14178.5**

Table 11 above gives the mass of catalyst in each bed. Considering bed by bed, the total mass of catalyst in the reactor is = 14178.5kg.

4.5 Cross Sectional Area Occupied by Catalyst
Cross sectional area of the reactor = 0.935m^2
The heat transfer area of the bed and heat exchanger is also equal to 0.935m^2

4.6 Height of the reactor
The height of the reactor equates the summation of the bed heights, + Height of distributing phase + Height of bottom feed.
Height of the reactor = 4.311 + 0.625 +0.203
= 5.139m

Table 12: Height of the beds

Bed	Height (m)
Bed 1	0.619
Bed 2	0.579
Bed 3	0.115
Bed 4 Height of distributing phase Height of bottom feed	1.958 0.54 0.22
Total height of the reactor	**5.139**

4.7 Gas velocity in the reactor
Using equations 27-30, the gas flow rate in the reactor was computed as 0.439m/s.

4.8: Summary of the Design Components
Summary of the design components is shown in the tables 13 below.

Table 13: Summary of the design components

Equilibrium conversion	**≅99%**
Volume of the reactor(m^3)	4.051
Mass of catalyst (kg)	14178.5
Cross sectional area of the reactor (m^2)	0.935
Height of the reactor (m)	5.231
Gas velocity in the reactor (m/s)	0.439

4.9. CONCLUSION

The synthesis of ammonia is a very important industrial process because of the extensive use of ammonia in the world today. The main constituent of ammonia is hydrogen and nitrogen present in the molar ratio of 3:1. There are also some traces of methane and argon. Because the reaction for the synthesis of ammonia is a reversible one, the optimum temperature progression is one, which subsequently reduces along the length of the reactor as the reaction progresses. The inlet temperature is usually at a high value. To achieve this progressive temperature reduction a packed bed reactor is employed. This helps in reducing to complexities in the heat transfer equipment while ensuring a progressive reduction in temperature from the first to the fourth bed. Subsequently there is a decrease in the composition of hydrogen and nitrogen from bed to bed and a corresponding increase in ammonia composition or conversion. The inlet operating conditions for the reactor were 15m^3/sec flow rate, pressure of 2.896 x 10^{7}Pa and temperature of 720k the diameter was calculated to be 1.5meters. The gas velocity of ammonia is equal to 0.439m/s. The reactor height is found to be 5.23m. The volume of the reactor zone is equal to the volume of catalyst in the beds which is 4.051m^3.

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