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Model prediction on the reliability of fixed bed reactor for ammonia production

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ABSTRACT

In this research work Haber process was employed to examine the reliability of the functional parameters and coefficient on ammonia production using the fixed bed reactor with hydrogen gas and nitrogen used as the main source of the reactant. Mathematical models were developed to monitor and predict the effectiveness factors, nitrogen fractional conversion, temperature, component mole fraction, hydrogen mole fraction, and ammonia mole fraction profile for the various cases considered during the investigation. The simulated parameters for case 1, 2 and 3 for components of total feed flow, pressure, reactor bed volume and feed composition influence the reliability of the functional parameters and the coefficient of the fixed bed reactor for optimum yield of ammonia. The developed models were simulated using Matlab program to evaluate the functional parameters and the results obtained from the system in terms of optimum yield factor indicate 30% to 34% increase in ammonia production. The increase in the performance evaluation concept revealed the reliability of the developed model in monitoring and predicting the rate of production of ammonia in a fixed bed reactor.

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Capsule Summary: Matlab program concept was applied to monitor, predict and simulate the reliability of the functional parameters and coefficients on ammonia production in a fixed bed reactor with hydrogen gas and nitrogen used as the only main source of the reactant (the approach of Haber process). The variation in the optimum production rate indicates the reliability of the developed model as well as the concept applied.

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INTRODUCTION

Ammonia is the initial chemical material for variety of industries; it is used in production of chemicals such as: fertilizers, explosive materials, polymers, acids and coolers. Ammonia is commercially produced through the reaction between hydrogen gas (H_2) and (N_2) in a well-known process (Haber process) which has not been changed fundamentally.

Industrial ammonia converters are mainly fixed bed catalytic reactors. The conversion obtained from the reactor is relatively low (15%-20%). This is mainly due to the following: Ammonia is produced by an exothermic reversible reaction of hydrogen and nitrogen. The ammonia synthesis shares the general problem of exothermic reversible reactions (Abashar, 2003, Einashaie et al., 1988, Sing et al., 1981; Ukpaka, 2012). That is, the conversion is limited by the thermodynamic equilibrium. Different approaches have been

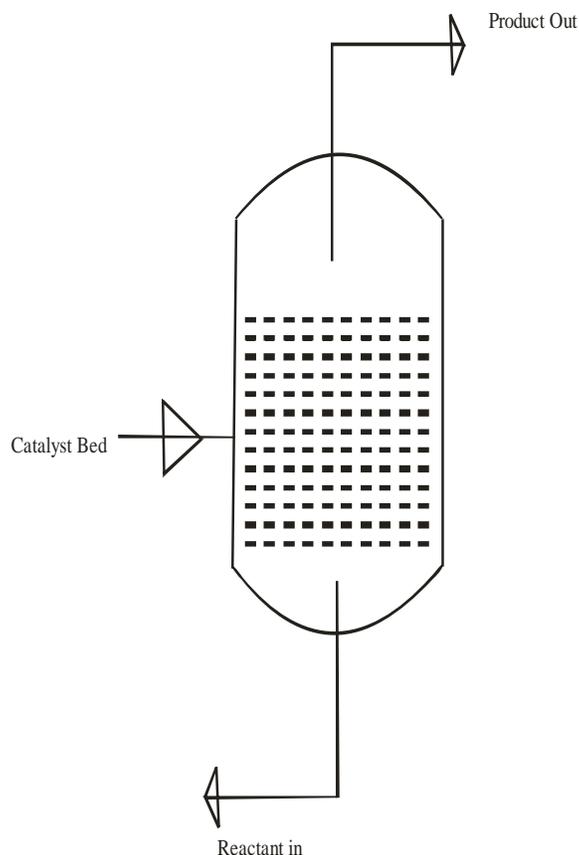


Fig. 1: Schematic representation of fluid movement in fixed bed reactor

considered to overcome the thermodynamic limits on the conversion by shifting the reaction from the thermodynamic equilibrium through direct quenching of reacting gases with fresh synthesis gas (e.g. the pullman-kellogg and chemico converters). Quenching of the reaction mixture by an external cooling (e.g. the montecatini Edison converters) and heat exchanger with reacting gases (e.g. the TVA converters). In a recent study, it has been shown that, considerable increase in the ammonia conversion is possible by the crossing of the reaction equilibrium, using internal heat exchanger and energy optimization. Many optimization studies have been reported in literature, which addressed the problem of maximizing the ammonia conversion by optimizing the temperature profile along the reactor length. However, it is quite difficult to implement this optimal temperature profile technically.

The effectiveness factor (η) is relatively small (0.3-0.6) along the length of the reactor. The concept of the effectiveness factor as a measure of importance of diffusion limitation for gas-solid catalytic reactions has gone a long way (Appl, 2007; Isla et al., 1993; Jennings, 1991; Shah, 1967; Butt, 2000., Dyson and Simon, 1968; Ukpaka, 2013). The ammonia reaction is diffusion limited within the catalyst pellet i.e. the existence of high diffusion resistances because concentration profiles inside the catalyst pellet, which reflect

the slow diffusion of the reactants and product. Both thermodynamic equilibrium and the diffusion resistances impose limitation on ammonia conversion.

The main characteristics of fixed bed catalytic reactors are: the catalyst pellets are held in place and do not move with respect to a fixed reference frame, since the gas has to pass over the material (catalyst), the reaction is limited by the available surface area, the reaction is exothermic, which means that, energy is released, in passing through fixed beds, gases approximately plug flow, effective temperature control of large fixed beds can be difficult because such systems are characterized by low heat conductivity, and fixed bed reactor is operated with high temperature and pressure (Butt, 2000; Dyson and Simon, 1968; Ukpaka, 2013).

A process plant is designed to work with optimization at the background; anything short of optimization is working at loss. Therefore reliability of ammonia production plant is to reduce risk of equipment failure, reduce cost of unreliability and increase in production. These three points above depends on maintenance key performance. The measurement of performance identifies current performance gaps between current and desired performance and provides indication of progress towards closing the gaps (Hill, 1977; Jennings, 1991).

Therefore, reliability is the probability of equipment or process to function without failure, when operated correctly, for a given interval of time, under stated conditions. Reliability numbers by themselves, the lack of meaning for making improvements for process plant, (ammonia plant). The financial issues of reliability is controlling the failures which waste money. Reliability issues are understandable when converted into monetary values by using actual plant data.

In general, reliability is a measuring index for great effect on the dependability and investment of such system. By definition, reliability is the probability that a device or system will perform its prescribed function adequately, for the period of time intended under specified operating conditions (Ukpaka, 2015).

Ammonia production plant make budget for their yearly operational or running cost with the aim of generating profits, but much can we afford to spend to fix the problem causing unreliability. Single and practical reliability tool for converting failure data into costs are available in the literature. When the process engineer can understand the problem on the one side of a sheet paper as reported, effort focuses on solving important problems are considered.

Information on other reliability data is needed, which will help in conversion of the figure - of - merit, performance induces using mean time between failures (MTBF). Reliability is experienced when the mean time between failures large compared to the mission time. Likewise, small values for mean time indices compares to the mission time reflect unreliability.

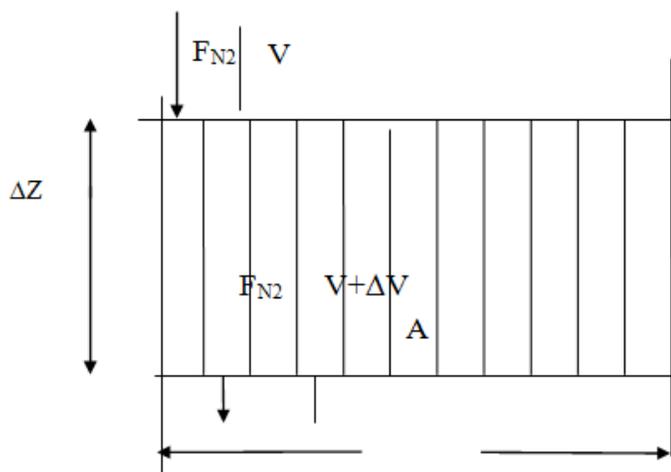


Fig. 2: Mass balance for reactor system

Accuracy of these single indices is improved when many data points are screened using well known statistical tools described in various literatures.

The failure of equipment or plant could be attributed to the following such as; depreciation, human error, corrosion error and lack of maintenance after start up.

To understand the performance of the reactors converting the raw feedstock (H_2 and N_2) into ammonia would require the simulation of the reaction through the development of mathematical models that are able to satisfactorily describe the reaction process. However, majority of the currently available models which describe the ammonia synthesis for fixed bed reactor and fluidized bed reactor are lacking. Therefore, the main focus of this study is to develop a feasible and reliable mathematical model which can describe the performance of fixed bed reactors for ammonia synthesis.

The aim of the research is to formulate the simulation models which require several expressions, such as, the individual chemical reaction steps defined by the stoichiometric equations along with the rate equations. Additionally, reaction phase equilibrium and also thermodynamic expressions are also utilized to develop the mathematical model. The aim of the research is to establish or evaluate the performance, reliability and risk assessment of fixed and fluidized bed reactors for ammonia synthesis. Mathematical model will be developed and necessary mathematical tools or techniques will be used for the simulation.

The overall objective of the study is to develop a mathematical model for both fixed and fluidized bed reactors, to evaluate their performance for ammonia synthesis. The specific objectives in order to achieve the above are: establishment of mathematical model using the first principle, to investigate the performance of the processes, to conduct a conceptual study of the processes and

establishment of reliability and risk assessment techniques in the processes.

The scope covered under this conceptual study involves: development of mass balance equations, development of energy balance equations, development of stoichiometric equations, development of reaction rate kinetics, development of liquid-vapor system equilibrium, reliability and risk assessment of the processes, and simulation of the model developed using the necessary mathematical tools or techniques and performance evaluation of the processes.

Industrial ammonia converter is mainly fixed bed catalytic reactor. The conversion obtained from the reactor is still relatively low (15-20%). To that effect, a mathematical model is developed for both fixed bed catalytic reactor and fluidized bed catalytic reactor for ammonia synthesis to evaluate their performance and make necessary recommendations to improve on the process.

MATERIAL AND METHODS

Research methodology

The main activity performed in this study covers the model development of the reaction process. Satisfactory model was developed which was simulated using the MATLAB Software. The mathematical model was simulated using industrial parameters and finally, the obtained profiles were compared to existing data to determine the model accuracy.

The Kinetic modeling was performed for fixed bed reactor for ammonia synthesis. The study of the reaction kinetics first begins with reading and studying the basic chemical reactions in the two processes. The rate laws was applied to formulate the rate equation for the reaction. This expression alongside with the mass balance equation will combined to develop the model needed to stimulate the reactions. Other useful expressions and equations for various parameters, such as the phase equilibrium and thermodynamics were used in the development of the model. The mass balance equations, in addition to the energy balance equations; this will finally give the reaction profiles of concentration, pressure and temperature to evaluate the two processes, as well as the component of reliability for the process.

Modeling fixed bed reactor for ammonia synthesis

A mathematical model is developed for the synthesis reactor temperature, concentration and pressure profiles are obtained.

The following assumptions are used in the derivation of the model.

1. The system is at steady state.
2. One - dimensional Cartesian co-ordinate has been considered along with the bulk flow.
3. The density is constant.

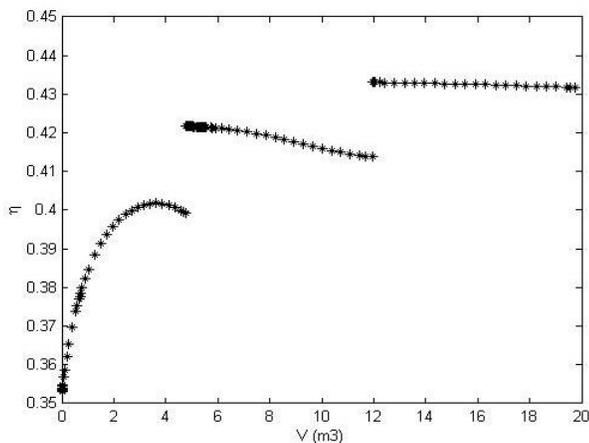


Fig. 3: Effectiveness factor profile – case 1

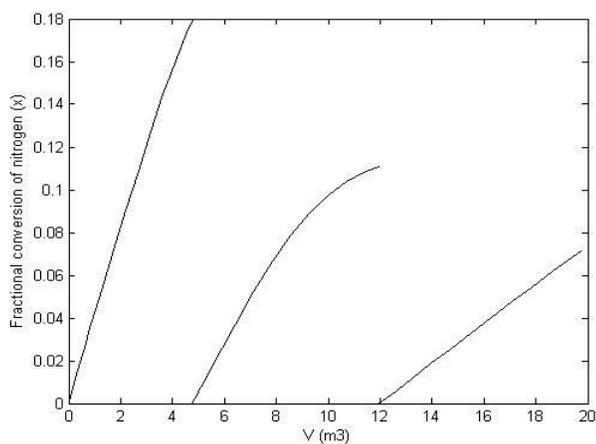


Fig. 4: Nitrogen fractional conversion profile – case 1

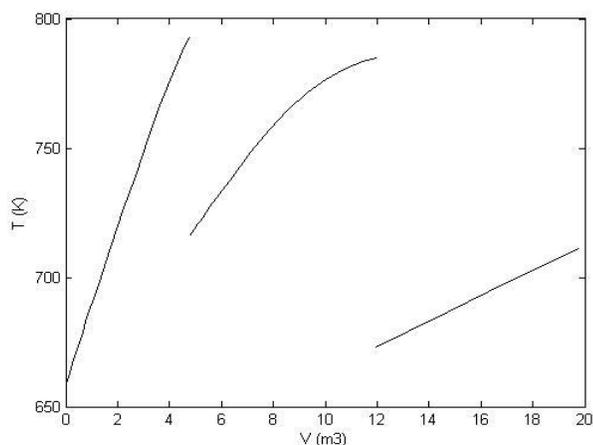


Fig. 5: Temperature profile – case 1

4. The concentration and temperature on catalyst surface and bulk of gas are equal.

5. Penetration of mass and heat is ignored, as the fluid velocity is very high.
6. The effects of penetration resistance in catalyst, temperature gradient and catalyst inside concentration have been incorporated in the equations by a coefficient.
7. Plug flow reaction

The stoichiometric reaction for ammonia production is defined as



Where, the conversion of N_2 (limiting reaction) is calculated by

$$X_{\text{N}_2} = \frac{F_{\text{N}_2}^0 - F_{\text{N}_2}}{F_{\text{N}_2}^0} \quad (2)$$

β is the feed ration of H_2 to N_2

$$\beta = \frac{F_{\text{H}_2}^0}{F_{\text{N}_2}^0} = 3 \text{ moles} \quad (3)$$

The exit flow rate of N_2 can be defined from equation (2) given as:

$$F_{\text{N}_2} = F_{\text{N}_2}^0 - F_{\text{N}_2}^0 X_{\text{N}_2} = F_{\text{N}_2}^0 (1 - X_{\text{N}_2}) \quad (4)$$

The conversion of the H_2 is given by

$$X_{\text{H}_2} = \frac{F_{\text{H}_2}^0 - F_{\text{H}_2}}{F_{\text{H}_2}^0} \quad (5)$$

The exit flow rate of H_2 can be defined from equation (5) given as:

$$F_{\text{H}_2} = F_{\text{H}_2}^0 - F_{\text{H}_2}^0 X_{\text{H}_2} \quad (6)$$

From equation (3) Substitute the feed ratio into equation (6) we have

$$F_{\text{H}_2} = \beta F_{\text{N}_2}^0 - 3 F_{\text{N}_2}^0 X_{\text{N}_2} \quad (7)$$

$$F_{\text{H}_2} = F_{\text{N}_2}^0 (\beta - 3 X_{\text{N}_2}) \quad (8)$$

$$F_{\text{NH}_3} = F_{\text{NH}_3}^0 - 2 F_{\text{N}_2}^0 X_{\text{N}_2} \quad (9)$$

$$F_{\text{CH}_4} = F_{\text{NH}_4}^0 \quad (10)$$

$$F_{\text{Ar}} = F_{\text{Ar}}^0 \quad (11)$$

$$F^0_{\text{total}} = F_{\text{N}_2}^0 + F_{\text{H}_2}^0 + F_{\text{NH}_3}^0 + F_{\text{CH}_4}^0 + F_{\text{Ar}}^0 \quad (12)$$

$$F_{\text{total}} = F_{\text{N}_2} + F_{\text{H}_2} + F_{\text{NH}_3} - 2 F_{\text{N}_2} X_{\text{N}_2} + F_{\text{CH}_4} + F_{\text{Ar}} \quad (13)$$

$$= F_{\text{N}_2} + F_{\text{H}_2} - 2 F_{\text{N}_2} X_{\text{N}_2} + F_{\text{NH}_3} + F_{\text{CH}_4} + F_{\text{Ar}}$$

$$= F_{\text{N}_2} + \beta F_{\text{N}_2} - 2 F_{\text{N}_2} X_{\text{N}_2} + F_{\text{NH}_3} + F_{\text{CH}_4} + F_{\text{Ar}}$$

$$F_{\text{total}} = F_{\text{N}_2} (1 + \beta - 2 X_{\text{N}_2}) + F_{\text{NH}_3} + F_{\text{CH}_4} + F_{\text{Ar}} \quad (14)$$

The mole fraction can then be calculated from flow rates as

For Nitrogen

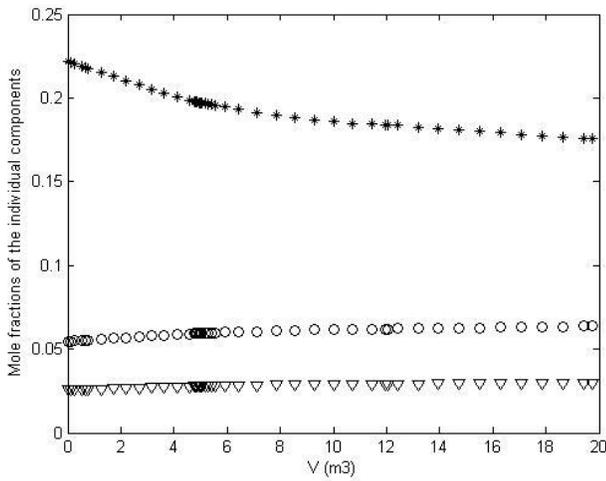


Fig. 6: Component mole fraction profile – case 1

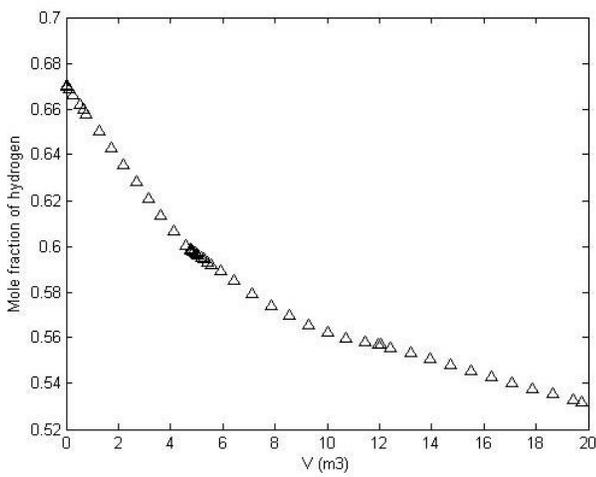


Fig. 7: Hydrogen mole fraction profile – case 1

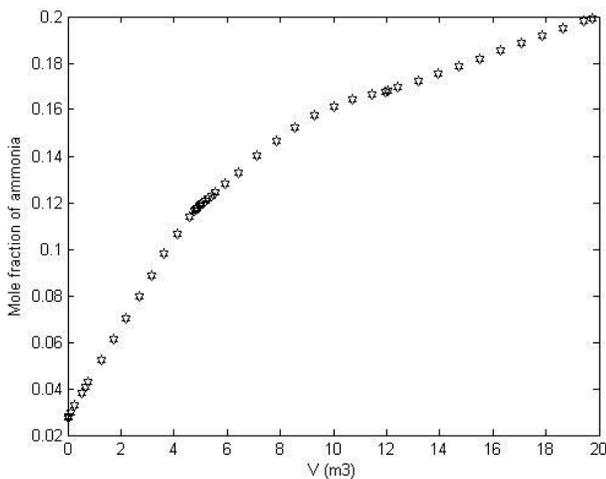


Fig. 8: Ammonia mole fraction profile - Case1

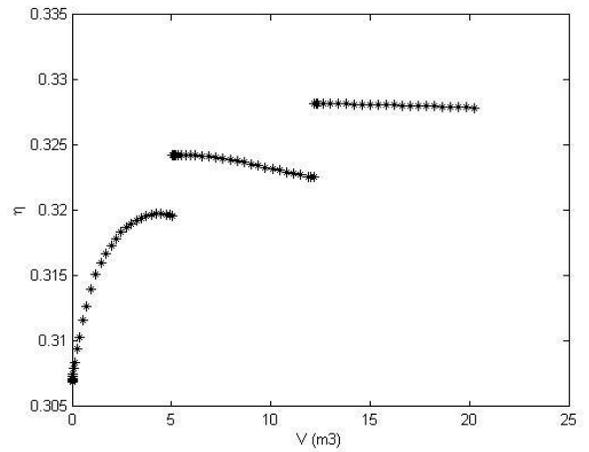


Fig. 9: Effectiveness factor profile –case 2

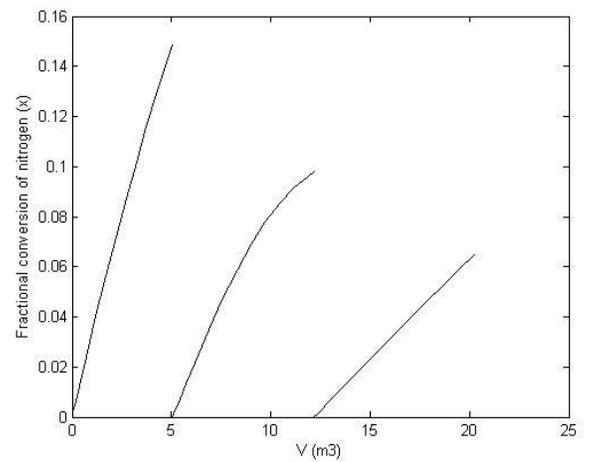


Fig. 10: Nitrogen fractional conversion profile - case 2

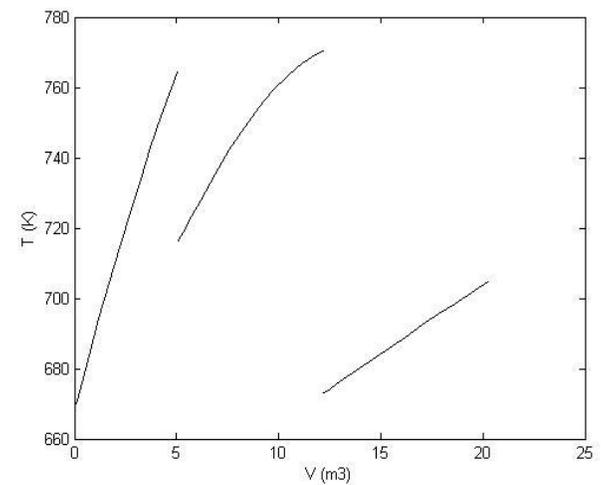


Fig. 11: Temperature profile - case 2

Table 1: Coefficient of the correction factor polynomial in terms of pressure

Pressure (Bar)	b ⁰	b ¹	b ²	b ³	b ⁴	b ⁵	b ⁶
150	-17.539096	0.07697849	6.900548	-1.08279e-4	-26.42469	4.927648e-8	38.937
225	-8.2125534	0.03774149	6.190112	-5.354571e-5	-20.86963	2.379142e-8	27.88
300	-4.6757259	0.02354872	4.687353	-3.463308e-5	-11.28031	1.540881e-8	10.46

Table 2: Coefficients of Cp polynomial for some component

Component	A	Bx10 ²	Cx10 ⁵	Dx10 ⁵
H ₂	6.952	-0.04567	0.09560	-0.2079
N ₂	6.903	-0.03753	0.193	-0.6861
CH ₄	4.75	1.2	0.303	-2.63
Argon	4.9675	-----	-----	-----

In 1967, Shah has developed an equation for determination of ammonia heat capacity which has been used in our modeling

Table 3: Simulation parameters for case 1

Total feed flow(Nm ³ /h)	242160				
Pressure (ATM)	226				
Reactor bed volume span(m ³)	4.75	7.2	7.8		
Feed composition	N ₂ 0.2219	H ₂ 0.6703	NH ₃ 0.0276	CH ₄ 0.0546	Ar 0.0256

Table 4: Simulation parameters for case 2

Total feed flow (Nm ³ /h)	180000				
Pressure (atm)	177				
Reactor bed volume span (m ³)	5.05	7.12	8.1		
Feed composition	N ₂ 0.1960	H ₂ 0.6510	NH ₃ 0.0320	CH ₄ 0.0740	Ar 0.0470

$$Y_{N_2} = \frac{F_{N_2}^0 - F_{N_2}^0 X_{N_2}}{F_{total}^0} \quad (15)$$

For hydrogen

$$Y_{H_2} = \frac{F_{H_2}^0 - F_{H_2}^0 X_{H_2}}{F_{total}^0} \quad (16)$$

$$Y_{H_2} = \frac{\beta F_{N_2}^0 - 3F_{N_2}^0 X_{N_2}}{F_{total}^0} \quad (17)$$

For ammonia

$$Y_{NH_3} = \frac{F_{NH_3}^0 + 2 F_{N_2}^0 X_{N_2}}{F_{total}^0} \quad (18)$$

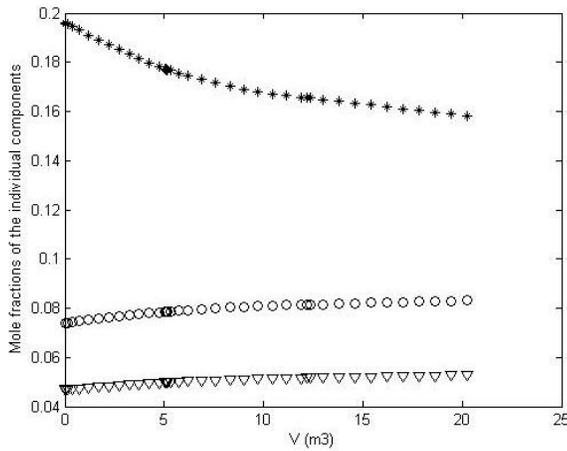


Fig. 12: Component mole fraction profile - case 2

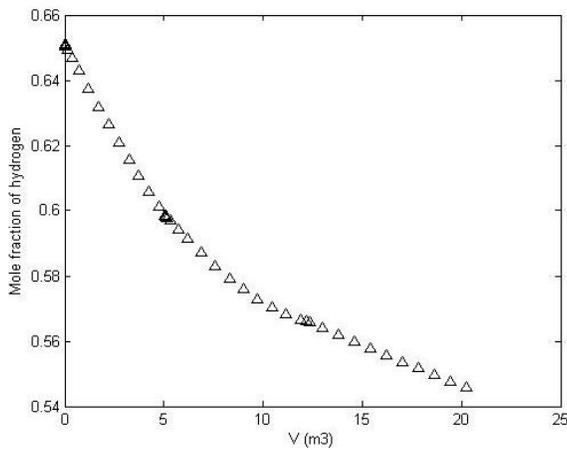


Fig. 13: Hydrogen mole fraction profile - case 2

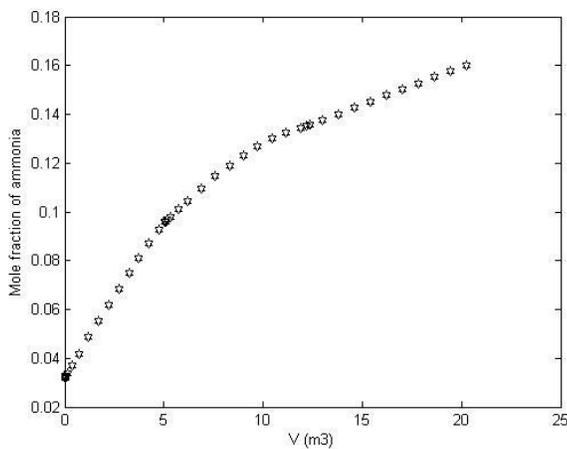


Fig. 14: Ammonia mole fraction profile - case 2

For methane

$$Y_{CH_4} = \frac{F_{CH_4}^0}{F_{total}^0} \tag{19}$$

For Argon

$$Y_{Ar} = \frac{F_{Ar}^0}{F_{total}^0} \tag{20}$$

Where, β is the feed ratio of H_2 to N_2 , X_{N_2} is the conversion of N_2 , X_{H_2} is the conversion of H_2 , $F_{N_2}^0$ is the inlet feed rate of N_2 (mol/sec), $F_{H_2}^0$ is the inlet feed rate of H_2 (mol/sec), F_{N_2} is the exit flow rate of N_2 (mol/sec), F_{H_2} is the exit flow rate of H_2 (mol/sec), F_{NH_3} is the exit flow rate of NH_3 (mol/sec), F_{total}^0 is the total inlet feed rate (mol/sec), F_{total} is the total exit flow rate (mol/sec).

Considering an element of differential volume with height ΔZ and cross sectional area (A) equal to that of the bed, We have

Accumulation = Input – output + generation – Consumption.

Accumulation is Zero under steady state.

Accumulation = input - output + generation- consumption

0 = input - output + generation.

Therefore, the above mass balance can be written as follows.

$$F_{N_2}|_V - F_{N_2}|_{V+\Delta V} + \Delta V (r_{N_2}) \eta = 0$$

$$F_{N_2}|_{V+\Delta V} - F_{N_2}|_V = \Delta V (r_{N_2}) \eta$$

Divide both sides by ΔV

$$\frac{F_{N_2}|_{V+\Delta V} - F_{N_2}|_V}{\Delta V} = (r_{N_2}) \eta$$

$$\frac{F_{N_2}|_{V+\Delta V} - F_{N_2}|_V}{\Delta V} = \left. \frac{dF_{N_2}}{dV} \right|_{V+\Delta V}$$

$$\left. \frac{dF_{N_2}}{dV} \right|_{V+\Delta V} = (r_{N_2}) \eta$$

Limit $\Delta V \rightarrow 0$

$$\frac{dF_{N_2}}{dv} = (r_{N_2}) \eta \tag{21}$$

From equation (9) substitute Nitrogen conversion percentage

$$F_{NH_3} = F_{NH_3}^0 - 2F_{N_2}^0 X_{N_2}$$

$$\frac{dF_{N_2}}{dv} = \frac{dF_{NH_3}}{dv} = - \frac{2F_{N_2}^0 dx}{dv} = - (r_{NH_3}) \eta$$

$$-2F_{N_2}^0 \frac{dx}{dv} = - (r_{NH_3}) \eta$$

$$\frac{dx}{dv} = \frac{(r_{NH_3}) \eta}{2F_{N_2}^0} \tag{22}$$

Where, $F_{N_2}^0$ is the inlet molar flow rate of Nitrogen (mol/sec), X is the limiting reactant (N_2) conversion, r_{NH_3} is ammonia reaction rate (mol/m³ sec), η is the effective factor and V is the reactor volume (m³).

Reaction rate

To calculate the rate of reaction, modified Temkin's equation offered by Dyson & Simon in 1968 has been used.

$$r_{NH_3} = 2k[K^2 a_{N_2} (a_{H_2}^3 / a_{NH_3}^2)^\alpha - (a_{NH_3}^2 / a_{H_2}^3)^{\alpha-1}] \quad (23)$$

where, K is the rate constant for the reverse reaction, K_a is the equilibrium constant of the reaction $N_2 + 3H_2 \leftrightarrow 2NH_3$, a is the activity of the component, which can be calculated using fugacity, α is the correlation parameter which has a constant of value 0.5 to 0.75 in literature.

Activation can be written in terms of activation coefficient as below

$$a_i = \frac{f_i}{f_i^0}$$

Where, f_i^0 : reference fugacity, f_i : fugacity of the component i , if the reference fugacity is considered to be 1 atm, then,

$$a_i = \frac{f_i = y_i \phi_i p}{1} \quad (24)$$

In this equation, ϕ_i is the fugacity coefficient and p is the total pressure. The equations for the experimental values of fugacity coefficient of hydrogen, nitrogen and ammonia are given below.

$$\phi_{H_2} = e^{[(p^{-3.8402T0.125+0.541}) P^{-e(-0.126T0.5-15.98)} P^{2+300} [e^{(-0.011901T-5.94)}] (e^{P/300})]} \quad (25)$$

$$\phi_{N_2} = 0.93431737 + 0.2028538 \times 10^{-3} T + 0.295896 \times 10^{-3} P - 0.270727 \times 10^{-6} T^2 + 0.4775207 \times 10^{-6} P^2 \quad (26)$$

$$\phi_{NH_3} = 0.148996 + 0.2028533 \times 10^{-2} T - 0.4487672 \times 10^{-3} P - 0.1142945 \times 10^{-5} T^2 + 0.2761216 \times 10^{-6} P^2 \quad (27)$$

The above equations, T is in terms of kelvin and p in terms of atmosphere.

The equation of reverse ammonia synthesis reaction has been considered in base of Arrhenius format.

$$K = k_0 \exp(-E/RT) \quad (28)$$

K_0 : Arrhenius coefficient equal to 8.849×10^{14}

E : Activation energy, which varies with temperature. Its mean value is 40765

(Kcal /kmol)

R : Gas constant

In 1930, Gillespie and Beattie have developed the following equation to calculate the equilibrium constant

$$\log K_a = -2.691122 \log T - 5051925 \times 10^{-5} T + 1.848863 \times 10^{-7} T^2$$

$$\frac{2001.6 + 2.689}{T} \quad (29)$$

Effective factor

To investigate the effects of temperature and density of the catalyst interior and the difference between these parameters with those of the catalyst surface, an effect factor called η has been defined. The general form of the equation defining this effect factor has been given below.

$$\eta = b_0 + b_1 T + b_2 Z + b_3 T^2 + b_4 Z^2 + b_5 T^3 + b_6 Z^3 \quad (30)$$

The above equation is in terms of temperature and density of the catalyst interior and the difference between these parameters with those of the catalyst surface, an effect factor called η has been defined. The general form of the equation defining this effect factor has been given below. The above equation is in terms of T and conversion percentages, the coefficient of this equation for three different pressures have been depicted in table below.

Heat capacitance

The following equation is used to determine the Heat capacitance.

$$C_{pi} = 4.184 (a_1 + b_1 T + c_1 T^2 + d_1 T^3) \quad (\text{kJ/kmol}) \quad (31)$$

$$6.5846 - 0.61251 \times 10^{-2} T + 0.23663 \times 10^{-5} T^2 -$$

$$1.5981 \times 10^{-9} T^3 + 96.1678 - 0.067571 p +$$

$$C_{PNH_3} = 4.184 (0.2225 + 1.6847 \times 10^{-4} P) T +$$

$$(1.289 \times 10^{-4} - 1.0095 \times 10^{-7} P) T^2 \quad (\text{kJ/kmol} \cdot \text{K}) \quad (32)$$

Reaction heat

ElNashare has developed a relation in 1981 for calculation of reaction heat which has been used in our modeling

$$\Delta H_r = 4.184 - [0.54526 + 846.609/T + 459.734 \times 10^6] p - 5.3468 5T -)$$

$$0.2525 \times 10^{-3} T^2 + 1069197 \times 10^{-6} T^3 - 9157.09 (\text{kJ/kmol} \cdot \text{K}) \quad (33)$$

Pressure drop

To calculate the pressure drop inside bed and Ergun equation has been applied and this relation for a one dimension flow is as below.

$$\Delta p = \frac{150(1-\epsilon)^2}{\epsilon^3} \times \frac{\mu u_{mf}}{d_p^2} + 1.75 \frac{(1-\epsilon)}{\epsilon^3} \times \frac{\rho u_{mf}^2}{d_p} \quad (34)$$

Where, Δp is pressure drop (atm), ϵ is bed voidage of the fluid velocity (dimensionless), μ is the viscosity of fluid (kg/m.sec),

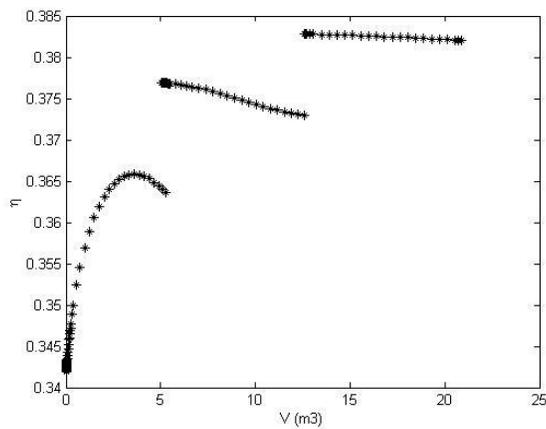


Fig. 15: Effectiveness factor profile - case 3

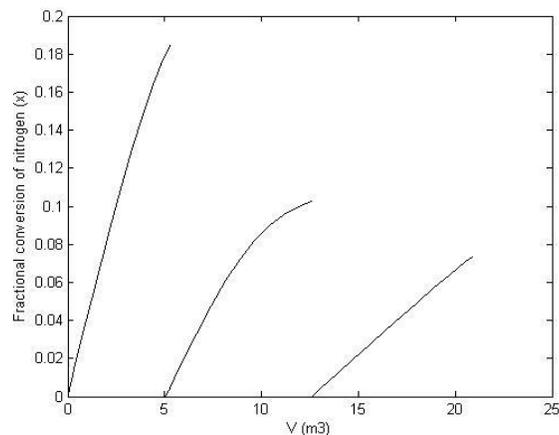


Fig. 16: Nitrogen fractional conversion profile - case 3

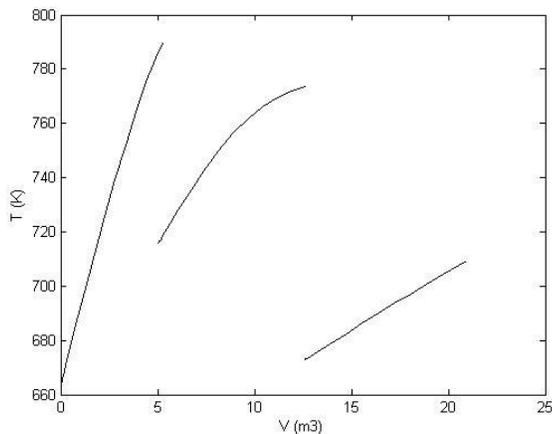


Fig. 17: Temperature profile - case 3

u_{mf} is minimum fluidization velocity (m/s), d_p is the diameter of the bed (m).

Energy balance

Energy balance is investigated on the same element on which mass balance has been considered.

Accumulation = input energy - output energy + generation energy - consumption energy.

In steady state, accumulation is zero, No energy is consumed as well as the consumption energy is zero.

$0 = \text{input energy} - \text{output energy} + \text{general energy}$

$$0 = F_T C_{p_i} T|_V - F_T C_{p_i} T|_{V+\Delta V} + (-\Delta H_r) r_{NH_3} \Delta V$$

$$F_T C_{p_i} T|_{V+\Delta V} - F_T C_{p_i} T|_V = (-\Delta H_r) r_{NH_3} \Delta V$$

Divide both sides by ΔV

$$\frac{F_T C_{p_i} T|_{V+\Delta V} - F_T C_{p_i} T|_V}{\Delta V} = \frac{(-\Delta H_r) r_{NH_3} \Delta V}{\Delta V}$$

$$F_T C_{p_i} T|_{V+\Delta V} - F_T C_{p_i} T|_V = (-\Delta H_r) r_{NH_3} \eta$$

$$\frac{F_T C_{p_i} T|_{V+\Delta V} - F_T C_{p_i} T|_V}{\Delta V} = (-\Delta H_r) r_{NH_3} \eta$$

$$\frac{T|_{V+\Delta V} - T|_V}{\Delta V} = \frac{(-\Delta H_r) r_{NH_3} \eta}{F_T C_{p_i}}$$

$$\frac{T|_{V+\Delta V} - T|_V}{\Delta V} = \frac{(-\Delta H_r) r_{NH_3} \eta}{F_T C_{p_i}}$$

Where

$$\frac{T|_{V+\Delta V} - T|_V}{\Delta V} = \frac{dT}{dV} \Big|_{V+\Delta V}$$

$$\frac{dT}{dV} \Big|_{V+\Delta V} = \frac{(-\Delta H_r) r_{NH_3} \eta}{F_T C_{p_i}}$$

Limit $\Delta V \rightarrow 0$

$$\frac{dT}{dV} = \frac{(-\Delta H_r) r_{NH_3} \eta}{F_T C_{p_i}} \quad (35)$$

With boundary conditions

$$T = T_f, V = 0$$

Where, $(-\Delta H_r)$ is the heat of reaction in J/k mol of NH_3 , F_T is the total mass flow rate in (kg/s) and C_{p_i} is the heat capacity of the components in (j/kg °K)

RESULTS AND DISCUSSION

Ammonia model for fixed bed reactor

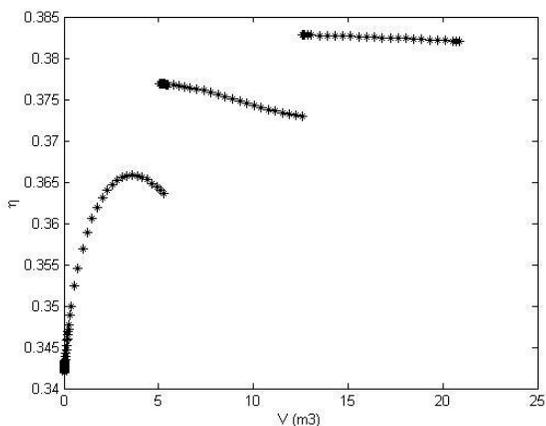


Fig. 15: Effectiveness factor profile – case 3

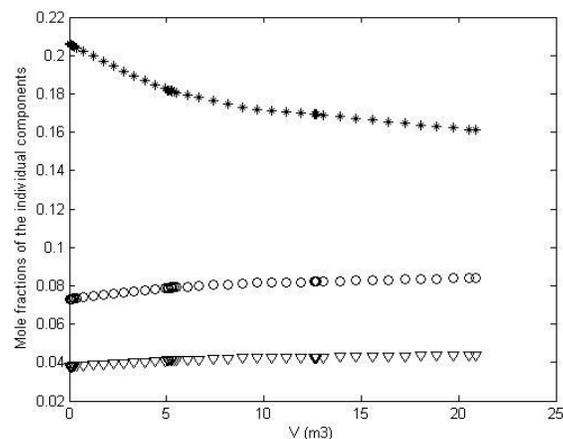


Fig. 18: Component mole fraction profile – case 3

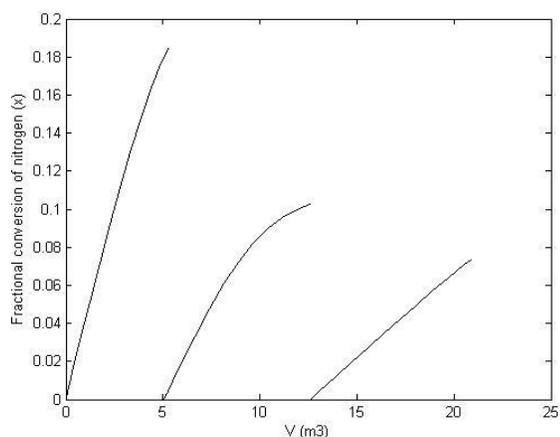


Fig. 16: Nitrogen fractional conversion profile – case 3

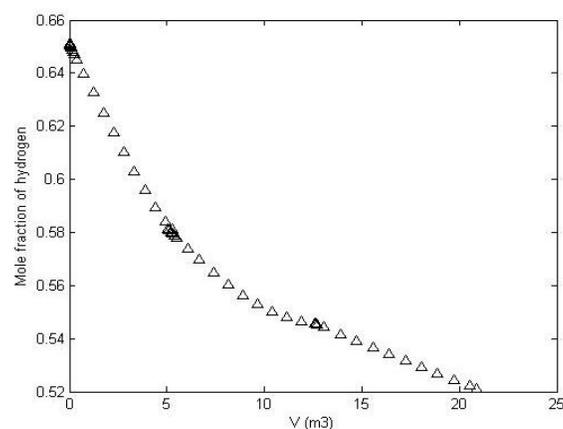


Fig. 19: Hydrogen mole fraction profile – case 3

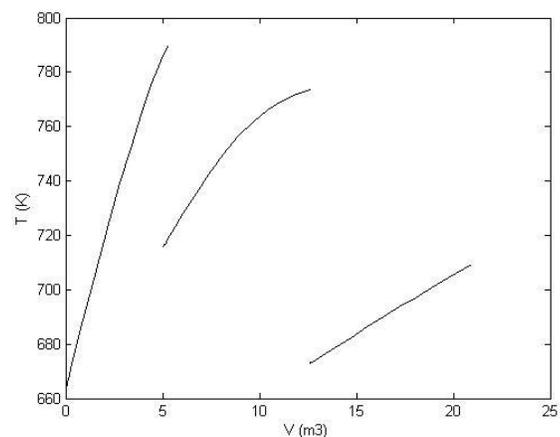


Fig. 17: Temperature profile – case 3

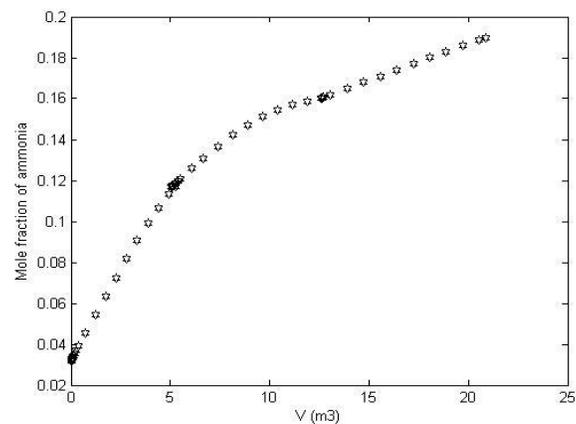


Fig. 20: Ammonia mole fraction profile – case 3

The individual model for fixed bed reactor for ammonia production process has been developed in to a suitable mathematical form for simulation in MATLAB. Simulation has been performed to determine the reactor performance for both fixed bed for ammonia production process using industrial data to obtain the concentration profiles as shown

below. The simulation was carried out using three different sets of reactor data and the results are as follow.

The simulation of the ammonia model provided six sets of profile which is the effectiveness factor of the catalyst against the volumetric span of the reactor. The same trend is observed on all 3 simulation cases whereby the effectiveness factor of the catalyst increases with each

Table 5: Simulation parameters for case 3

Total feed flow (Nm ³ /h)	195000				
Pressure (atm)	207				
Reactor bed volume span (m ³)	5.25	7.35	8.3		
Feed composition	N ₂	H ₂	NH ₃	CH ₄	Ar
	0.2060	0.6510	0.0320	0.0730	0.0380

Table 6: Industrial data of ammonia reactor

Case	Bed1		Bed2		Bed3	
	Inlet Temp(°C)	Outlet Temp(°C)	Inlet Temp(°C)	Outlet Temp(°C)	Inlet Temp(°C)	Outlet Temp(°C)
1	385	507	433	502	415	455
2	395	496	442	502	404	440
3	390	512	443	502	400	439

reactor bed but decreases with volume on each individual bed. The higher the overall inlet flow rate increases the effectiveness factor as well as presented Figure 3, 9 and 15.

The next profile obtained was the fractional conversion of nitrogen against the volumetric span of the reactor. The conversion of nitrogen decreases with each bed as the concentration of nitrogen decreases as it enters each bed. The conversion within each bed also slows down as the concentration of nitrogen decreases as the product concentration increases as presented in Figure 4, 10 and 16.

The third profile obtained is the temperature profile against the volumetric span of the reactor and results obtained are presented in Figure 5, 11 and 17. The results of the component mole fraction for various cases are shown in Figure 6, 12 and 18. Increase in product formation with decrease in reactant consumed upon increase in reactor volume. Decrease in hydrogen mole fraction was observed with increase in reactor volume as presented in Figure 7, 13 and 19. But in the case of ammonia mole fraction, increase was observed with increase in reactor volume as presented in Figure 8, 14 and 20. This profile is obtained from the energy balance of the system and is used to determine the performance of the model developed by the means of comparison with industrial data. Comparison shows that the model developed approximates the actual condition of the reactor adeptly. The data is as below

CONCLUSIONS

The simulation for the fixed bed reactor for ammonia production has been modeled using matlab, providing the concentration and temperature profiles. Additionally, the effect of temperature on the conversion and reaction rate is

also studied. In comparison with an operational industrial fixed bed ammonia converter showed that, for the same three bed configuration, the conversion can be improved from 30.91% to 34.2% (10.4% over the industrial fixed bed).

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