SIMULATION OF AN AMMONIA SYNTHESIS CONVERTER

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ABSTRACT

Steady state one dimensional pseudo-homogeneous models of an axial flow industrial catalytic packed bed ammonia converter have been developed. The converter is a vertical four catalytic bed reactor with varying volumes of catalysts. Effects of temperature changes on the catalyst surface and in its interior were incorporated in the model by an effectiveness factor. The models were used to predict conversions, concentrations of reactant/product mixtures and temperature profiles along the catalyst beds. The developed models consisted of ordinary differential equations which were solved numerically using the 4th order Runge-Kutta algorithm implemented with MatLab ode45 solver. The accuracy of the models was ascertained with industrial plant data from Notore Chemical Industry, Onne, Rivers State. The results obtained from solutions to the models compared favorably with output plant data of the ammonia converter with a maximum deviation between models predictions and actual plant data of 6.7%. Consequently, simulation studies of the converter was performed varying operating parameters such as feed flow rates, inlet temperatures and pressures to determine their effects on the performance of the converter.

Keywords: Modeling, ammonia converter, effect of feed flow rate and inlet temperature.

INTRODUCTION

Ammonia is a widely used raw material for the production of nitrogen compounds of vital importance, such as urea, nitric acid, fertilizer, explosive materials, pharmaceuticals, polymers and coolants; thus its synthesis is an important industrial process. It is produced following the Haber-Bosch process by the reaction between gaseous nitrogen (from air) and hydrogen (from natural gas). The diversification policy of the Nigerian Government aimed at increasing awareness and improvement in mechanized agriculture has resulted in increased agricultural activities across the country and increasing the demand for fertilizers a key requirement/ingredient for agricultural productivity. A sustained availability of fertilizer will be achieved through the efficient operation of exiting fertilizer plants and the construction of new plants of which the converter used for ammonia synthesis a precursor for the manufacture of nitrogenous fertilizers is very vital. The development of suitable models that can be used for simulation studies of the converter is vital in achieving this policy as the simulation would provide a wide range of operating conditions and design possibilities of the converter for prospective investors.

A typical ammonia production process consists of (a) production of the synthesis gas, (b) compression of the gas to the required pressure and (c) synthesis loop in which its conversion to ammonia takes place. This work is focused on the converter of the synthesis loop.

MODEL DEVELOPMENT

Process description

The hydrogen for the synthesis process is obtained from steam reforming of natural gas (chiefly methane) thereafter a shift conversion takes place to produce more hydrogen from reaction of carbon monoxide with water. Carbon dioxide is removed by absorbing in a potassium carbonate solution before passing the process gas to a methanation section where carbon monoxide and carbon dioxide are converted back to methane. The nitrogen input is obtained from the atmosphere through air liquefaction. After passing these stages the process gas is compressed (make-up gas) and sent to the ammonia converter where a portion of the synthesis gas is converted to ammonia in a catalytic reaction. Iron catalyst is used promoted with potassium oxides. The single-pass conversion is not more than 25%. A portion of the effluent emerging from the reactor exit is purged to remove inert contents while the other portion is sent to ammonia separation section where ammonia is condensed out at about -23°C. After separation, the gas is recycled and mixed with fresh makeup gas. A typical four bed ammonia converter in Notore Chemical Industry Limited operating at Onne in Rivers State is depicted in figure 1.

Kinetic Model

Various kinetic models for ammonia synthesis have been proposed over the years. These models were based either on mechanistic considerations or on empirical evaluations and include the works of ICI, 1970; Temkin, 1979; Nielsen, 1981; Boudart, 1981; Ull-mann's, 1985; Appl,

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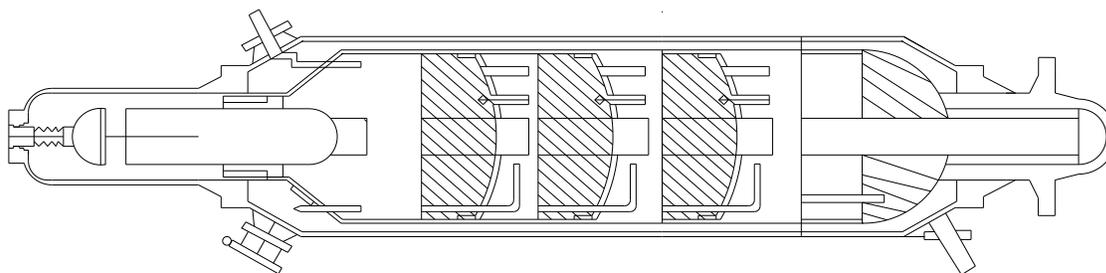
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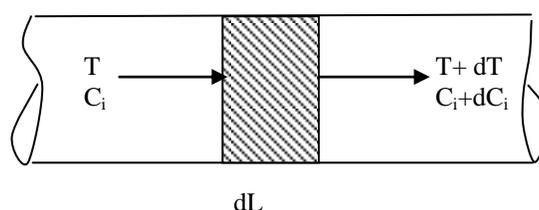
Fig. 1. Typical four Bed Ammonia Converter.

Fig. 2. Elemental portion of the packed bed reactor.

1992, 1997; Aparicho and Dumesic, 1994. The kinetics of ammonia synthesis over various catalyst has also been reported; over Ni-doped CeO2 and Ru/CeO2 catalyst respectively (Izumi*et al*., 1996); over a ruthenium catalyst supported on active carbon (Zbigniew *et al*., 1996) with barium-promoted iron-cobalt alloys (Hagen *et al*., 2003) and over a bimetallic catalyst Fe and Mo supported HZSM-5 catalyst at atmospheric pressure and high temperature (Unde and Gaikwad, 2007). These studies produced reaction rates expressions for the synthesis reaction with varying complexities and operating conditions. However, the rate expression of Temkin – Pyzhez (1940), (Temkin, 1990) is believed and widely accepted to accurately represent the ammonia synthesis reaction over wide and varying conditions; the modified form of the Temkin- Pyzhez equation expressed in activities as developed by Dyson and Simon (1986) will therefore be used in this work. The reaction rate expression is represented as:

$$R_{NH_3} = 2k\left(K_a^2 a_{N_2}\left[\frac{a_{H_2}^3}{a_{NH_3}^2}\right]^{\alpha} - \left[\frac{a_{NH_3}^2}{a_{H_2}^3}\right]^{1-\alpha}\right) \quad (1)$$

Where k is the rate constant for the reverse reaction, K_a is the equilibrium constant, a_i is the activity of component i and α is a constant which takes a value from 0.5 to 0.75 (Dashti*et al*., 2006).

The reaction rate equations for the reactants were determined using the stoichiometry of the reaction:

$N_2 + 3H_2 \leftrightarrow 2NH_3$ to relate the individual rates of reactions as follows:

$$-R_{N_2} = -\frac{1}{3}R_{H_2} = \frac{1}{2}R_{NH_3} \quad (2)$$

Reactor Model
To predict the performance of the converter, a mathematical model was developed. The conventional classification of reactor models contains two main categories (Reddy and Husairi, 1982): the pseudo-homogeneous and heterogeneous models. Pseudo-homogeneous models that do not account explicitly for the presence of catalyst can be used by modifying the intrinsic rate of reaction by multiplying it by an effectiveness factor. The empirical relation (Dyson and Simon, 1986) which relates the effectiveness factor at any point along the length of the catalyst bed to the temperature and conversion at that specific point is therefore incorporated in the model to be developed.

Model Assumptions
The following conditions are imposed on the synthesis converter in the development of its mathematical model:
The converter operates at steady state, the flow through it is assumed to be plug flow which means concentration varies along the length (bed) of the reactor. One-dimensional Cartesian coordinate was considered along the bulk flow. (Radial effects were not considered), density of the gas is constant and the effects of

penetration resistance in catalyst, temperature gradient and catalyst inside concentration have been incorporated in the rate equation by a coefficient. Based on these assumptions a pseudo-homogeneous one-dimensional model was developed for the reacting species by applying the principle of conservation of mass and energy on an elemental section (differential section) of the converter as shown in figure 2.

Mass Balance (Molar)

$$u\frac{dC_i}{dL} = \eta R_i \tag{3}$$

This equation can be written for the limiting reactant (nitrogen) as:

$$u\frac{dC_{N_2}}{dL} = \eta R_{N_2} \tag{4}$$

Where u = velocity of gas (m/s)
A = cross-sectional area of the bed (m^2)
C_{NH3} = Exit concentration of ammonia (NH$_3$) (moles/m^3)
L = Length of bed (reactor) (m)
R_{NH_3} = Rate of depletion of nitrogen (N$_2$)
η = Effectiveness factor

Expressing equation (4) in terms of nitrogen conversion (X) and initial flow rate $F_{N2,0}$ (mole/hr) as follows:

$$\frac{dX}{dL} = -\eta\frac{(R_{N_2})A}{F_{N_{2O}}} \tag{5}$$

Equation (5) can be expressed in terms of rate for ammonia production using the relationship in equation (2) to give:

$$\frac{dX}{dL} = \eta\frac{(R_{NH_3})A}{2F_{N_{2O}}} \tag{6}$$

Energy Balance

$$\frac{dT}{dL} = \eta\frac{(-\Delta H_R)R_{NH_3}A}{mC_{p_{mix}}} \tag{7}$$

Where:
m = total mass flow rate of (kg/hour)
$(-\Delta H_R)$ = Heat of reaction (KJ/kmol)
T = Temperature variable in the reactor (K)
Cp_{mix} = Specific heat capacity of the gas mixture (kJ/kmol)

MATERIALS AND METHODS

The component activities in the reaction rate equation were expressed in terms fugacity as:

$$a_i = \frac{f_i}{f_i^0} \tag{8}$$

Where:
f_i^0 = reference fugacity. Taken to be 1 atm
The fugacity of component i (fi) can be determined from the expression of the dimensionless fugacity coefficient:

$$\emptyset_i = \frac{f_i}{P_i} \text{ as:}$$

$$f_i = \emptyset_i P_i \tag{9}$$

The component partial pressures were converted to molar concentrations using the expression:

$$P_i = Y_i P_T = \left(\frac{N_i}{\sum N_i}\right)P_T \tag{10}$$

Substituting these, the component activities can be expressed as:

$$a_i = \emptyset_i Y_i P_T \tag{11}$$

The molar concentrations of each component (Y_i) were expressed in terms of fractional conversion of the limiting reactant nitrogen (X) using the expressions in Appendix 1 developed by performing a mole balance on the converter; thus expressing the component activities in terms of fraction conversion of the limiting reactant nitrogen. The respective component activities were substituted into the rate expression to yield the reaction rate expression in terms of fractional conversion of the limiting reagent (nitrogen).

$$R_{NH_3} = 2k\left(K_a^2 \emptyset_{N_2}\frac{Y_{N_{2,o}}(1-X)}{1-2XY_{2o}}P\left[\frac{\left(\emptyset_{H_2}\frac{(Y_{H_{2,o}}-3XY_{N2o})}{1-2XY_{2o}}P\right)^3}{\left(\emptyset_{NH_3}\frac{(Y_{NH_{3,o}}+2XY_{N2o})}{1-2XY_{2o}}P\right)^2}\right]^\alpha - \left[\frac{\left(\emptyset_{NH_3}\frac{(Y_{NH_{3,o}}+2XY_{N2o})}{1-2XY_{2o}}P\right)^2}{\left(\emptyset_{H_2}\frac{(Y_{H_{2,o}}-3XY_{N2o})}{1-2XY_{2o}}P\right)^3}\right]^{1-\alpha}\right) \tag{12}$$

Further simplification yields:

$$R_{NH_3} = 2k\left(K_a^2 \emptyset_{N_2}\frac{Y_{N_{2,o}}(1-X)}{1-2XY_{2o}}P\left[\frac{P(\emptyset_{H_2}(Y_{H_{2,o}}-3XY_{N2o}))^3}{(1-2XY_{2o})(\emptyset_{NH_3}(Y_{NH_{3,o}}+2XY_{N2o}))^2}\right]^\alpha - \left[\frac{(1-2XY_{2o})(\emptyset_{NH_3}(Y_{NH_{3,o}}+2XY_{N2o}))^2}{P(\emptyset_{H_2}(Y_{H_{2,o}}-3XY_{N2o}))^3}\right]^{1-\alpha}\right) \tag{13}$$

Substituting the reaction rate expression (eqn. 13) into the model equations (eqn. 6 and 7) gives the model equations in terms of fractional conversion of the limiting reactant nitrogen.

The MatLab 7.5 ODE45 solver from Mathworks for non stiff ordinary differential equations which uses the 4th order Runge Kutta algorithm was employed in solving the resulting ordinary differential equations of the model equations using data given in Table 1from the industrial ammonia converter of Notore Chemical Industry Limited operating at Onne in Rivers State, Nigeria. The industrial ammonia converter operates on a 4 catalyst beds system.

The outputs (results) from each catalyst bed were used as inputs into the successive bed and the process re-initiated. This was done for all four (4) catalyst beds until the final fractional conversion, concentrations (of reactants and product) and outlet bed temperature were determined at the end of the last bed (catalyst bed #4). To replicate the industrial converter accurately where the products from catalyst beds 1 and 2 were quenched (cooled) while the products from bed 3 were heated before entering the successive beds respectively, the industrial bed entry temperatures were used for beds 2, 3 and 4.

The results of the model equations gave the fractional conversions of the limiting reactant and temperature progression along each catalyst bed. The exit concentrations (mole %) of the reactants and product at each catalyst bed were obtained using the expressions in Appendix 1.

DETERMINATION OF PARAMETERS

To solve the model equations developed requires the determination of certain constants and parameters. These were determined as follows:

Component Fugacity Coefficient
The fugacity coefficients for Hydrogen (H_2), Nitrogen (N_2) and Ammonia (NH_3) were determined using the expressions given by Dyson and Simon (1986) as:

$$\varnothing_{H_2} = \left(exp \left(\begin{array}{l} exp(-3.802T^{0.125} + 0.541)P - exp(-0.1263T^{0.5} - 15.98)P^2 \\ + \left(300\left(exp(-0.011901T - 5.941)\left(exp\frac{P}{300}\right)\right)\right) \end{array} \right) \right)$$
(14)

$$\varnothing_{N_2} = \left(\begin{array}{l} 0.93431737 + 0.2028538x10^{-2}T + 0.295896x10^{-3}P \\ -0.270727x10^{-6}T^2 + 0.4775207x10^{-6}P^2 \end{array} \right)$$
(15)

$$\varnothing_{NH_3} = \left(\begin{array}{l} 0.1438996 + 0.2028538x10^{-2}T - 0.4487672x10^{-3}P \\ -0.1142945x10^{-5}T^2 + 0.2761216x10^{-6}P^2 \end{array} \right)$$
(16)

Reaction Rate Constant
The rate constant for the reverse reaction was obtained using the Arrhenius relation with values for the synthesis reaction given by (Dashti et al., 2006):

$$K = k_0 \exp\left(-\frac{E}{RT}\right)$$
(17)

Where:
K_0 = Arrhenius coefficient; (8.849 x1014)
E= Activation energy with temperature its mean value is 40765 Kcal/kmol
R=Universal Gas constant R (8.314 kJ/kmol.K)

Equilibrium Constant K_a
The equilibrium constant was obtained using the expression in Dashti et al. (2006):

$$logK_a = \left(\begin{array}{l} -2.69112logT - 5051925x10^{-5}T + \\ 1.848863x10^{-7}T^2 + \frac{2001.6}{T} + 2.689 \end{array} \right)$$
(18)

Effectiveness Factor (η)
The effect of temperature, conversion on the length of catalyst bed was accounted for by the expression given by (Babu and Reddy, 2012):

$$\eta = b_0 + b_1T + b_2X + b_3T^2 + b_4X^2 + b_5T^3 + b_6X^3$$
(19)

The coefficients for this equation are given by Babu and Reddy (2012).

Specific Heat Capacity
The specific heat capacity of the reactant gas mixture was obtained using the equation:

$$C_{P_{mix}} = \sum_{i=1}^{n} Y_i C_{P_i}$$
(20)

Where: y_i = mole fraction of component i,
Cp_i = specific heat capacity of component i

The heat capacities of the components of the reactant gases were obtained with the expression by Elverse et al. (1993):

$$C_{p_i} = 4.1884(a_i + b_iT + c_iT^2 + d_iT^3)$$
(21)

Where a_i b_i c_i and d_i are constants with values given in table 1.
The heat capacity of the product (ammonia) was obtained with the equation in Elverse et al. (1993)

$$C_{P_{NH_3}} = \left(\begin{array}{l} 6.5846 - 0.61251x10^{-2}T + 0.23663x10^{-5}T^2 - 1.5981x10^{-9}T^3 + 96.1678 \\ -0.067571P + (0.2225 + 1.6847x10^{-4}P)T + (1.289x10^{-4} - 1.0095x10^{-7}P)T^2 \end{array} \right)$$
(22)

Heat of Reaction
The equation developed by Mahfouz et al. (1987) was used to calculate the exothermic heat of reaction.

$$\Delta H_R = 4.184 \left(\begin{array}{l} -\left(0.54426 + \frac{846.609}{T} + \frac{459.734x10^6}{T^3}\right)P - 5.34685T \\ -0.2525x10^{-3}T^2 + 1069197x10^{-6}T^3 - 9157.09 \end{array} \right)$$
(23)

Determination of Feed Properties and Operating Conditions
Feed composition and converter bed properties from an industrial ammonia converter (Notore Chemical Industry) at Onne in Rivers State, Nigeria are given in tables 2 and 3.

Table 1. Coefficients of C_p polynomial for feed components.

	Component			
	H_2	N_2	CH_4	Ar
A	6.952	6.903	4.75	4.9675
b x 10^2	-0.04567	-0.03753	1.2	-
C x 10^5	0.095663	0.193	0.303	-
d x 10^5	-0.2079	-0.6861	-2.63	-

Table 2. Feed Composition.

FEED COMPOSITION (%mole)						FLOW RATE	
H_2	N_2	CH_4	NH_3	Ar	H_2/N_2	FEED (Kg/Hr)	N_2 (Kmole/hr)
63.32	21.01	10.48	2.08	3.11	2.78	289661	5828

Table 3. Ammonia converter Bed Properties.

	BED #1	BED #2	BED #3	BED #4
INLET TEMPERATURE	439 ^{o}C	448 ^{o}C	412 ^{o}C	453 ^{o}C
VOLUME (M3)	9.2	11.9	17.8	25
Reactor Diameter	9'8" (2949mm)			
Reactor Pressure	122.44 Bar (120.84 atm)			

RESULTS AND DISCUSSION

The results obtained from the solution of the model equations are presented as follows:

Fractional Conversions along the Reactor Beds
The fractional conversion of the limiting reactant (N_2) along the catalyst beds is shown in figure 3.

Figure 3 shows that the conversion of the limiting reactant (Nitrogen) increases along the length of the reactor from catalyst BED 1 to BED 4as a result of the reaction of the reactants (N_2 and H_2) to form the product (NH_3).

Reactants/Product Concentrations
The concentrations of the reactants and product across each catalyst bed are shown in figure 4.

Figure 4 shows that the concentrations of the reactants (N_2 and H_2) decreases steadily as they are being converted into the product (NH_3), while the concentration of the product (NH_3) increases from its initial value as it is being formed as the reaction proceeds along the length of the reactor beds.

Temperature Profile
The temperature progression along the four catalyst beds using industrial inlet temperatures of each bed and model prediction of effluent concentrations of preceding bed is shown in figure 5. The temperature along each bed increases due to the exothermic reaction of ammonia synthesis leading to the release of heat.

Model Validation
The comparison of model predictions of ammonia converter outputs (exit concentrations of ammonia, nitrogen, hydrogen and temperature of bed 4) and industrial plant outputs are shown in Table 4.

Table 4 shows that the maximum deviation between model prediction and industrial plant outputs is 6.7%. Hence the models developed matched the industrial converter accurately and can be used for simulation studies of the ammonia converter.

The model prediction of the outlet bed temperature was very close to the industrial plant value with a deviation of 1.5% as the temperature was re-initialized at the entrance of the second and third beds using actual industrial data hence the error from the previous bed was not propagated across subsequent beds. However the model prediction of the concentration of reactants and product had a maximum deviation of 6.7% as the exit concentration of the preceeding bed was the entry to the next bed resilting in the propagation of the error across the beds.

PROCESS SIMULATION

The 1st catalyst bed was selected for simulation studies because the products from catalyst beds 1 and 2 were quenched (cooled) while the products from bed 3 were heated before entering the successive beds respectively.

Effect of Feed Flow Rate
The influence of feed flow rate on the converter performance is presented in figures 6 and 7. When the

Table 4. Comparison of plant data with model results.

S/N	PARAMETER	PLANT DATA	MODEL RESULT	%DEVIATION
1	NH_3(Mole %)	11.50	11.81	2.7%
2	N_2(Mole %)	18.19	19.46	6.7%
3	H2 (Mole %)	54.90	53.17	3.2%
4	Outlet Temperature (K)	754	754.87	1.5%
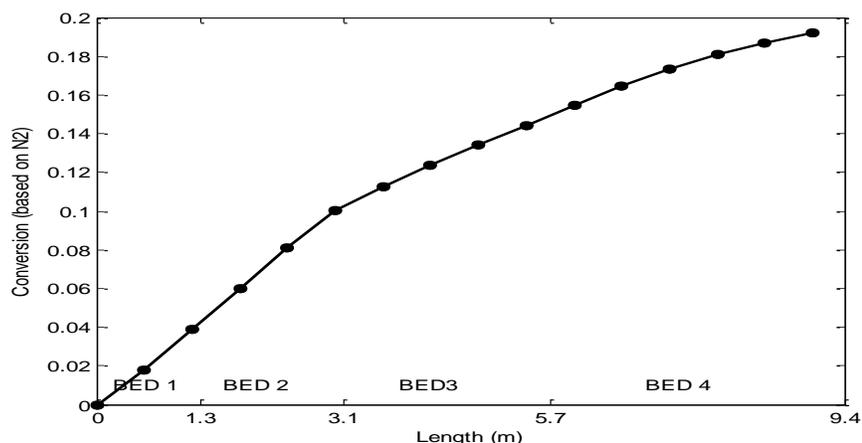
Fig. 3. Fractional Conversion of N_2 along the catalyst bed length.
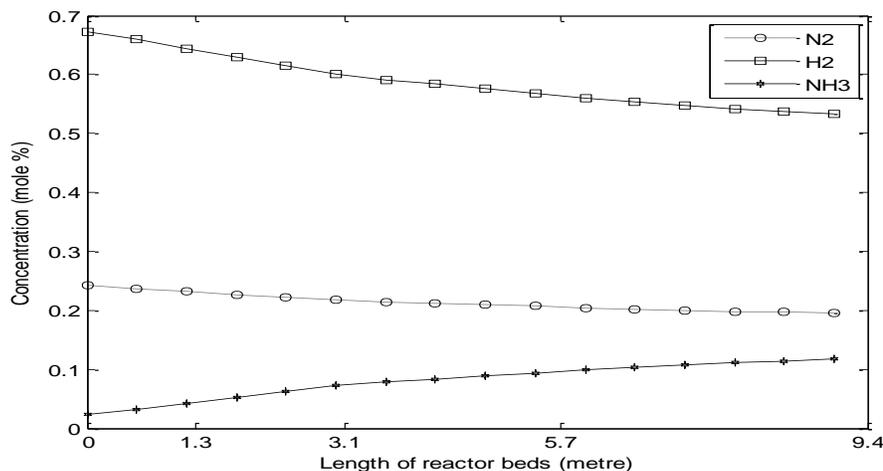
Fig. 4. Concentration (mole percent) of reactants and product along catalyst beds.

feed flow rate is increased, its velocity increases (reactants move faster) and the contact time of the reactants with the catalyst is reduced, resulting in a decrease in conversion and more reactants leaving the bed un-reacted. These trends the model predicts as shown in figure 6 where the reactants concentration increased slightly, the product (ammonia) concentration and conversion decreased with increase in feed flow rate. The decrease in conversion results in a decrease in exothermic heat released as reaction proceeds and subsequent

reduction in bed temperatures. This trend model predicts as shown in figure 7.

Effect of Feed Temperature
The effects of feed input temperature into BED 1 on the performance of the converter are shown in figure 8.

For an exothermic equilibrium reaction such as ammonia synthesis, Le Chetalier's principle predicts that when there is a reduction in feed temperature, the system will
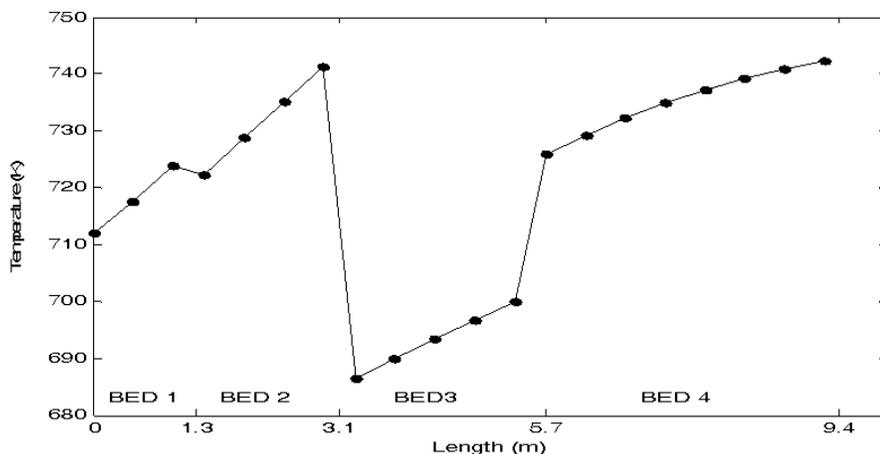
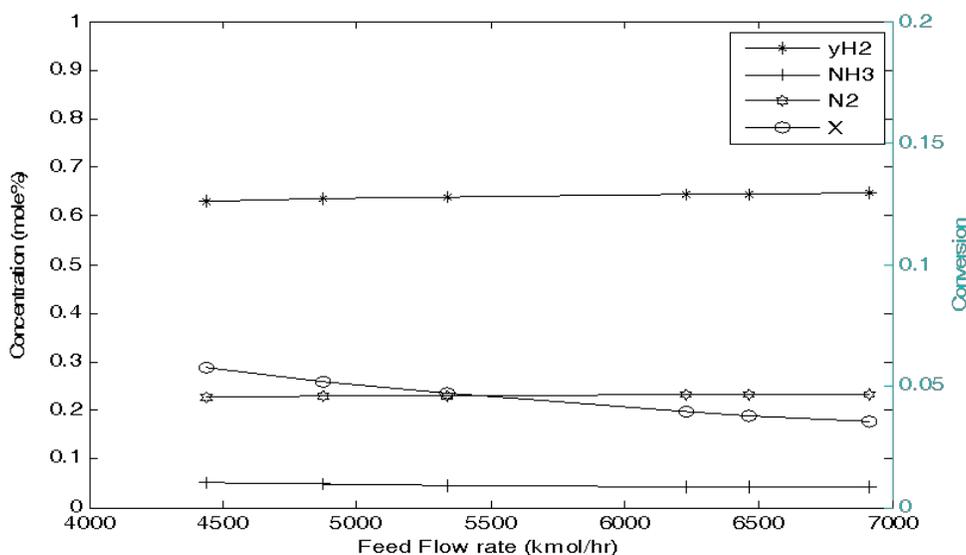Fig. 5. Temperature profiles along catalyst beds.

Fig. 6. Effect of Feed Flow rate on concentration and conversion.

adjust to annul the effect of this change, which is towards the production of more heat hence the equilibrium shifts to the right leading to the production of more ammonia. Similarly, when feed temperature is increased, the reaction rate is increased, but equilibrium shifts to the left resulting in decreased conversion of reactants and lower yield of ammonia. These trends the model accurately predicts as shown in figure 8.

The rates of reaction at low temperatures are extremely slow and catalyst deactivation leading to loss of iron surface area and activity is reported (Ye*et al*., 2001) to occur by thermal sintering at high temperature. Therefore, in practice a temperature range of 400-500°C is a compromise designed to achieve an acceptable yield of

ammonia within an acceptable time period (Nikola*et al*., 2010).

Effect of Input Pressure
Figure 9 shows the effect of input pressure of the feed on conversion and the reactant and product concentration.

The Ammonia synthesis reaction proceeds with a reduction in gas molecules (volume). According to Le Chetalier's Principle if the pressure of the converter is increased, the system adjusts to reduce the effect of this increase, that is, to reduce the pressure by having fewer gas molecules. Hence equilibrium shifts to the right resulting in higher conversion of reactants (decrease in concentration) and higher yield of ammonia. Higher yield
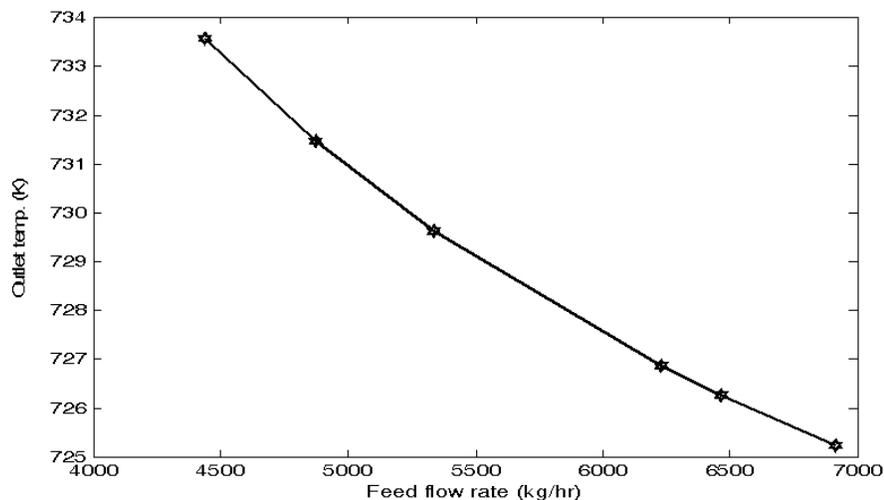
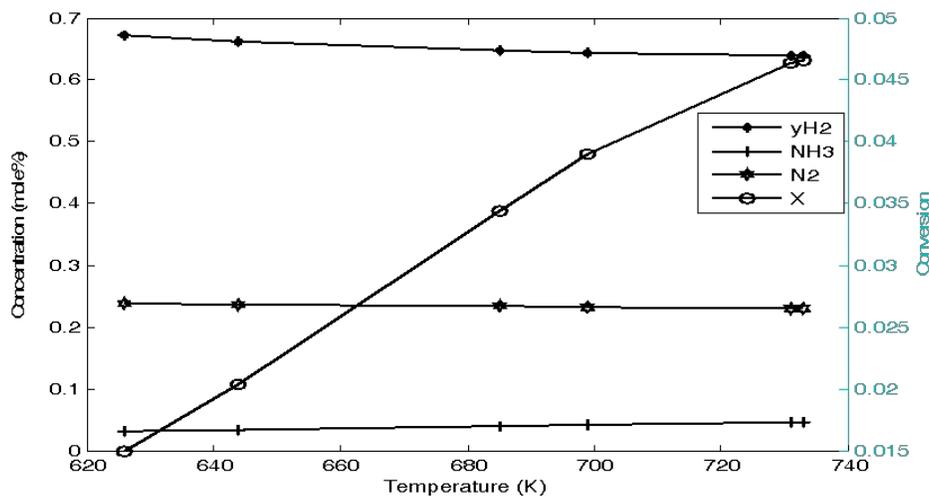Fig.7. Effect of Feed Flow Rate on Outlet Temperatures.

Fig. 8. Effect of Input Temperature on conversion and reactants concentration.

of ammonia means an increase in exothermic reaction leading to the release of more heat and resulting in an increase in outlet temperatures. Similarly, a decrease in pressure causes the equilibrium to shift to the left resulting in lower conversion of reactants and lower yield of ammonia; that is, a decrease in exothermic reaction resulting in a decrease in outlet temperatures. These trends the model accurately predicts as shown in figures 9 and 10 respectively. Although high pressure favors higher conversion, containing larger amounts of materials at high pressures are extremely difficult (Ye*et al*., 2001), therefore relatively low pressures are used industrially.

CONCLUSION

Model equations were developed from first principles by performing material and energy balances on the converter

to obtain one dimensional model equations that were used to predict the conversion and temperature variations within the catalyst bed of an ammonia converter. The developed models consisted of two coupled ordinary differential equations with a host of other algebraic/polynomial equations for determining various parameters in the models. The model equations were solved numerically using the 4th order Runge-Kutta algorithm implemented with MatLab ode45 solver. Data from an industrial ammonia converter at Notore - a chemical industry that produces urea and other nitrogenous fertilizer from ammonia, located at Onne in Rivers state, Nigeria were obtained and used in solving the model equations. The results obtained from solutions to the models were compared with output plant data of the ammonia converter and a maximum deviation between outputs from solved models and actual plant data
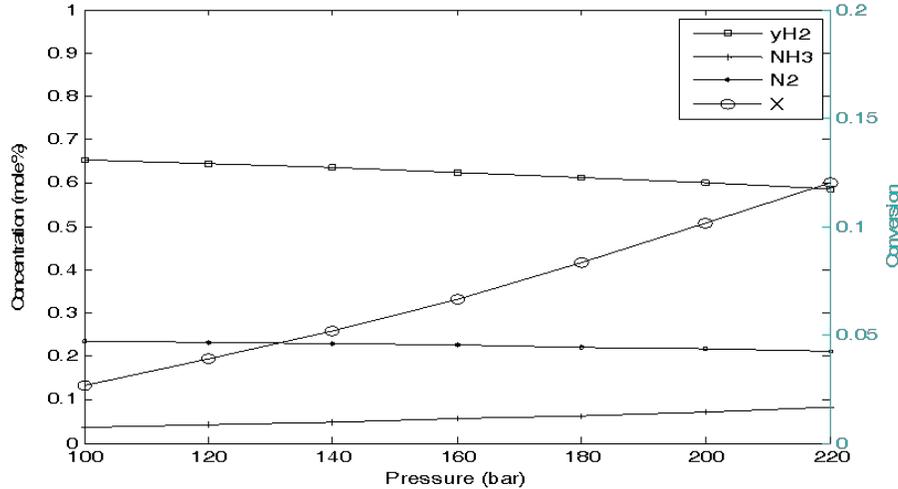
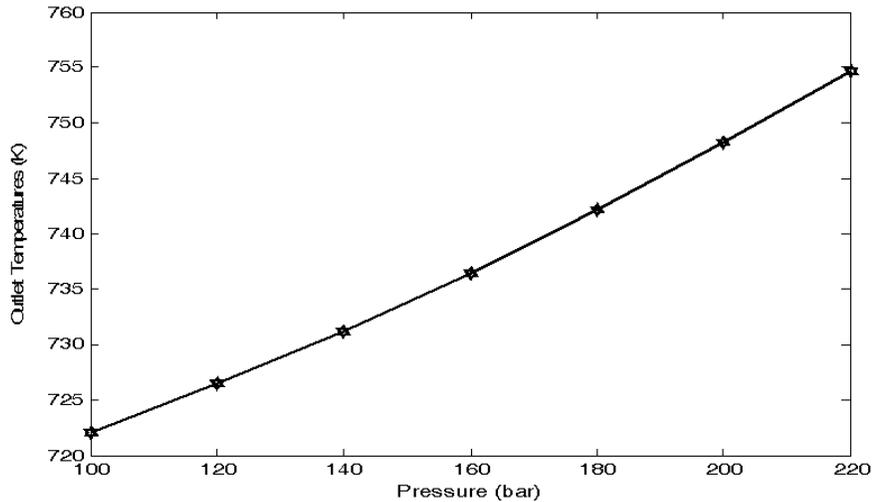Fig. 9. Effect of Input Pressures on different parameters.

Fig.10. Effect of feed input pressure on the outlet temperatures.

of 6.7% was obtained. Having validated the models, the models were used to simulate the ammonia converter. Parameters such asfeed flow rates, input/quench stream temperatures, and pressures into the first catalyst bed (BED #1) were simulate to investigate their effect the performance of the converter. Consequently, the effect of these variations on conversions, outlet temperature progression and reactants/product mixture concentrations along the reactor beds were determined.

NOMENCLATURE

A	Cross sectional area
a_i	activity of component i
C_i	Concentration of component i
C_{p_i}	Specific heat capacity of component i
Cp_{mix}	Specific heat capacity of gas mixture (KJ/Kml)
E	Activation Energy
Fi_o	Initial flow rate of component i
f_i	Fugacity of component i
f_i^0	Reference fugacity
K	rate constant for the reverse reaction
K_a	Equilibrium constant
K_o	Arrhenius coefficient
L	Length of converter bed (m)
M	Total mass flow rate
N_i	mole of component i
N_T	Total moles of reactants and product
P	Operating Pressure
P_i	Partial pressure of component i
P_T	Total Pressure
R	Universal gas constant
R_i	rate of reaction with respect to component i

T	Temperature
U	velocity reactant gases (m/s)
X	Fractional conversion of Nitrogen
Y_i	mole fraction of component i
ΔH_R	Heat of reaction
η	Effectiveness factor
$\emptyset_i$	Dimensionless fugacity coefficient of component i

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APPENDIX1. Mole Model (Stoichiometric) Table.

COMPONENT (symbol)	INITIAL MOLAR CONC. (MOLE/Hr)	AMOUNT OF REACTANT USED /PRODUCT PRODUCED	EXIT MOLAR CONC.	MOLE FRACTION (y_i)
(N_2)	$FY_{N2,0}$	$-FXY_{N2,0}$	$F(Y_{N2,0}-XY_{N2,0})$	$\dfrac{Y_{N2,0}(1-X)}{1-2XY_{N2,0}}$
(H_2)	$FY_{H2,0}$	$-3FXY_{N2,0}$	$F(Y_{H2,0}-3XY_{N2,0})$	$\dfrac{Y_{H2,0}-3X\,Y_{N2,0}}{1-2YN_{2,0}}$
(CH4)	$FY_{CH4,0}$	0	$FY_{CH4,0}$	$\dfrac{Y_{CH4,0}}{1-2XY_{N2,0}}$
(Ar)	$FY_{Ar,0}$	0	$FY_{Ar,0}$	$\dfrac{Y_{Ar,0}}{1-2XY_{N2,0}}$
(NH_3)	$FY_{NH3,0}$	$2FX\,Y_{N2,0}$	$F(Y_{NH3,0}+2XY_{N2,0})$	$\dfrac{Y_{NH3,0}+2YX_{N2,0}}{1-2XY_{N2,0}}$
Total	$(\sum_{i=1}^{5} Y_i) = F(1-2XY_{N2,0})$			