

Optimization of an Ammonia Synthesis Converter

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Abstract

A scheme that optimizes the converter of an ammonia synthesis plant to determine optimal inlet temperatures of the catalyst beds has been developed. The optimizer maximizes an objective function—The fractional conversion of nitrogen on the four catalyst beds of the converter subject to variation of the inlet temperature to each catalyst bed. An iterative procedure was used to update the initial values of inlet temperature thus ensuring accurate results and quick convergence. Converter model results obtained with optimized operating conditions showed significant increase in fractional conversion of 42.38% (from 0.1949 to 0.2586), increased rate of reaction evident in a 13.18% (0.5317 to 0.4616) and 23.84% (0.1946 to 0.1482) reduction in reactants (hydrogen and nitrogen) concentration respectively and a 56.48% increase (from 0.1181 to 0.1838) in ammonia concentration at the end of the fourth catalyst bed compared to results obtained with industrial operating conditions.

Keywords

Ammonia Synthesis Converter, Optimization, Optimal Inlet Bed Temperatures

1. Introduction

The need to operate process equipments at optimal conditions that ensures efficient performance and economic competitiveness of products of similar industries is a growing challenge to process designers and entrepreneurs of industries. An optimal set of design and operating parameters ensures that the industry/system functions in the most efficient way. One way of achieving this is through optimization. Optimization is a widely used engineering tool for enhancing efficiency and performance of systems. It is the process of determining the operating

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conditions of a process/system's parameters that ensures the most efficient operation of the system/process by adjusting the process parameters so as to maximize some specified set of parameters or one or more of the process specifications while keeping all others within their constraints. The improved efficiency/performance can be measured by the reduction in production cost, increase in profit or increase in the quantity of products produced. Operating parameters usually optimized include process variables such as flow rates, pressures, temperatures or equipment size such as volume, length and catalyst volume.

Optimization involves minimizing or maximizing an objective function; in most optimization problems, the objective function could be an economic return or term based on some parameters of the system, minimizing a cost function or maximizing a profit function; Optimizing the efficiency of the system by minimizing or maximizing parameters that indicates performance of the system viz: minimize specific energy consumption [1], optimize maximum energy output [2], minimum catalyst volume obtained to satisfy the production capacity at specified operating conditions [3], maximum mass flow rate of production using a generic algorithm at optimal conditions of inlet temperature, total feed flow rate and operating pressure [4], optimize reactor performance by varying its quench flows: Temperature and flow rate [5], obtain optimum reactor length [6] [7] that gives the maximum profit with objective function being: a function of the process parameters (heating value of product and feed gas) and reactor capital cost [8].

The ammonia synthesis converter is a major component of the ammonia synthesis loop. Steady state one dimensional pseudo-homogeneous models of an axial flow four catalyst bed ammonia synthesis converter were successfully developed by Akpa and Raphael [9]. The industrial plant data of Notore Chemical Industries Limited, located in Onne, Rivers State, Nigeria was used to run the developed simulation program (converter simulator) [9]. The developed model predicted a fractional conversion of 19.49% against the industrial plant output of 18.19%. This low output has necessitated the need for the optimization of the converter aimed at improvement in the converter performance by investigating new operational conditions/parameters that will result in improved higher conversion of the reactants to product.

In this work, a parameter that indicates directly the efficiency of the converter—the fractional conversion of the reactants to products is optimized. The model equation that predicts the fractional conversion of reactants to products is used as the objective function to be maximized.

2. Methodology

In an earlier work by Akpa and Raphael [9], models that accurately predicted the performance (concentration of reactants and products, fractional conversion and Temperature progression along the catalyst beds) of the converter were developed. In the simulation study performed on the converter, effects of process parameters (feed flow rate, inlet temperature and pressure) on the converter performance were investigated. The inlet temperatures of each catalyst bed were observed to be very sensitive to the performance of the converter. The outlet temperature of a previous bed obtained from model equation was quenched to correspond to the industrial value of the inlet temperature of the next bed.

However in this optimization; an optimum inlet temperature of each bed which will result in the highest fractional conversion, lowest reactant concentration and highest product concentration was determined.

A constrained non-linear optimization procedure was used to determine the optimum inlet temperatures of the four catalyst beds which maximize the objective function (model equation that predicts the fractional conversion of the ammonia converter).

The objective function to be maximized is:

$$F(T) = \frac{dX}{dL} = -\eta \frac{(R_{\text{NH}_3})A}{2F_{\text{N}_2\text{O}}} \quad (1)$$

Subject to the values of the inlet Temperature:

$$T_{\text{ind.}} \leq T_{\text{inlet}} \leq T_{\text{Design}} \quad (2)$$

where A = cross-sectional area of the bed (m^2); X = fractional conversion of Nitrogen; $F_{\text{N}_2\text{O}}$ = initial flow rate (mole/hr) of nitrogen reactant; L = length of bed (reactor) (m); R_{NH_3} = rate of production of ammonia (NH_3); η = effectiveness factor; $T_{\text{ind.}}$ = industrial plant inlet temperature; T_{Design} = design inlet temperature; T_{inlet} = inlet temperature of bed.

Where the reaction rate expression of Temkin-Pyzhez expressed in terms of activities by Dyson and Simon [10] had been expressed in terms of fractional conversion of the limiting reagent (nitrogen) by Akpa and Raphael [9] as:

$$R_{\text{NH}_3} = 2k \left(K_a^2 \phi_{\text{N}_2} \frac{Y_{\text{N}_2,0} (1-X)}{1-2XY_{2,0}} P \left[\frac{P(\phi_{\text{H}_2} (Y_{\text{H}_2,0} - 3XY_{\text{N}_2,0}))^3}{(1-2XY_{2,0})(\phi_{\text{NH}_3} (Y_{\text{NH}_3,0} + 2XY_{\text{N}_2,0}))^2} \right]^\infty - \left[\frac{(\phi_{\text{NH}_3} (Y_{\text{NH}_3,0} + 2XY_{\text{N}_2,0}))^2}{P(\phi_{\text{H}_2} (Y_{\text{H}_2,0} - 3XY_{\text{N}_2,0}))^3} \right]^{1-\infty} \right) \quad (3)$$

Other parameters in this equation can be obtained following the methods outlined in Akpa and Raphael [9].

The industrial values of the inlet temperature of each bed were used as starting guesses, with maximum possible value being the maximum value of the design temperature for the reactor and catalyst (823 K) above which the catalyst would begin to sinter [11]. Having established the lower and upper bounds of the constraint; a bracketing procedure [12] was employed to narrow the bracket until the inlet temperature value which satisfies (maximizes) the objective function was obtained. This ensures quick convergence and reasonable values of the inlet temperatures. The bisection method [13] was used to update the initial values of the inlet temperature of each bed using two initial guesses thus:

$$T_{i+1,j} = \frac{T_{i,j} + T_{\text{Design}}}{2} \quad (4)$$

where:

$T_{i+1,j}$ is the present value of the inlet Temperature of Bed j .

$T_{i,j}$ is the previous value of the inlet Temperature of Bed j .

T_{Design} is the value of design inlet Temperature.

An algorithm developed to solve this optimization problem is shown below:

Process Optimization Algorithm

Step 1: Guess initial inlet temperature of bed (industrial inlet temperature of each bed)

Step 2: Optimize converter bed j ($j = 1, 2, 3, 4$)

Determine converter performance:

Solve objective function to obtain fractional conversion of reactants in Bed j : Equation (1)

$$F(T_{i,j}) = \frac{dX}{dL} = -\eta \frac{(R_{\text{NH}_3})A}{2F_{\text{N}_2,0}}$$

using the program "CONVERTER SIMULATOR" [9].

The converter simulation program [9] also solves the model equation for the temperature progression along any catalyst Bed j :

$$\frac{dT}{dL} = \eta \frac{(-\Delta H_R) R_{\text{NH}_3} A}{mC_{p,\text{mix}}} \quad (4)$$

Equation (4) gives the outlet temperature of each bed.

Step 3: Update value of the inlet temperature using the bisection method

$$T_{i+1,j} = \frac{T_{i,j} - T_{\text{Design}}}{2}$$

Step 4: Optimize converter Bed j using present inlet temperature value

Solve objective function to obtain fractional conversion of reactants in Bed j : Equation (1)

$$F(T) = \frac{dX}{dL} = -\eta \frac{(R_{\text{NH}_3})A}{2F_{\text{N}_2\text{O}}}$$

using the program “CONVERTER SIMULATOR” [9].

The converter simulation program [9] also solves the model equation for the temperature progression along any catalyst Bed j : Equation (4)

$$\frac{dT}{dL} = \eta \frac{(-\Delta H_R) R_{\text{NH}_3} A}{mC_{p_{\text{mix}}}}$$

Step 5: Check if objective function has been maximized:

Compare present $F(T_{i+1,j})$ and previous $F(T_{i,j})$ values of the objective function.

Step 6: If answer to Step 5 is “YES”:

Optimum inlet of Bed j has been obtained.

If answer to Step 5 is “NO”:

Repeat Steps 3, 4, 5 and 6.

The steps above were followed to develop the optimization algorithm flow chart shown in **Figure 1**. A Math-Lab program was developed (Converter Optimizer) to solve the constrained nonlinear optimization problem following the algorithm flow chart.

Having obtained the optimum input/quench temperatures to Bed 1, 2, 3 and 4, these values (optimum temperatures) were then used to run the converter simulator program [9] to obtain the conversion, temperature variations and concentrations of the reactants (nitrogen N_2 , hydrogen H_2) and product (ammonia NH_3) at any point in the converter. The maximum conversion recorded at the end of Bed 4 is now taken as the optimum for the converter.

3. Discussion of Results

3.1. Effect of Inlet Temperature on Conversion in Each Bed

The result of optimization of the four catalyst beds of the converter by solving the objective function at varying inlet bed temperatures to obtain outlet fractional conversion for each catalyst bed is shown in **Figure 2**.

Figure 2 shows that the fractional conversion on each catalyst bed increases with increase in inlet temperature to a maximum point where further increase in inlet temperature results in a decrease in conversion. Thus it establishes the inlet temperature corresponding to this optimum conversion. The inlet temperature corresponding to the maximum conversion in a given bed is the optimum temperature of that bed. These optimum inlet temperatures from **Figure 2** are: Bed 1: 740 K with a maximum conversion of 5.70%; Bed 2: 750 K with a maximum conversion of 11.75%; Bed 3: 720 K with a maximum conversion of 17.66%; Bed 4: 700 K with a maximum conversion of 25.86%.

3.2. Effect of Optimum Inlet Temperatures on Percent Conversion

Having obtained the optimum inlet temperatures for each catalyst bed, the simulation program earlier developed by Akpa and Raphael [9] was used to obtain the optimum conversion, temperature progression and reactant and product concentrations along each catalyst bed. These converter performance parameters are shown in **Figures 3-5** respectively.

Figure 3 shows a steady increase in conversion along each catalyst bed and **Figure 4** shows the entire temperature of the four catalyst beds of the ammonia converter—temperature at the inlet, within and at the outlet of the catalyst beds while **Figure 5** shows the concentrations of the reactants (hydrogen and nitrogen) and product (ammonia) along each catalyst bed of the converter. The reactants decreased in concentration while the concentration of the product increased.

A comparison of the model prediction of converter performance using values of inlet bed temperatures from optimization results and industrial plant values [9] are presented in **Table 1** (fractional conversion and inlet and outlet temperature) and **Table 2** (concentration of reactants (Nitrogen and Hydrogen) and product (Ammonia)).

Table 1 and **Table 2** show the possible improvements in the converter performance when operated at the optimum conditions as predicted from the optimization performed on the converter.

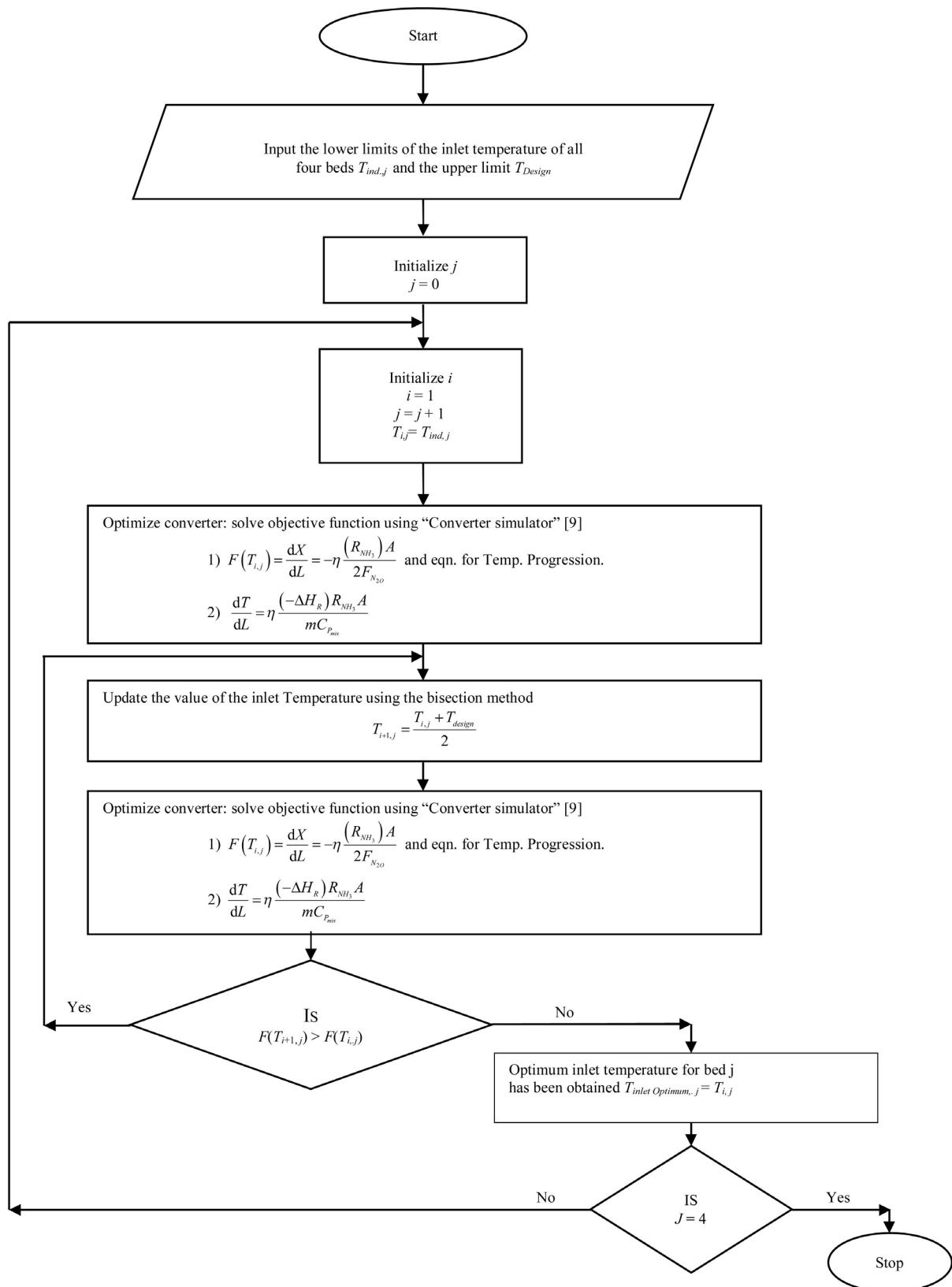


Figure 1. Flow algorithm for converter optimization.

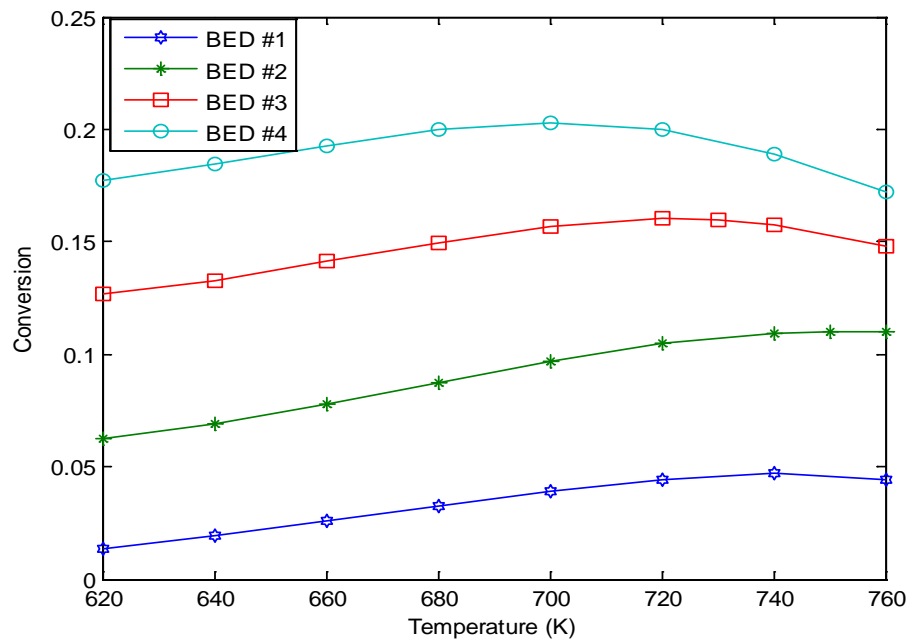


Figure 2. Effect of inlet temperature on conversion at the end of each catalyst bed.

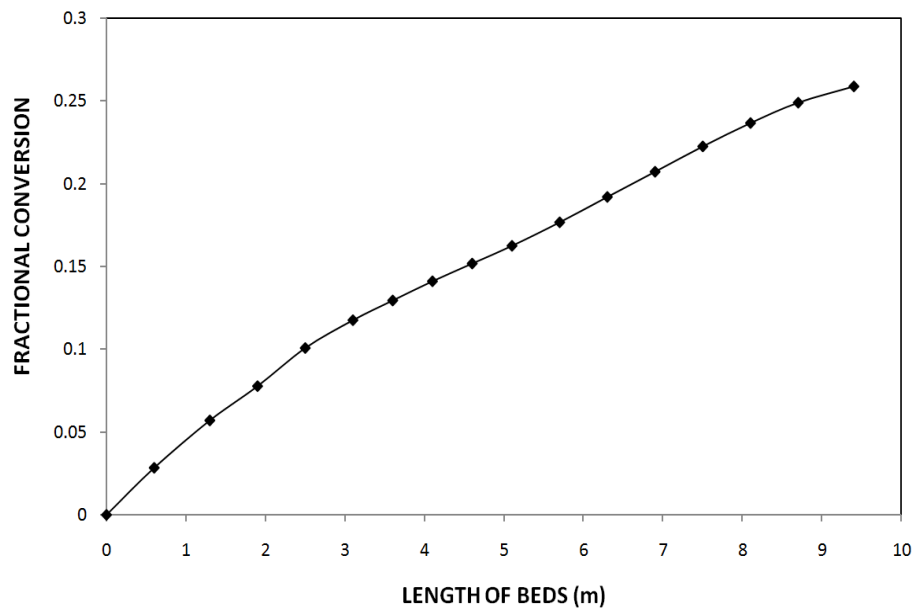


Figure 3. Fractional conversion along the catalyst beds.

Table 1. Comparison of optimization results with model prediction.

Bed	Bed Length (m)	Conversion		Inlet Temperature (K)		Outlet Temperature (K)	
		Model	Optimization	Model	Optimization	Model	Optimization
1	1.3	0.0427	0.057	712	740	727.96	757.22
2	1.8	0.1034	0.1175	721	750	743.50	773.66
3	2.6	0.1493	0.1766	685	720	702.48	739.52
4	3.7	0.1949	0.2586	726	700	742.88	716.60

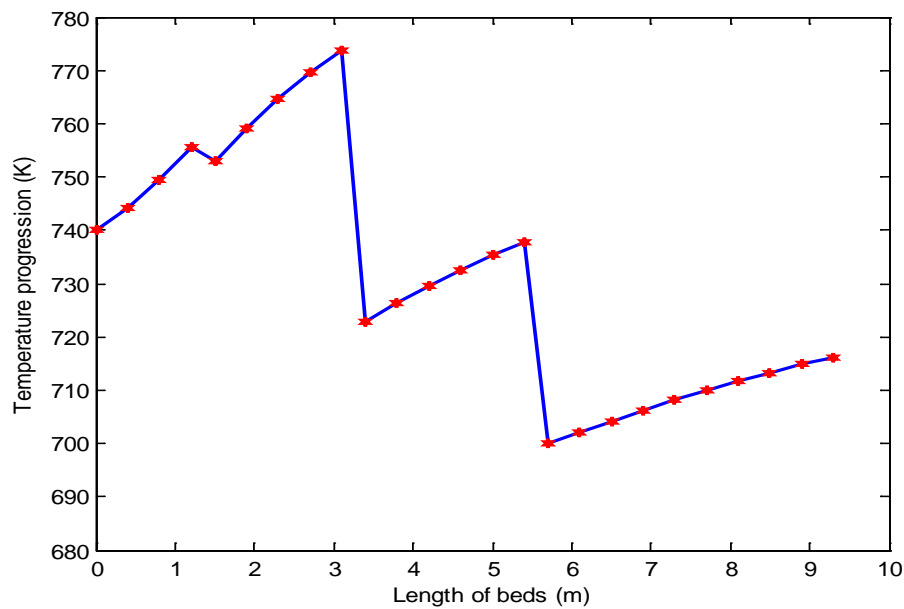


Figure 4. Temperature variation along the catalyst beds.

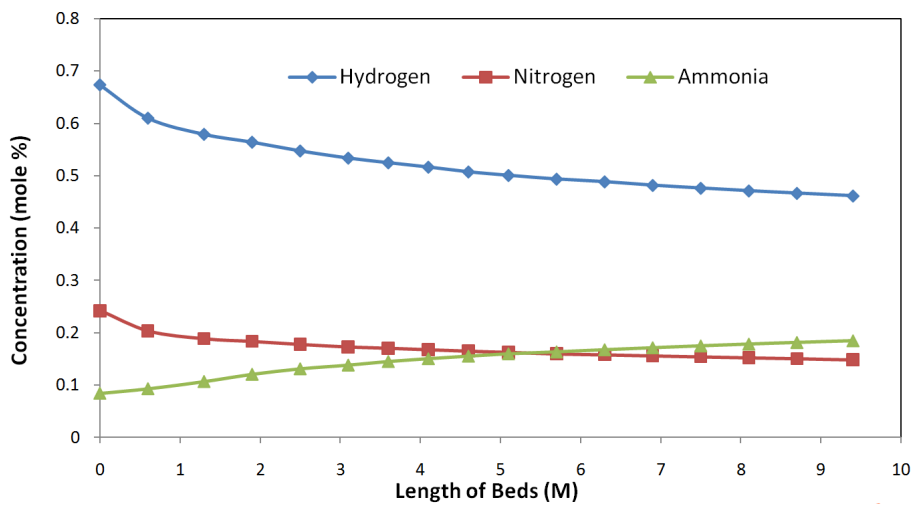


Figure 5. Concentration of reactants and product along the beds at optimum inlet temperatures.

Table 2. Comparison of optimization results with model prediction.

Bed	Concentration (mole %)					
	Hydrogen		Nitrogen		Ammonia	
	Model	Optimization	Model	Optimization	Model	Optimization
1	0.6395	0.5789	0.2314	0.1884	0.0445	0.1006
2	0.5967	0.5336	0.2167	0.1729	0.0748	0.1381
3	0.5621	0.4936	0.2056	0.1596	0.0978	0.1935
4	0.5317	0.4616	0.1946	0.1482	0.1181	0.1848

Table 1 shows that operating the converter at optimum conditions obtained from the optimization program results in an increase in the fractional conversion of the reactants to product from 0.1949 as predicted by model using industrial conditions to 0.2586 using optimized conditions. This corresponds to a 42.38% increase from

predictions using industrial conditions. The inlet temperatures at the optimum conditions were higher for the first three beds and lower for the fourth bed when compared with the industrial inlet temperatures. Increase in optimum inlet temperatures were also reported in the works of Saddiq *et al.* [2]. The outlet temperature at the end of the fourth catalyst bed also decreased from 742.87 K to 716.60 K indicating more efficient heat utilization resulting in a reduction in temperature.

Table 2 also shows that operating converter at optimized conditions result in reduction in reactants concentration in each bed (increased rate of reaction) culminating in a 13.18% (0.5317 to 0.4616 for the Hydrogen) and 23.84% (0.1946 to for the Nitrogen) concentration respectively at the end of the fourth catalyst bed; while the concentration of ammonia (the product) increased by 56.48% (from 0.1181 to 0.1838).

These results (increase in fractional conversion, reduction in reactants concentration and increase in product concentration) show improvements in converter efficiency when operated at optimized conditions.

4. Conclusions

One dimensional model was used for the optimization of the optimizations of an ammonia converter was performed to determine optimal inlet temperatures of the catalyst bed that will maximize an objective function—model equation that predicts the fractional conversion of the catalyst beds of the converter. The optimum inlet temperatures of the catalyst beds obtained were used as operating conditions for the converter. The converter model equations using these new optimum inlet temperatures predicted improved efficiency (42.38% increase in fractional conversion and 56.48% increase in ammonia concentration) compared with results obtained using industrial inlet catalyst bed temperature values.

An unsteady state and or two dimensional model of the ammonia converter are proposed for future study and simulation of the converter. The optimization procedure developed in this work can also be used for optimization of processes/systems.

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Nomenclature

- A : Cross sectional area (m^2)
 $C_{p_{mix}}$: Specific heat capacity of gas mixture (KJ/Kml)
 K : Rate constant for the reverse reaction
 K_a : Equilibrium constant
 L : Length of converter bed (m)
 M : Total mass flow rate (KJ/kmol)
 P : Operating pressure (Bar)
 R_i : Rate of reaction with respect to component i
 T : Temperature (K)
 X : Fractional conversion of nitrogen
 Y_i : Mole fraction of component i
 ΔH_R : Heat of reaction (KJ/kmol)
 η : Effectiveness factor
 ϕ_i : Dimensionless fugacity coefficient of component i
 α : Constant