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# Chemical Plant Design for the Production of Ammonia through Haldor Topsoe Process Route: Simulation using Plant Design Management System

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**Abstract:** Chemical plant design for the production of ammonia through Haldor Topsoe process route is presented. It involves the simulation of ammonia production plant with high energy efficiency and lower production cost. Material and energy balances of the complete process were determined using laws of conservation of mass and energy respectively. The material balance was taken to determine the quantities of raw materials required and ammonia produced. And the energy requirements were obtained from the energy balances. Plant Design Management System (PDMS) was used to simulate the process flow diagram. Economic tools of rate of return and payback period were used to determine the viability of the plant. Safety and plant location factors were considered. From the design analysis, plant production capacity of 640,288.800 metric tonnes per year was obtained. The energy required by the converter for the ammonia production is -241412233.8 kJ/hr (-68974.94 kW). The overall reaction is highly exothermic, and the primary reforming process is characterized by a low pressure. Plant Design Management System software is adequate for the simulation process. The plant required a total investment cost of #63.68 x $10^{10}$ (\$1.8 x $10^{9}$) with 5.17% rate of return, and payback period of six years. Procedure for hazard communication standard, that will ensure adequate safety, was recommended. Emene (in Enugu State, Nigeria) is found suitable for the installation of the ammonia plant. The geographical location of Emene will contribute immensely to the success of ammonia business venture.

**Keywords:** Ammonia Production, Plant Design, Simulation

## I. INTRODUCTION

Ammonia ($NH_3$) is one of the most vital chemicals used for the production of a variety of industrial products [1]. The critical temperature and pressure of ammonia is 132.4$^{o}$C and 111.3 atm with its heat of fusion, vapourisation and heat of combustion as 58.1 kJ/mol, 23.3 kJ/mol and -316 kJ/mol respectively. It is a colourless substance with a melting point of -77.7$^{o}$C and boiling point of -33.35$^{o}$C [2]. Considering the chemical properties, ammonia is a weak base with high affinity in water. It is a strong reducing agent that is quite reactive. Its volatility increases with increase in pH. Ammonia has numerous applications. It is used in the production of nitric acid, soda ash, cleaning agents, explosives, fertilizers, food and beverages. Its applications extends to leather tanning, petroleum refining, pulp and paper industry, textiles, refrigeration, rubber and synthetic resin industries [3, 4]. There is tremendous increase in ammonia demand by fertilizers and allied industries. At such, there is need to design large ammonia production plant with well-developed heat and cold recovery units. Suitable units will ensure improvement in heat utilisation and reduction of the refrigeration costs.

Direct ammonia synthesis is accomplished by passing a 3:1 mixture of hydrogen and nitrogen at elevated pressure and temperature over a catalytic material [5]. The production of ammonia requires the formation of molecular hydrogen followed by contacting the hydrogen with molecular nitrogen over a catalyst for ammonia synthesis. According to Kirova-Yordanova [6], exergy consumption of ammonia production plants depends strongly on the ammonia synthesis loop design. Thus, to increase the degree of conversion of hydrogen–nitrogen mixture to ammonia, the industrial ammonia synthesis should be designed as a recycle process (ammonia synthesis loop). The first breakthrough in large scale synthesis of ammonia resulted from the development of Haber process in 1913 in which ammonia was produced by direct combination of nitrogen and hydrogen, in the presence of catalyst [2, 4].

$$N_2 + 3H_2 \rightarrow 2NH_3 \qquad (1)$$

Intermittently, research efforts are made to improve ammonia production process. Ruthenium metal has been reported as active catalyst for the synthesis of ammonia from dihydrogen and dinitrogen at temperatures between 300 and 450$^{o}$C and at atmospheric pressure [7]. Kirova-Yordanova [6] applied exergy method to estimate the effect of the most important process parameters on the exergy efficiency of industrial ammonia synthesis. Also, Ilenia et al [8] carried out a set of kinetic tests on Ru/C catalyst for ammonia synthesis, under industrially relevant reaction conditions (temperature of 370-460 $^{o}$C, and pressure of 50-100 bar). The optimized parameters were obtained by modifying the Temkin equation with the addition of $H_2$ and $NH_3$ absorption terms. Better design and operation of ammonia synthesis reactors using Ru/C catalyst was achieved. It was observed that using Ru/C catalyst (instead of Fe based catalyst), working pressure decreased by 40-50%, with corresponding increase in productivity. Furthermore, Nikifor and Kardhish [9] reported continuously and batch wise production of ammonia by lithium-mediated electrochemical methods.

For the ammonia production, nitrogen is obtained through the air, while the hydrogen is produced by steam-methane autothermal reforming or by partial oxidation processes from natural gas or coal. That is, the synthesis gas for manufacture of $NH_3$ is produced by steam reforming or partial oxidation of hydrocarbon feed (natural gas or coal). Coal can be gasified with oxygen and steam to produce the syngas [10, 11, 12, 13]. The various processes used commercially in industries for production of Ammonia are; Haldor Topsoe process, Kellogg Brown and Roots Advanced Ammonia Process (KAAP), Krupp Uhde GmbH ammonia Process, The Linde Ammonia Concept (LAC) ammonia process, Haber process and Braun Purifier process. In this design work, naphtha from Enugu coal is chosen as source of hydrogen. Enugu coal (sub-bitummous and non-coking coal) is very rich in waxes and resins. It is a potential raw material for production of various chemicals. Naphtha is a flammable liquid hydrocarbon mixture which can be produced from natural gas condensates, petroleum distillates, and the distillation of coal tar and peat. Syngas, a mixture of hydrogen and carbon monoxide can also be produced from coal [10, 12]. The main sections for ammonia production are; hydrofining or desulphurization, steam reforming, shift CO conversion, $CO_2$ removal, final purification, ammonia synthesis, recovery, cracking, and liquefaction and storage.

Several research reports on ammonia production process exist [3, 14, 15, 16]. And the scientific reviews showed that energy efficiency and lower production cost are serious challenges to ammonia production. There is need to synthesis ammonia in an optimized manner; smarter, safer and more profitable way, with significantly reduced environmental impact. Thus, the aim of this study is to design a chemical plant for production of ammonia using Haldor Topsoe method. The process route was chosen because Topsoe's ammonia plant designs have good characteristics of being highly energy efficient and economically viable. Topsoe's low energy ammonia process scheme can be optimized for a wide range of operating conditions by selecting proper process technology and by adjusting the process parameters. Simulation of such process can be aided by Plant Design Management System (PDMS). PDMS is a 3-D Pipe Drafting software. It is used for engineering designs (including chemical and process plants) and construction projects.

## II. DESIGN METHOD

Material balances formed the basis of the process design [17, 18, 19]. The material and energy balances of the complete process were determined. A material balance was taken over the complete process in order to determine the quantities of raw materials required and product produced. Balances over individual process units set the process stream flows and compositions. The general law of conservation of mass was used to determine the material balances. The following estimates were used to determine the material balance data:

Estimated quantity of naphtha needed to be used, $C_8H_{18}$ = 650,000 metric tons/yr.), and the estimated quantity of Ammonia to be produced, $NH_3$ = 700,000 metric tons/yr.

Energy balances over individual process units were determined. Law of conservation of energy was adopted in the determination of the energy requirement data. Then the chemical process diagram was simulated using Plant Design Management System. The capital budgeting analysis started with the determination of all feasible alternatives [20]. And economic tools of rate of return and payback period (obtained from plot net cumulative cash inflow versus time) were used to determine the viability of the plant. More so, safety and plant location considerations were made.

## III. ANALYSIS OF THE PROCESS PLANT

### 3.1 Material balance of the plant

The flow streams for the material balance of each of the units are presented in Figures 1-7, while the corresponding complete data for the material balances are presented in Tables 1-7. In Figure (1), reaction of desulfurized naphtha and steam in a primary reformer (tubular reforming furnace) gave $C_8H_{18}$, $H_2$, CO and $CO_2$. The flow rates of these compositions are presented in Table 1. In the secondary reformer, the gases from the primary reformer react with air (Figure 2). The remaining hydrocarbon was further reformed, thereby increasing the overall hydrogen yield. The compositions of the secondary reformer are shown in Tables 2. The essence of adding air is to form a mixture of $H_2$ and $N_2$ for the ammonia synthesis process. As shown in Figures (4) and (5), Concentration of CO was reduced through its conversion to $CO_2$, in two stage converter. The material balances of the High Temperature Shift Converter and Low Temperature Shift Converter are presented in Tables (3) and (4) respectively. The gas leaving the high temperature converter was cooled and sent to low temperature converter where the gas passes over copper catalyst. In the shift convertor, the remaining CO was converted to $CO_2$. The flow streams of the counter current absorption column are shown in Figure (5). Flow rates of the absorber components are shown in Table 5. Carbon monoxide and Carbon dioxide which may act as catalyst poisons in the synthesis loop were removed by conversion into methane in the methanator (Figure 6). Then, the streams of the ammonia production by the reaction of nitrogen and hydrogen are shown in Figure (7). And 88,929.56 kg/hr (640,288.800 metric tonnes per year) of ammonia production is shown in Table (7)

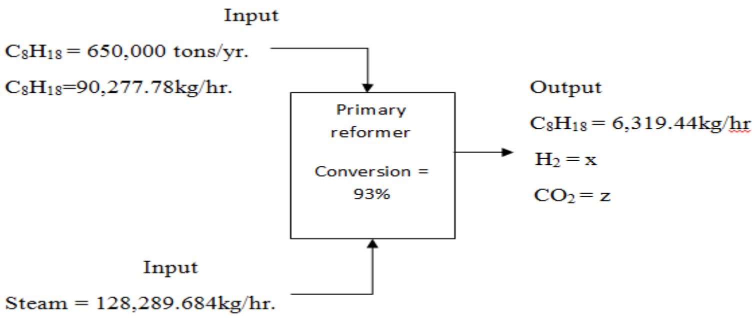


**Figure 1 Compositions and Flow Streams of the Primary Reformer**

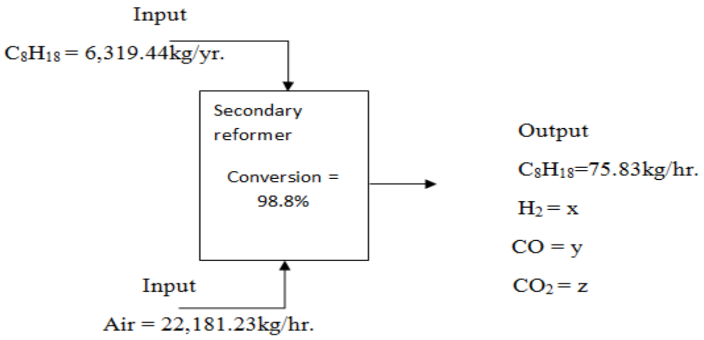


**Figure 2: Compositions and Flow Streams of the Secondary Reformer**

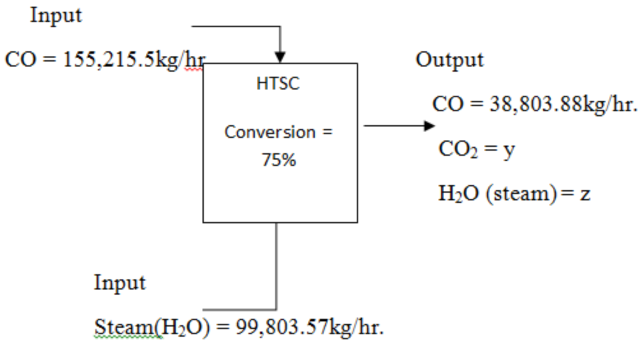


**Figure 3: Compositions and Flow Streams of the High Temperature Shift Converter (HTSC)**

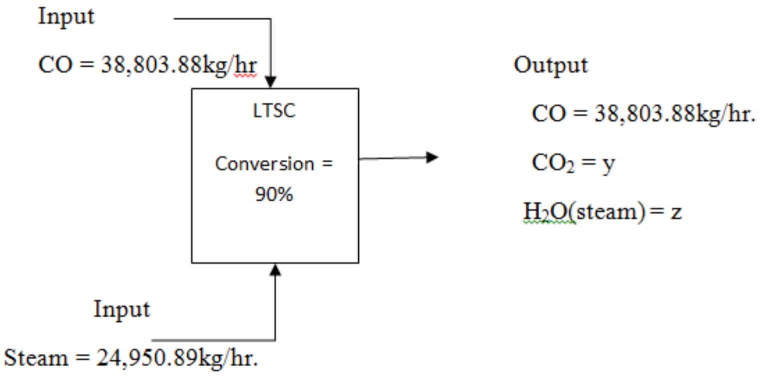


**Figure 4: Compositions and Flow Streams of the Low Temperature Shift Converter (LTSC)**

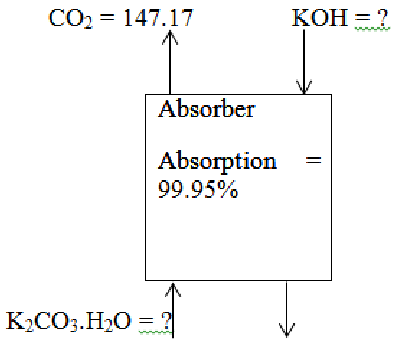


**Figure 5: Compositions and Flow Streams of the Absorber**

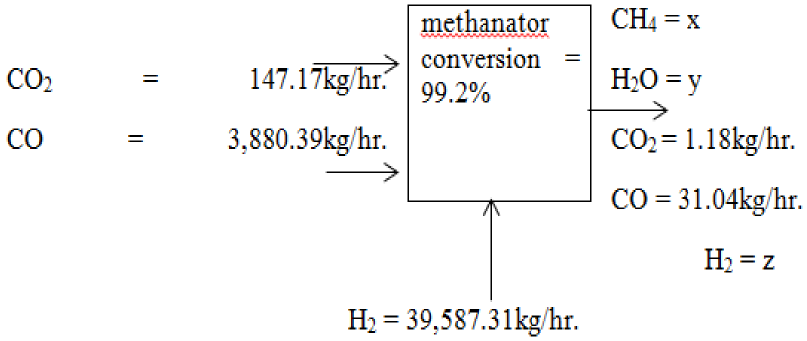


**Figure 6: Compositions and Flow Streams of the Methanator**

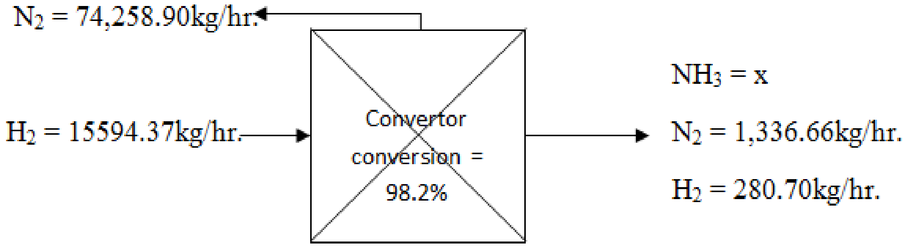


**Figure 7: Compositions and Flow Streams of the Convertor**

**Table 1: Material Balance of the Primary Reformer**

| INPUT | | OUTPUT | |
|---|---|---|---|
| Components | Flow rate (kg/hr) | Components | flow rate (kg/hr) |
| $C_8H_{18}$ | 90,277.78 | $C_8H_{18}$ | 6,319.44 |
| $H_{2O}$ | 128,289.684 | $H_2$ | 28,508.8 |
| | | CO | 155,215.5 |
| | | $CO_2$ | 34,843.2 |

**Table 2: Material Balance of the Secondary Reformer**

| INPUT | | OUTPUT | |
|---|---|---|---|
| Components | flow rate (kg/hr) | Components | flow rate(kg/hr) |
| $C_8H_{18}$ | 6,319.44 | $CO_2$ | 19,280.44 |
| Air | 22,181.23 | $H_2O$ | 8,873.39 |
| | | $O_2$ | 8,158.57 |
| | | $N_2$ | 74,258.90 |
| | | $C_8H_{18}$ | 75.83 |

**Table 3: Material Balance of the HTSC**

| INPUT | | OUTPUT | |
|---|---|---|---|
| Components | flow rate (kg/hr) | Components | flow rate (kg/hr) |
| CO | 155,215.5 | CO | 38,803.88 |
| Steam | 99.803.57 | $CO_2$ | 184,780.37 |
| | | $H_2$ | 8,512.39 |
| | | $H_2O$ | 23,426.38 |

**Table 4: Material Balance of the LTSC**

| INPUT | | OUTPUT | |
|---|---|---|---|
| Component | flow rate (kg/hr) | Component | flow rate (kg/hr) |
| CO | 38,803.88 | CO | 3880.39 |
| Steam | 24,950.89 | $CO_2$ | 55,434.11 |
| | | $H_2$ | 2,566.12 |
| | | $H_2O$ | 1,874.52 |

**Table 5: Material Balance of the Absorber**

| INPUT | | OUTPUT | |
|---|---|---|---|
| components | flow rate (kg/hr) | components | flow rate (kg/hr) |
| $CO_2$ | 294,338.12 | $CO_2$ | 147.17 |
| KOH | 750,562.21 | $K_2CO_3.H_2O$ | 1,045,500.52 |

**Table 6: Material Balance of the Methanator**

| INPUT | | OUTPUT | |
|---|---|---|---|
| Components | flow rate (kg/hr) | Components | flow rate (kg/hr) |
| $CO_2$ | 147.17 | $CH_4$ | 2,252.72 |
| CO | 3,880.39 | $H_2O$(steam) | 2,590.79 |
| $H_2$ | 39,587.31 | $H_2$ | 38,739.13 |
| | | $CO_2$ | 1.18 |
| | | CO | 31.04 |

**Table 7: Material Balance of the Convertor**

| INPUT | | OUTPUT | |
|---|---|---|---|
| Components | flow rate (kg/hr.) | Components | flow rate (kg/hr.) |
| $N_2$ | 74,258.90 | $NH_3$ | 88,929.56 |
| $H_2$ | 15,594.37 | $N_2$ | 1,336.66 |
| | | $H_2$ | 280.70 |

### 3.2 Energy balance of the plant

The energy balances over each of the equipment are presented in Tables (8) – (14). Each Table revealed the energy requirements of the process. It showed the heating, cooling, and power required for the plant operation. Initially the carbon monoxide burned in air to produce carbon dioxide, with increased temperature. Then adiabatic reaction of methane with steam occurred, and the outlet temperature decreased. The tabulated data revealed the pattern of energy usage. The energy required by the converter for the ammonia production is -241412233.8 kJ/hr (-68974.94 kW). The overall reaction is highly exothermic and the primary reforming process is characterized by a low pressure.

**Table 8: Energy Balance of the Primary Reformer**

| INPUT | | OUTPUT | | |
|---|---|---|---|---|
| Components | Flow rate (mole/hr.) | Components | Flow rate (mole/hr.) | Molar enthalpy (kJ/hr.) |
| $C_8H_{18}$ | 791,910.35 | $C_8H_{18}$ | 55,433.68 | 202.98 |
| $H_{2O}$ | 712,7204.67 | $H_2$ | 14,254.400 | 0.0298 |
| | | CO | 554,3410.71 | 0.0391 |
| | | $CO_2$ | 791,890.91 | 0.0521 |
| | | $H_2O$ | | 0.0361 |

Q = 757,408,537.1 W or 757,408.54 kW

**Table 9: Energy Balance of the Secondary Reformer**

| INPUT | | OUTPUT | | |
|---|---|---|---|---|
| Components | flow rate (mole/hr.) | Components | flow rate(mole/hr.) | Molar enthalpy(kj/hr. |
| $C_8H_{18}$ | 55433.68 | $CO_2$ | 438,191.82 | 0.0547 |
| Air | 693,163.44 | $H_2O$ | 492,966.11 | 0.0412 |
| | | $O_2$ | 254,955.31 | 0.0393 |
| | | $N_2$ | 2,652,103.57 | |
| | | $C_8H_{18}$ | 665.18 | 100.48 |

Q = -81612483.06W or 81612.48KW.

**Table 10: Energy Balance of the HTSC**

| INPUT | | OUTPUT | |
|---|---|---|---|
| Components | flow rate (mole/hr) | Components | flow rate (mole/hr) |
| CO | 5543410.71 | CO | 1385852.86 |
| Steam | 5544642.78 | $CO_2$ | 4199553.86 |
| | | $H_2$ | 4256195.0 |

Q = - 3.24 x $10^{10}$ kJ/hr.

**Table 11: Energy Balance of the LTSC**

| INPUT | | OUTPUT | |
|---|---|---|---|
| Component | flow rate (mole/hr) | Component | flow rate (mole/hr) |
| CO | 1385852.86 | CO | 1385852.86 |
| Steam | 1386160.56 | $CO_2$ | 1259866.14 |
| | | $H_2$ | 1283060 |
| | | $H_2O$ | 104140 |

Q = - 367730081.6k J/hr. = - 105065.74 kW

**Table 12: Energy Balance of the Absorber**

| INPUT | | OUTPUT | |
|---|---|---|---|
| Component | flow rate (mole/hr) | Component | flow rate (mole/hr) |
| $CO_2$ | 294338.12 | $CO_2$ | 147.17 |
| KOH | 750562.21 | $K_2CO_3.H_2O$ | 1045500.52 |
| Total | 1044900.33 | | 1044900.33 |

**Table 13: Energy Balance of the Methanator**

| INPUT | | OUTPUT | |
|---|---|---|---|
| Components | flow rate (mole/hr) | Components | flow rate (mole/hr) |
| $CO_2$ | 147.17 | $CH_4$ | 2252.72 |
| CO | 3880.39 | $H_2O$(steam) | 2590.79 |
| $H_2$ | 39587.31 | $H_2$ | 38739.13 |
| | | $CO_2$ | 1.18 |
| | | CO | 31.04 |

Q = 40333422.08kJ/hr.= 11523.835Kw

**Table 14: Energy Balance of the Convertor**

| INPUT | | OUTPUT | |
|---|---|---|---|
| Components | flow rate (mole/hr.) | Components | flow rate (mole/hr.) |
| $N_2$ | 74258.90 | $NH_3$ | 88929.56 |
| $H_2$ | 15594.37 | $N_2$ | 1336.66 |
| | | $H_2$ | 280.70 |

Q = -241412233.8 kJ/hr. = -68974.94 kW

### 3.3 The process plant design layout

The process plant design layout is shown in Figure 8, with the corresponding labelled view in Figure 9. It revealed the ammonia production plant layout. Plant Design Management System software is adequate for the simulation process.

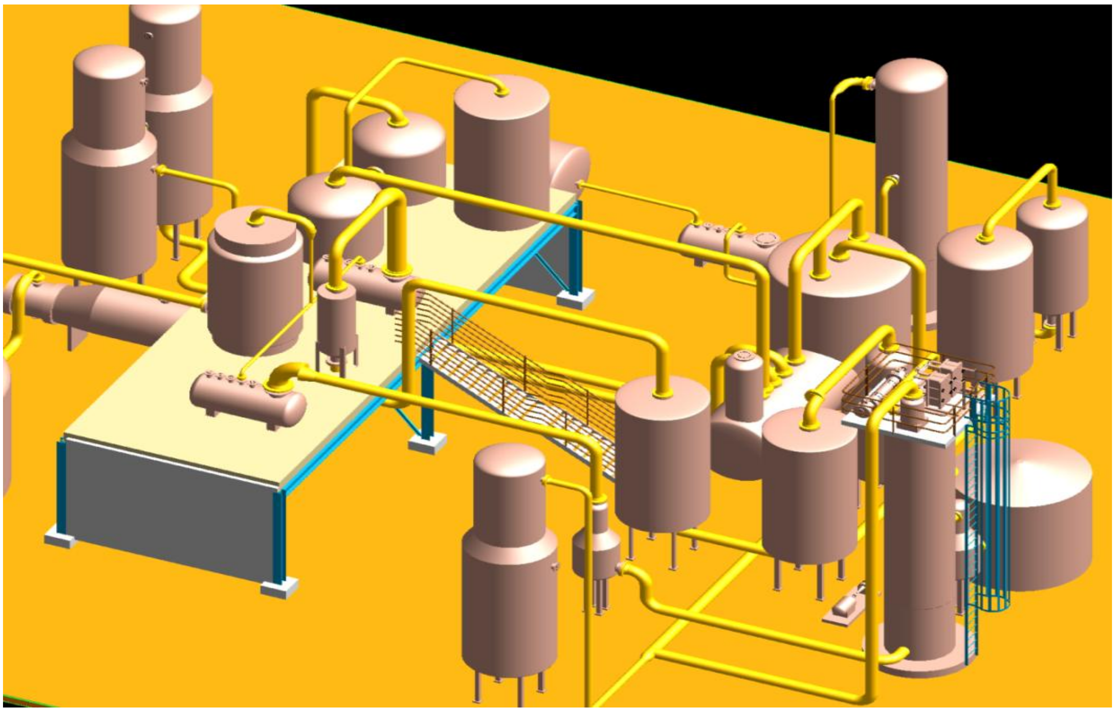


**Figure 8: Simulated Process Flow Diagram for the Ammonia Production (Isometric View)**

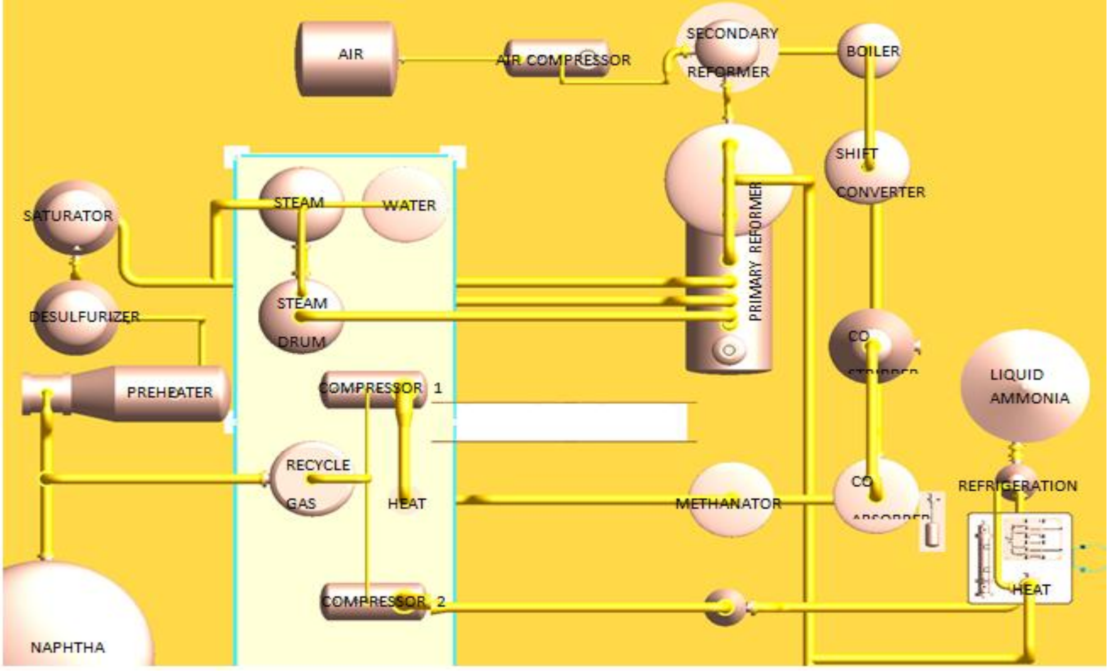
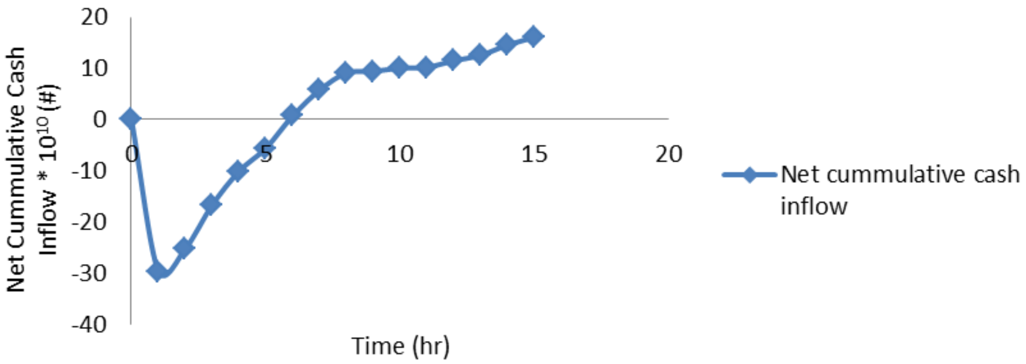


**Figure 9: Simulated Process Flow Diagram (with labels) for the Ammonia Production**

### 3.4 The economic analysis of the plant

Fundamental principles that give rise to the rationale of capital allocation were considered [18, 20]. From the economic analysis, the plant required a total investment cost of 63.68 x $10^{10}$ Nigerian naira (which is equivalent to 1.8 x $10^{9}$ USD), with 5.17% rate of return. The plot of Net Cumulative Cash Inflow (NCCI) versus time is presented in Figure 10. It revealed a payback period of six years (that is, breakeven point of 6 years). The progressive NCCI after the breakeven point confirmed the economic viability of the plant.



*# stands for Nigerian naira.*

### 3.5 Safety considerations and plant location

Safety issues of hazard identification, risk assessment and accident prevention were considered in this design work. Procedure for hazard communication standard was recommended. It is the responsibility of the ammonia manufacturers, importer and distributors to evaluate the hazards of the product and convey hazards information through labels and material safety data sheets to the employees and customers. This measure will ensure adequate safety. Emene is the selected place for the installation of the Plant. Emene is in Enugu East Local Government Area of Enugu State, Nigeria.

Naphtha (the basic raw material for ammonia production) can be sourced from Enugu coal. And Emene is the industrial area of Enugu State. The considered factors for the site of the plant include; nearness to source of raw material, proximity to market, availability of communication and transportation networks, water supply, labour supply, safety and environmental issues, Government industrial policy and characteristics of the geographical location [17, 18, 19]. The choice of Emene as the plant site will minimize cost of production and distribution. Consequently, the geographical location of Emene will contribute immensely to the success of ammonia business venture.

## IV. CONCLUSION

From the design analysis, the following conclusions can be made:

- The plant production capacity is 640,288.800 metric tonnes per year.
- The energy required by the converter for the ammonia production is -241412233.8 kJ/hr. The overall reaction is highly exothermic.
- Plant Design Management System software is adequate for the simulation process.
- The plant required a total investment cost of \$1.8 x $10^9$ with payback period of six year. The plant is economically viable.
- Emene (in Enugu State, Nigeria) is found suitable for the installation of the ammonia plant. The geographical location of Emene will contribute immensely to the success of ammonia business venture.
- Procedure for hazard communication standard, that will ensure adequate safety, was recommended.

## ACKNOWLEDGEMENTS

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