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# DESIGN AND SIMULATION OF HYDRO-DESULPHURIZATION UNIT IN AN AMMONIA PLANT

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**ABSTRACT**
The research work considered the design and simulation of 200 tons per year hydro-desulphurization plant for the removal of sulfur in the form of H2S in the cracked natural gas. The process flow diagram for the hydro-desulphurization plant consists of an absorber column and two fixed bed reactors in series aimed at absorbing the H2S using the MDEA/H2O as solvent and then removal of the sulphide from the absorbent through the series fixed bed reactors respectively. The models were simulated with plant data using MATLAB and Aspen HYSYS. The results from the various simulations showed that the absorber height, diameter, number and height of transfer units, and pressure drop gave values of 7.06m, 2.36m, 6 and 0.843m, and 18.43kN/m2 respectively. The cost results for the absorber gave $44,000 while cost for fixed bed reactor 1 gave $12,000 as well as cost for fixed bed reactor 2 gave $100,000. Finally, the models were validated with plant data and result showed that the models developed were reliable and good predictor of the process since the percentage deviations are of range 0 to 5, except H2S component which gave 66.7 when compared the final value with the plant composition. The design results for the absorber column and the reactors gave the diameters and heights of 2.36m and 5.06m; 2.3m and 6.74m; and 1.8m and 6.74m respectively. It was observed that the pressure drop of the fixed bed reactors were 0.7bar. Simulated models performed better and reliable as the models developed predicted the process well since the results from the simulations gave good values.

**Keywords:** Hydro-desulphurization Unit, Natural Gas, Ammonia Plant, Design

## 1. INTRODUCTION

Many natural and industrial gases contain H2S. The presence of H2S usually prohibits the direct use of these gases because of its toxic properties, the formation of SO2 upon combustion (acid rain), and the problems it (usually) gives in downstream processing (e.g. catalyst poisoning and corrosion of pipelines and process equipment). This means that it is often necessary to remove H2S from the gas stream prior to use. If any CO2 is present in the gas, simultaneous removal of CO2 from the gas stream can occur (Nima et al., 2021).

In the past a number of processes have been developed to utilize the precipitation reaction of metal ions with sulfide. So far, the main utilization of this reaction is found in the removal of heavy metal ions from e.g. electroplating waste streams. In these cases, the primary interest was the efficient removal of metal ions from the waste stream (Ray et al., 2013).

In the regeneration step copper sulfide is oxidized to CuSO4 in the presence of ammonium ions in a pressure vessel at a temperature of approximately 100 - 200 °C, and an oxygen partial pressure of 1.5 Bara. The product of this type of process is, apart from a cleaned-up steam flow, a concentrated stream of ammonium sulfate. The application of this process is rather limited because the process cannot

operate in a closed loop manner if under stoichiometric amounts of ammonia are present in the gas stream to be cleaned. (Maddox, 2010).

Bakhshi & Ebrahim, (2021), posited that nowadays, protecting the environment is of utmost importance worldwide, and sulfur dioxide is one of the main pollutants in the atmosphere. Their work proposed a new method for simultaneous SO2 removal by MgO, and production of magnesium sulfate in a packed bed reactor for which breakthrough curves have been obtained.

Dushyant et al., (2004), in their study, investigated the use of activated carbon for odorant removal from natural gas to be used for synthesis gas production for fuel cells. The odorants used in their study were dimethyl sulfide, tetrahydrothiophene, methyl mercaptan, and t-butyl mercaptan.

Nawaree, (2009), defined natural gas as a mixture of variable hydrocarbons and many contain other contaminants such as nitrogen, carbon dioxide and sulfur. The undesirable compound such as hydrogen sulfide must be removed to prevent corrosion and environmental problems.

Apoorva et al., (2018), suggested that the poor quality of crude oil obviously leads to high sulfur contents of oil products, and the technology for desulfurization of crude oil is urgently needed so that the sulfur contents in petroleum product could be reduced from the root.

Ramiar & Matthaus, (2019), intimated that, Sulfur, and in particular, H2S removal is of significant importance in gas cleaning processes in different applications, including biogas production and biomass gasification. H2S removal with metal oxides is one of the most viable alternatives to achieve deep desulfurization. This process is usually conducted in a packed bed configuration in order to provide a high solid surface area in contact with the gas stream per unit of volume.

Zhang et al., (2020), stated that order to realize zero discharge of desulfurization wastewater, spray drying technology of desulfurization wastewater was used in 660MW unit of a power plant. Its principle was to use a rotary atomizer for atomization, and a part of hot flue gas was drawn from the SCR denitrification reactor and air preheater into the drying tower, the heat was used to evaporate the desulfurization wastewater in a spray drying tower.

The specific objectives of the study are the develop design equations for the process through the application of the principle of conservation of mass and energy, Solve the developed models using MATLAB and Carry out Sensitivity Analysis on the functional parameters of the reactors.

Appropriate steps was taken to achieve the research goal: From the foregoing several gaps are still needed to be filled from all various literatures cited so far in this work. While many of the researchers mainly focused on the modeling and simulation of desulfurization from gas feeds there is still the need to include a comprehensive design of the various equipment modeled and determine functional parameters like volume, height, diameter, residence time of process equipment used in the developed models. While most researchers limited their study to the use of a single fixed bed reactor, no one has yet considered the use of multiple fixed bed reactor in series to further reduce the Sulphur content in the gas stream before processing it. Finally, a case study of Indorama Petrochemical Ltd. has not been considered. But in all of these researches published, no researcher has yet to comparatively investigate the design and simulation of Hydrodesulphurization Unit for Natural Gas Treatment in an Ammonia Plant.

Hence, this study is aimed at investigating the design and simulation of Hydrodesulphurization Unit for Natural Gas Treatment in an Ammonia Plant.

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## 2. MATERIALS AND METHOD

### Materials

Materials for the study were Calculator, laptop, reference books (text books, & journals) and Physiochemical data of the plant (Indorama Petrochemical Company and shall consist of process flow diagrams of natural gas desulphurization unit made up of majorly absorption and reactor sections, operating conditions for feed streams and other utilities).

### Methods

The development of the design equations for the absorber column and the fixed bed reactor for the hydro-desulphurization unit for natural gas in ammonia plant is carried out. The process flow diagram as shown in Figure 2.1 indicates the hydro-desulphurization unit which comprises of the absorber column where the H2S/CH4 gas mixture enters the absorber and the bottom and the absorbent (MDEA/H20) enters the column at the top counter currently for efficient absorption of the H2S from the gas mixture. The absorbed gas together with the solvent enters the first fixed bed reactor for the removal or treatment of the waste mixtures to generate the solvent back and the pollutant (H2S) separated from the waste mixture. Since the separation is not carried out completely, the second reactor is then used to completely separate the gas from the solvent. The method used for the development of the design models were based on the principle of material balance. The development of the models were also based on the works of Green et al., (2019) and Fogler, (2021) for the fixed bed reactor.

### Design of the Absorber

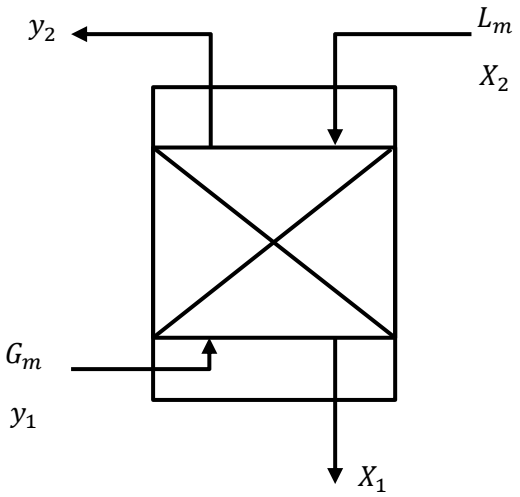



**Figure 2.1: Schematic diagram for material Balance on the Absorber Column**

For purity of the solvent,

$$X_2 = 0$$

$$Y = \frac{L_m}{G_m}X + Y_2 \qquad (2.1)$$

where, G_m is determinant based on the actual or theoretical value. Any of this value which is smaller is chosen for the absorber design. The slope, m of the equilibrium line is given as,

$$y_e = \frac{Y_e}{1+Y_e} \qquad (2.2)$$

$$x_e = \frac{X_e}{1+X_e} \qquad (2.3)$$

$$V_w^* = \left[\frac{K_4\rho_g(\rho_L-\rho_g)}{13.1F_P\left(\frac{\mu_L}{\rho_l}\right)^{0.1}}\right]^{\frac{1}{2}} \qquad (2.4)$$

where, $F_P$ is the packing factor size for the type of packing used in the absorption, $\mu_L$ is the liquid viscosity of the absorbent.

The column area $A_C$ is given or calculated in terms of $V_w^*$ as:

$$A_C = \frac{G_m}{V_w^*} \quad (2.5)$$

Column diameter is obtained as:

$$D_C = \left(\frac{4A_C}{\pi}\right)^{\frac{1}{2}} \quad (2.6)$$

The height of the absorber column is determined based on the overall gas transfer height, $H_{OG}$. This parameter is calculated based on the film transfer coefficients or film resistances for the liquid, $K_{OL}$ and gas, $K_{OG}$. These parameters are linked using correlation from Onda *et al*., (1968) as stated thus:

$$\frac{a_w}{a} = 1 - exp\left\{-1.45\left(\frac{\sigma_C}{\sigma_L}\right)^{0.75}\left(\frac{L_w^*}{a\mu_L}\right)^{0.1}\left(\frac{L_w^* a}{\rho_L^2 g}\right)^{-0.05}\left(\frac{L_w^{*\,2}}{\rho_L \sigma_L a}\right)^{0.2}\right\} \quad (2.7)$$

where, $a$ is actual area of packing per unit volume $\frac{m^2}{m^3}$, $a_w$ is effective interfacial area of packing per unit volume, $\frac{m^2}{m^3}$, $\sigma_C$ is critical surface tension for the particular packing material, $\sigma_L$ is liquid surface tension, N/m and g in acceleration due to gravity, $\frac{9.81m}{s^2}$, $L_w^*$ is liquid mass flow rate per unit column cross-sectional area $\frac{kg}{m^2.s}$.

The mass transfer coefficients, $K_L$ and $K_G$ are defined as,

$$K_L = 0.0051\left(\frac{L_w^*}{a_w\mu_L}\right)^{\frac{2}{3}}\left(\frac{\mu_L}{\rho_L D_L}\right)^{\frac{-1}{2}}(adp)^{0.4}\left(\frac{\rho_L}{\mu_L g}\right)^{\frac{-1}{3}} \quad (2.8)$$

where, $K_L$ is overall liquid film mass transfer coefficient, $\frac{kmol}{m^2}\left(\frac{kmol}{m^3}\right)$, $D_L$ is liquid diffusivity of the absorbent, $\frac{m^2}{s}$ and dp is the packing size, mm.

$$K_G = \frac{aD_V}{RT}K_5\left(\frac{G_m^*}{a\mu_V}\right)^{0.7}\left(\frac{\mu_V}{\rho_g D_V}\right)^{\frac{1}{3}}(adp)^{-2.0} \quad (2.9)$$

where, $K_G$ is overall gas film mass transfer coefficient $\frac{kmol}{m^2 s.atm}$ or $\frac{kmol}{m^2}s$ bar, $D_V$ is the vapoour diffusiity of the absorbent, $\frac{m^2}{s}$ $K_5$ is 5.23 for packing sizes above 15mm and 2.00

for packing sizes below 15mm, $G_m^*$ is gas mass flow rate per unit column cross-sectional area, $\frac{kg}{m^2 s}$ and $\mu_V$ is the vapour viscosity of the absorbent, Pa.s.

The film transfer unit heights are given by,

$$H_{OG} = \frac{G_m}{K_G a_w P} \quad (2.10)$$

$$H_{OL} = \frac{L_m}{K_L a_w C_t} \quad (2.11)$$

where, $P$ is column operating pressure, atm or bar, $C_t$ is total concentration $\frac{kmol}{m^3}\left(\frac{\rho_L}{M_{MDEA/water}}\right)$, $M_{MDEA/water}$ is molecular weight of the solvent (aqueous MDEA and water) and $G_m$ and $L_m$ are the molar flow rates per unit area cross-sectional flow for gas and liquid $\frac{kmol}{m^3}s$

$H_{OG}$ can also be calculated from the following equations as,

$$H_G = \frac{G}{k_G a_w P} \quad (2.12)$$

$$H_L = \frac{L}{k_L a_w C_t} \quad (2.13)$$

where, $K_G$ is gas film mass transfer coefficient $\frac{kmol}{m^2 s.atm}$ or $\frac{kmol}{m^2} s$ bar, $k_L$ is liquid film mass transfer coefficient $\frac{kmol}{m^2}\left(\frac{kmol}{m^3}\right)$

$$H_{OG} = H_G + \frac{mG_m}{L_m} H_L \quad (2.14)$$

The height of absorber column is this given as,

$$Z = N_{OG} H_{OG} \quad (2.15)$$

Including allowances, the total height, $Z_T$ is given as,

$$Z_T = 1.3Z \quad (2.16)$$

**Development of Design Equation for Fixed Bed Reactor**

**Design Assumptions**

The following assumptions are necessary for the design of a packed bed reactor.

i. The reactor is operated at unsteady state
ii. The composition of the reacting mixture is uniform only in the radial direction
iii. Balance can be made about a differential volume of reactor
iv. No conversion of reactant prior to inflow to the reactor volume.
v. The process is non-isothermal

***Volume of the Reactor***

$$V = F_{AO} \int_{\propto_{A0}}^{\propto_A} \frac{d\propto_A}{-r_A} \quad (2.17)$$

***Weight of Catalyst***

$$W = \rho F_{AO} \int_{\propto_{A0}}^{\propto_A} \frac{d\propto_A}{-r_A} \quad (2.18)$$

***Length of Reactor***

$$L_R = \frac{4F_{AO}}{\pi D^2} \int_{X_{A0}}^{X_A} \frac{dX_A}{(-r_A)} \quad (2.19)$$

***Space Time***

$$\tau = C_{A0} \int_{\propto_{A0}}^{\propto_A} \frac{d\propto_A}{-r_A} \quad (2.20)$$

***Space Velocity***

$$S_V = \frac{1}{\tau} \quad (2.21)$$

***Heat Load***

$$q = \frac{Q}{V_R} \quad (2.22)$$

where

$$Q = \Delta H_{rA} F_{A0} \propto_A \quad (2.23)$$

***Heat of Reaction***

$$\Delta H_{RA} = \Delta H_{RA}^{o} + \int_{T0}^{T} V \Delta C_p \, \Delta T \quad (2.24)$$

***Mechanism and Kinetics***

Thiols and sulphides react to form hydrogen sulphide and HC,

$$RSH + \rightarrow H_2 \rightarrow RH + H_2S \quad (2.25)$$

Mechanical Design Models for the Hydro-Desulphurization Plant

***Cylindrical shell thickness***

$$t_i = \frac{P_i D_i}{2fJ - P_i} + e \quad (2.26)$$

where, $t_i$ is the thickness of the unit to be designed, J is 100% fully radiographed, and e is the corrosion allowance

***Design of flat ends***

$$t_p = C_P D_e \sqrt{\frac{P_i}{f}} + e \quad (2.27)$$

where, $C_P$ is fully face gasket, 0.4, and $D_e$ is the bolt circle diameter which is also the design diameter.

**Doomed Head Design**

***Ellipsoidal head***

$$t_i = \frac{P_i D_i}{2fJ - 0.2P_i} + e \quad (2.28)$$

***Torispherical head***

$$t_i = \frac{P_i D_i C_s}{2fJ + P_i(C_s - 0.2)} + \quad (2.29)$$

where,C_s is stress concentration factor for torespherical head

## 3. RESULTS AND DISCUSSION

The result obtained from the taking material balance around the entire absorber and reactors and solving them via MATLAB R2022a is presented in Tables 4.2 to 4.3 and Figures 4.1 to 4.4. The absorber has two inlets (inlet Gas and inlet solvent) streams and two outlet streams (Gas outlet and Liquid Outlet). The output from the absorber were sent to the two reactors configured to operate in series for the purpose of reducing the amount of $H_2S$ to the barest minimum. The validation of the models results with plant is displaced in Table 4.1 and the sensitivity results of the volumetric flow rate effect on the functional parameters results of the reactors is shown in Figures 4.5 to 4.9.

**Model Validation with Plant Data**

**Table 1: Comparison of Model Prediction with Plant Data**

| Stream Component | Plant Data | Model Prediction | % Deviation |
|---|---|---|---|
| **$CH_4$** | 0.8 | 0.83509 | 4.4 |
| **$C_2H_6$** | 0.0288 | 0.029966 | 4 |
| **$C_3H_8$** | 0.02 | 0.020763 | 3.815 |
| **$C_4H_{10}$** | 0.01 | 0.010361 | 3.61 |
| **$CO_2$** | 0.08 | 0.075478 | 5.65 |
| **$O_2$** | 0.001 | 0.001045 | 4.5 |
| **$N_2$** | 0.01 | 0.010446 | 4.46 |
| **$H_2S$** | 0.05 | 0.016641 | 66.7 |
| **He** | 0.0001 | 0.000104 | 4 |
| **Ne** | 0.0001 | 0.000105 | 5 |
| **MDEA** | 0 | 1.08E-06 | 0 |
| **$H_2O$** | 0 | 0 | 0 |

**Table 2: Results obtained from Material Balance Result for the Absorption of $H_2S$ from Natural Gas**

| | Input 1 | | Input 2 | | Output 1 | | Output 2 | |
|---|---|---|---|---|---|---|---|---|
| Component | S1 (mol) | S1 (mol/h) | S2 (mol) | S2 (mol/h) | S3 (mol) | S3 (mol/h) | S4 (mol) | S4 (mol/h) |
| $CH_4$ | 0.8 | 7728.80 | 0 | 0.00 | 0.83509 | 7722.91 | 0.002136 | 2120.80 |
| $C_2H_6$ | 0.0288 | 278.24 | 0 | 0.00 | 0.029966 | 277.13 | 0.000413 | 76.35 |
| $C_3H_8$ | 0.02 | 193.22 | 0 | 0.00 | 0.020763 | 192.02 | 0.00045 | 53.02 |
| $C_4H_{10}$ | 0.01 | 96.61 | 0 | 0.00 | 0.010361 | 95.82 | 0.000296 | 26.51 |
| $CO_2$ | 0.08 | 772.88 | 0 | 0.00 | 0.075478 | 698.02 | 0.028234 | 212.08 |
| $O_2$ | 0.001 | 9.66 | 0 | 0.00 | 0.001045 | 9.66 | 7.46E-07 | 2.65 |
| $N_2$ | 0.01 | 96.61 | 0 | 0.00 | 0.010446 | 96.60 | 4.05E-06 | 26.51 |
| $H_2S$ | 0.05 | 483.05 | 0 | 0.00 | 0.016641 | 153.90 | 0.124177 | 132.55 |
| He | 0.0001 | 0.97 | 0 | 0.00 | 0.000104 | 0.96 | 4.98E-07 | 0.27 |
| Ne | 0.0001 | 0.97 | 0 | 0.00 | 0.000105 | 0.97 | 0 | 0.27 |
| MDEA | 0 | 0.00 | 1 | 2238.00 | 1.08E-06 | 0.01 | 0.844289 | 0.00 |
| $H_2O$ | 0 | 0.00 | 0 | 0.00 | 0 | 0.00 | 0 | 0.00 |
| TOTAL | 1 | 9661.00 | 1 | 2238.00 | 1 | 9248.00 | 1 | 2651.00 |

**Table 3: Results obtained from Sizing and Specification of Absorber Unit**

| Parameter | Value | Unit |
|---|---|---|
| $N_{OG}$ | 6 | |
| Cross Sectional Area | 4.3704 | $m^2$ |
| Diameter | 2.3589 | m |
| $H_{OG}$ | 0.8431 | m |
| Height (Z) | 5.0586 | m |
| Allowance for Liquid Distribution | 1 | m |
| Allowance for Liquid Redistribution | 1 | m |
| Total Height of Absorber | 7.0586 | m |
| Degree of Wetting | $1.99 \times 10^{-5}$ | $m^3/m.\ sec$ |
| Pressure Drop | 18.43 | $KN/m^2$ |
| Volume of Packing/plates | 31 | $m^3$ |

Table 3 shows the sizing/design result for fixed bed reactor 1, the sizing parameters considered includes diameter, cross sectional area, residence time, space velocity, reactor volume, and volumetric flow rate whose values are shown in Table 5.

**Table 4: Results obtained from Sizing of Fixed Bed Reactor 1**

| Parameter | Value | Unit |
|---|---|---|
| Operating Temperature | 60 | $^oC$ |
| Operating Pressure | 30 | bar |
| Height of Reactor | 6.74 | m |
| Diameter | 2.3 | m |
| Cross sectional area | 4.154 | $m^2$ |
| Residence time | 8.3 | mins |
| Space Velocity | 0.12 | $min^{-1}$ |
| Reactor Volume | 249 | $m^3$ |
| Corrosion allowance | 2 | mm |
| Design Pressure Drop | 0.7 | bar |
| Material of Construction | Carbon Steel | |
| Volumetric flow Rate | 30 | $m^3/h$ |

Table 4 shows the sizing/design result for fixed bed reactor 1, the sizing parameters considered includes diameter, cross sectional area, residence time, space velocity, reactor volume, and volumetric flow rate whose values are shown in Table 6.

**Table 5: Results obtained from Sizing of Fixed Bed Reactor 2**

| Parameter | Value | Unit |
|---|---|---|
| Operating Temperature | 400 | $^oC$ |
| Operating Pressure | 42 | bar |
| Height of Reactor | 6.74 | m |
| Diameter | 1.8 | m |
| Cross sectional area | 2.544 | $m^2$ |
| Residence time | 4.3 | mins |
| Space Velocity | 0.2380 | $min^{-1}$ |
| Reactor Volume | 129 | $m^3$ |
| Corrosion allowance | 2 | mm |
| Design Pressure Drop | 0.7 | bar |
| Material of Construction | Carbon Steel | |
| Volumetric flow Rate | 30 | $m^3/h$ |

**Table 6: Results obtained from Mechanical Design for the Absorber Column**

| Parameter | Value | Unit |
|---|---|---|
| Operating Pressure | 42 | Bar |
| Design Pressure | 45.1 | Bar |
| Design Temperature | 400 | $^oC$ |
| Maximum Allowable Stress | 92.39 | $N/mm^2$ |
| **Cylindrical Section** | | |
| Thickness | 18.9 | mm |
| Corrosion Allowance | 2 | mm |
| **Flat Head** | | |
| Thickness | 45.44 | mm |
| Corrosion Allowance | 2 | mm |
| **Domed Head** | | |
| **Standard Dished Head** | | |
| Crown radius | 2.4 | mm |
| Knuckle Radius | 0.144 | mm |
| Thickness | 87 | mm |
| **Standard Ellipsoidal Head** | | |
| Thickness | 18.88 | mm |

**Table 7: Results obtained from Mechanical Design of a Fixed Bed Reactor 1**

| Parameter | Value | Unit |
|---|---|---|
| Operating Pressure | 42 | Bar |
| Design Pressure | 45.1 | Bar |
| Design Temperature | 400 | $^oC$ |
| Maximum Allowable Stress | 153.46 | $N/mm^2$ |
| **Cylindrical Section** | | |
| Thickness | 90.8 | Mm |
| Corrosion Allowance | 2 | Mm |
| **Flat Head** | | |
| Thickness | 117.3 | mm |
| Corrosion Allowance | 2 | mm |
| **Domed Head** | | |
| **Standard Dished Head** | | |
| Crown radius | 2.4 | mm |
| Knuckle Radius | 0.144 | mm |
| Thickness | 240.7 | mm |
| **Standard Ellipsoidal Head** | | |
| Thickness | 90.7 | mm |

**Table 8: Results obtained from Mechanical Design for Fixed Bed Reactor 2**

| Parameter | Value | Unit |
|---|---|---|
| Operating Pressure | 42 | Bar |
| Design Pressure | 45.1 | Bar |
| Design Temperature | 400 | $^oC$ |
| Maximum Allowable Stress | 92.39 | $N/mm^2$ |
| **Cylindrical Section** | | |
| thickness | 22.9 | mm |
| Corrosion Allowance | 2 | mm |
| **Flat Head** | | |
| thickness | 33 | mm |
| Corrosion Allowance | 2 | mm |
| **Domed Head** | | |
| **Standard Dished Head** | | |
| Crown radius | 2.4 | mm |
| Knuckle Radius | 0.144 | mm |
| Thickness | 66 | mm |
| **Standard Ellipsoidal Head** | | |
| Thickness | 22.4 | mm |

**Table 9: Results obtained from Costing of Absorber**

| Parameter | Value | Unit |
|---|---|---|
| Material of Construction | Stainless Steel | |
| Operating Pressure | 17 | Bar |
| Pressure Factor | 1.1 | |
| Material Factor | 2.0 | |
| Bare Cost | 20,000 | USD |
| Bare Cost | 15,270,600 | Naira |
| Purchased Cost | 44,000 | USD |
| Purchased Cost | 33,595,320 | Naira |

**Table 10: Results obtained from Costing of Fixed Bed Reactor 1**

| Parameter | Value | Unit |
|---|---|---|
| Material of Construction | Stainless Steel | |
| Operating Pressure | 42 | Bar |
| Pressure Factor | 2.0 | |
| Material Factor | 2.0 | |
| Bare Cost | 30,000 | USD |
| Bare Cost | 34,350,000 | Naira |
| Purchased Cost | 120,000 | USD |
| Purchased Cost | 137,400,000 | Naira |

**Table 11: Results obtained from Costing of Fixed Bed Reactor 2**

| Parameter | Value | Unit |
|---|---|---|
| Material of Construction | Stainless Steel | |
| Operating Pressure | 42 | Bar |
| Pressure Factor | 2.0 | |
| Material Factor | 2.0 | |
| Bare Cost | 25,000 | USD |
| Bare Cost | 28,625,000 | Naira |
| Purchased Cost | 100,000 | USD |
| Purchased Cost | 114,500,000 | Naira |

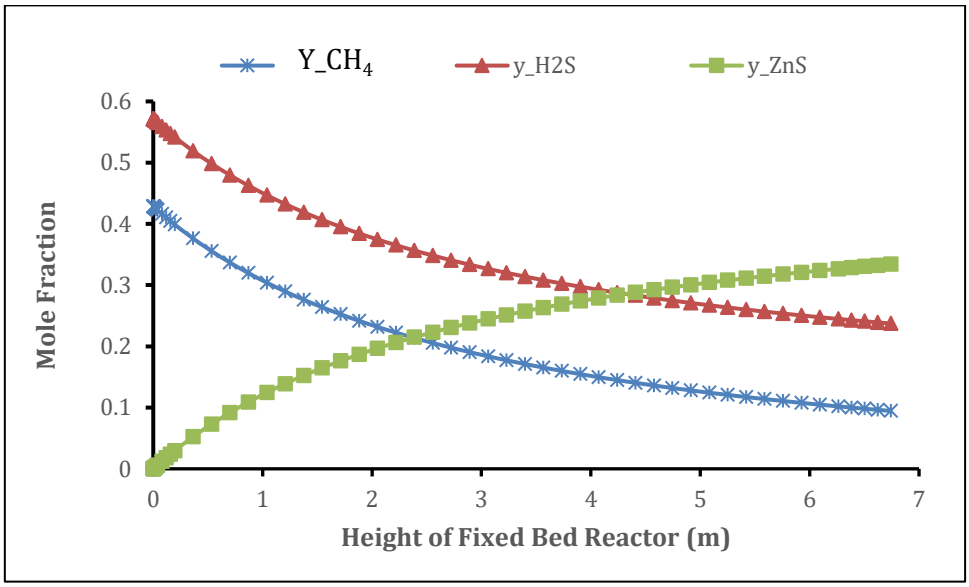



Figure 3: Profile Plot of Mole Fraction Versus Reactor 1 Height

Figure 3 depicts the profile plot of mole fraction of reactants (CH4 and H2S) and desired product (ZnS) changing along the height of the reactor. A careful examination of Figure 3 reveals that the result obtained from simulation of developed model equations capable of predicting the mole fraction of reactants and products with reactor height is in agreement with trend. The first reactant component which is $CH_4$ started the reaction with an initial mole fraction of 0.42 and this value continued to decrease to a final mole fraction was 0.09.

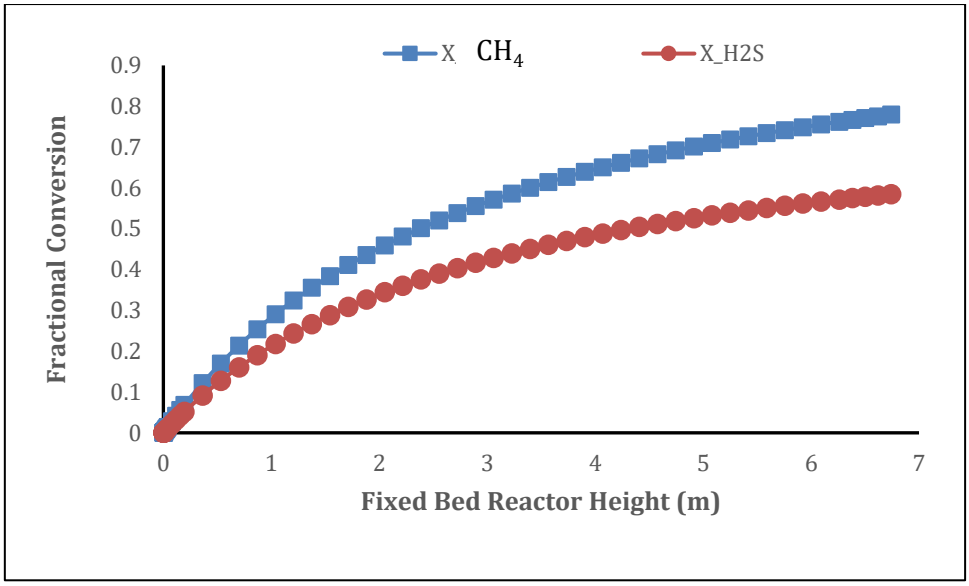



Figure 4: Profile Plot of Conversion Versus Reactor 1 Height

Figure 4 shows the plot of conversion of reactants along the height of the fixed bed reactor, after the absorption of H2S from the absorption unit, the unabsorbed $H_2S$ is sent to the reactor section where ZnO which acts as the catalyst in this reaction reacts with $H_2S$ to further reduce the concentration of H2S. From the results obtained from the simulation, the conversion of ZnO rose from 0 to 78% while that of $H_2S$ rose from 0 to 58%.

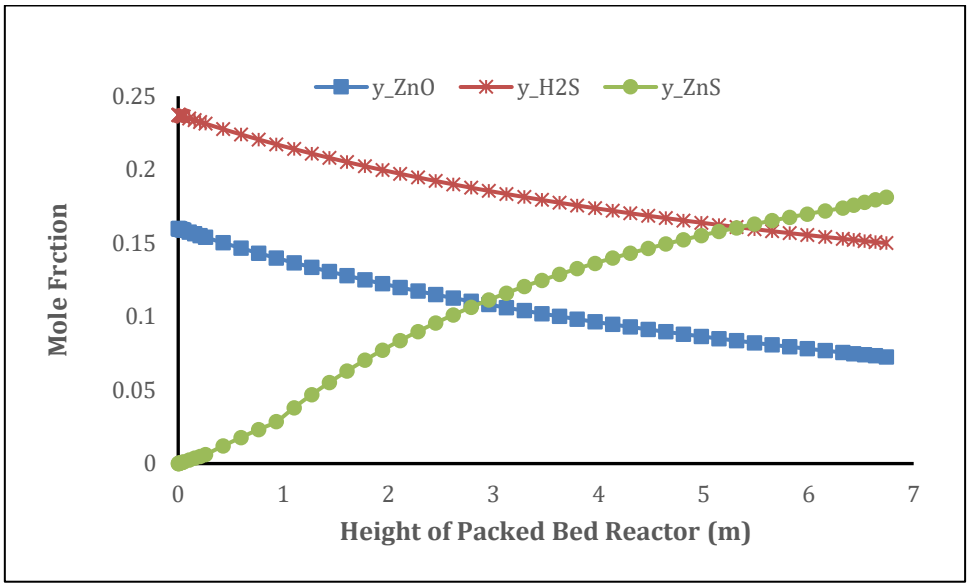



Figure 5: Profile Plot of Mole Fraction Versus Reactor 2 Height

Figure 5 depicts the profile plot of mole fraction of reactants (CH4/ZnO and H2S) and desired product (ZnS) changing along the height of the reactor. A careful examination of figure 4.3 reveals that the result obtained from simulation of developed model equations capable of predicting the mole fraction of reactants and products with reactor height is in agreement with trend in chemical reaction engineering where mole fraction of reactants decreases and mole fraction of products increases.

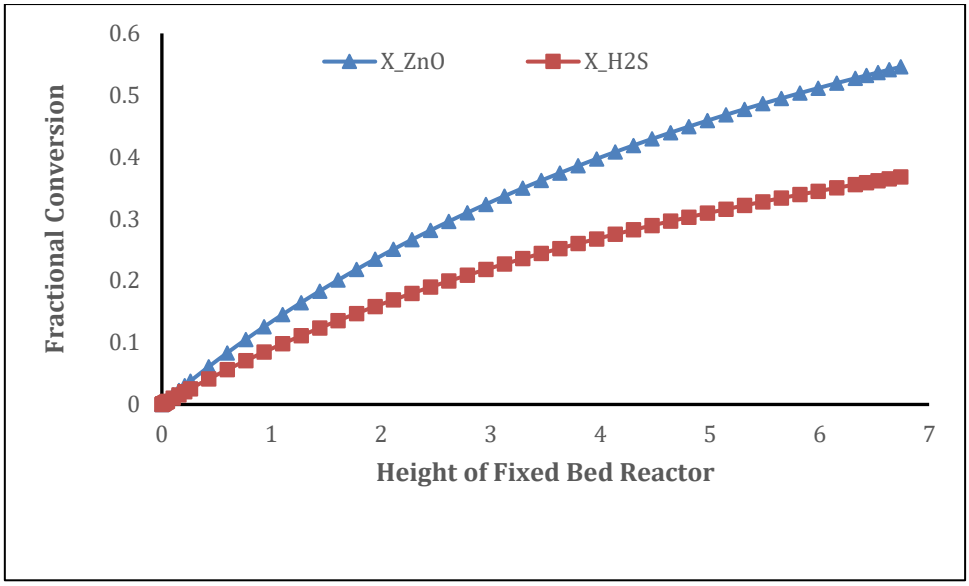



Figure 6: Profile Plot of Conversion Versus Reactor 2 Height

Figure 6 shows the plot of conversion of reactants along the height of the fixed bed reactor, after the absorption of H2S from the absorption unit, the unabsorbed $H_2S$ is sent to the fixed bed reaction section where ZnO which acts as the catalyst in this reaction reacts with H2S to further reduce the concentration of H2S. From the results obtained from the simulation, the conversion of ZnO rose from 0 to 55% while that of $H_2S$ rose from 0 to 37%.

## 4. CONCLUSION

The simulation and design of 200 tons per year of desulphurization plant was carried out in this work. The design started by developing a process flow diagram of the plant which contains an absorber unit and two fixed bed reactors configured in series to reduce the amount of H2S absorbed from the absorber unit to the barest minimum.

Design/sizing equations were also developed for each unit of the plant. The developed equations were then solved via MATLAB and Aspen HYSYS and the results obtained were presented in terms of material balance, energy balance, sizing/Design of equipment, mechanical design and equipment costing.

The design results for the absorber column and the reactors gave the diameters and heights of 2.36m and 5.06m; 2.3m and 6.74m; and 1.8m and 6.74m respectively. It was observed that the pressure drop of the fixed bed reactors were 0.7bar.

It was carefully observed that in all cases, all variables had a direct relationship with the volumetric flow rate except for residence time which had an inverse relationship with volumetric flow rate.

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