

# Simulation of Absorption Column for H<sub>2</sub>S Removal from Sour gas in Khartoum Refinery

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**Abstract-** The presence of H<sub>2</sub>S in sour gas gives dangerous effect on environment. Therefore, H<sub>2</sub>S must be eliminated from the sour gas, and the corresponding phenomena of mass transfer with chemical reaction in sieve tray column have to be studied.

Mass transfer was carried out theoretically by developing the mathematical model of mass transfer phenomena with chemical reaction in chemical absorption of H<sub>2</sub>S into Fe<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub> solution in a sieve trays column. The mass transfer process was described by film model, that yielding the second order differential equation solved numerically by orthogonal collocation to estimate enhancement factor. The mass balance model in sieve trays column consists of differential mass balance of H<sub>2</sub>S in gas phase and Fe<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub> in liquid phase giving system of non-linear first order differential equations that were solved numerically by Fourth order Runge-Kutta method under MATLAB Software.

This study assumed steady state and isothermal conditions. The system was stud in a sieve trays column 70 cm in diameter, number of trays 8, the height of 450 cm. The gas flow rate was 2401 kg/hr, pressure was 1 atm, liquid flow rate was 10000 cm<sup>3</sup>/s, the concentration of aqueous Fe<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub> solution is 0.002 mol/cm<sup>3</sup>.

It was that the percentage of absorbed H<sub>2</sub>S can be enhanced by increasing the temperature, liquid flow rate, Fe<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub> concentration, and decreasing sour gas flow rate. Gas side resistance actually is more than that solution; it means that the absorption process is dominated by gas side resistance than the liquid side resistance.

**Keywords-** Sour gas purification, H<sub>2</sub>S removal, Fe<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub>

## I. INTRODUCTION

The two main purposes for removing H<sub>2</sub>S from sour gas streams are to purify sour gas and to achieve air pollutants control. For these goals, numerous methodologies have been developed, and more than half a dozen have been demonstrated commercially. hydrogen sulfide is being produced by many industrial activities such as petroleum refining, natural gas and petrochemical plants, viscose rayon manufacturing craft, pulp manufacturing, food processing, aerobic and anaerobic wastewater treatments and many other industries [1]. Sour gas contains hydrogen sulfide gas and ammonia. The existence of hydrogen sulfide in sour gas is very disturbing, besides it smells bad, on combustion it will evolve (SO<sub>2</sub>) gas which pollutes environment, in global, it will cause acid rain. So that, it needs to be eliminated from sour gas.

Therefore, it is necessary to purify the sour gas first before combustion. The research is executed at Khartoum Refinery Company (KRC). Because hydrogen sulfide in the (KRC) is controlled by combustion process and hydrogen sulfide (2.401t/h) is converted to sulfur dioxide, which is also an air pollutant, in combustion process, it is not the better method to remove hydrogen sulfide by combustion. To operate a successful refinery you need to have a clean production, clean technology and be environmentally friendly.

Sour gas is split into two streams to enter the burner of sour gas incinerator. One stream comes from sour water stripping (SWS) unit(1670 t/h), the other path coming from Resid Fluid Catalytic Cracking RFCC (594t/h) and Delayed Coking DCU (137t/h) units passes through sour gas knockout drum for liquid separation, then each stream enters the burner separately. The flow rate and composition of sour gas (KRC) is shown in Table 1.

Table 1. Flowrate and composition of sour gas from KRC

Unit	H <sub>2</sub> S kg/h	NH <sub>3</sub> kg/h	CO <sub>2</sub> kg/h	H <sub>2</sub> O kg/h	Total kg/h
SWS	625	620.6	8.4	416	1670
RFCC	356.4	237.6	-	-	594
DCU	82.2	54.8	-	-	137
Total	1036.6	913	8.4	416	2401

Affected areas west and south-west of the Khartoum Oil Refinery in the weather stable even a distance of 4 km gas ammonia and sulphur dioxide (including residential complex for employees of the refinery Sudanese and Chinese), and in the event of a thunderstorm and sandy (June - July - August - September) up effect ammonia and sulphur dioxide until the parties to the village of

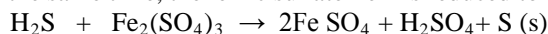
Gilin (18 - 20 kilometers southwest of the refinery), causing harassment and complain about odors from which most of the residents of the village of Gilin. Health, safety and environment of great importance in human life, therefore, the pollutants that result from petroleum products and their effect on air, water and land should be explained.

Currently, H<sub>2</sub>S removal is one of the most important aspects for the development of a new oil-gas field due to the reduction of the conventional oil resources (J.S.Gudmundsson, 2011). H<sub>2</sub>S must be removed both to protect workers and environment health (an H<sub>2</sub>S concentration equal to 600 ppm quickly causes breathing problems and death among the exposed people), and because it reduces the economic value of the oil-gas field. In fact, oil companies must use special materials for equipments, like metal and corrosion resistant alloys, whose costs are about 10 times greater than the common carbon steel piping. In addition, the sulphur that exists in the sour gas stream can be extracted and marketed on its own (J.S.Gudmundsson, 2011).

However, direct combustion of sour gas without removal of H<sub>2</sub>S leads to the formation of sulphur dioxide (SO<sub>2</sub>), which is another toxic pollutant and a major contributor to acid rain in the atmosphere. Gas must be very clean to reach pipeline quality, and must be of the correct composition for the local distribution network such as Carbon dioxide, Water, hydrogen sulfide and particulates must be removed if present.

There are many kinds of process that stated in literature for removing H<sub>2</sub>S gas [2]. These can be divided into two methods; those are chemical absorption and adsorption. Chemical absorption is an absorption which is followed by chemical reaction when the absorbed gas is reacted with the reactant in liquid phase, while adsorption is absorption on the surface of solid particle which is called adsorbent. In using H<sub>2</sub>S gas, the adsorbent in which commonly used is ZnO that reacts H<sub>2</sub>S into ZnS. Some researchers have learnt about the removing process of H<sub>2</sub>S gas in biogas flowing by changing it that it becomes more stable sulfur [2], [3] stated that gas desulphurization with Ferric Chelate is more stable than EDTA and HEDTA. Al stated that the H<sub>2</sub>S changing process becomes sulfur is by reaction with zinc natrium ferric (Asai, 1990). While Hix and Lynn stated that the absorption process of H<sub>2</sub>S gas into SO<sub>2</sub> solution in polyglycol ether (Horikawa, 2004) proposes removing process of gas H<sub>2</sub>S from biogas with changing it to become sulfur (S) applies absorption process into soluble chelate iron from at EDTA. [2]

In this study, the chemical absorption of hydrogen sulfide into aqueous ferric sulfate has been studied on a sieve trays column has not done yet. In this process an aqueous Fe<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub> solution is used an absorbent. The basic process involves putting in contact, in an absorber, a ferric sulfate solution Fe<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub>, counter-current with sour gas, contaminated with hydrogen sulfide. H<sub>2</sub>S is absorbed and oxidized into elemental sulfur [4]. At the same time, the ferric sulfate Fe<sup>+3</sup> is reduced to Fe<sup>+2</sup> (FeSO<sub>4</sub>), according to



Depending on the gas flow rate and the efficiency required several types of absorbers are suitable, such as plat towers or packed towers. The sulfur separator can include filter pres, settler and sulfur melters, Depending on quality of elemental sulfur required [5]. The theoretical study is important for column design and column performance analysis [5]

## II. MATERIALS AND METHODS

This study is done in simulation to determine sieve trays column performance in absorption of H<sub>2</sub>S gas into Fe<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub> solution. Theoretical study is divided to into parts. The first part developed transfer model between phases to estimate the value of enhancement factor (E) that yielding the ordinary differential equation system in second order and it is solved by the orthogonal collocation method. Estimation of the value of (E) required several data; there are reaction kinetics data, solubility data, and mass transfer data, after that the value of (E) is applied for sieve trays column model of chemical absorption of H<sub>2</sub>S yielding of ordinary differential equation system of first order solved by using Runge Kutta method. Output of sieve trays column model is % Recovery H<sub>2</sub>S, concentration distribution of A in gas phase, concentration distribution of B in liquid phase.

Ferric sulfate solution is used for H<sub>2</sub>S absorption the reaction rate can be expressed as [4]

$$r = k C_{\text{H}_2\text{S}} C_{\text{Fe}^{3+}}$$

(1)

By assuming that the kinetic constant varies with temperature according to an Arrhenius function, the activation energy can be calculated. In this process an aqueous Fe<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub> solution is used an absorbent.

Therefore the reaction rate constant values were obtained as a function of temperature [4]

$$\log k = 9.3855 - \frac{2636.6}{T} \quad (2)$$

### Mathematical Model Expansion

#### Development of Mass transfer Model between Phases to Estimate the Enhancement Factor

The expansion of mass transfer model between Phases to estimate the value of Enhancement with reaction that is represented below by irreversible second order reaction.

Mass balance for component A (H<sub>2</sub>S) (Film Model)

$$\frac{d^2 A}{dX^2} - MAB = 0 \quad (3)$$

Mass balance for component B (Fe<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub>)

$$\frac{d^2 B}{dX^2} - \frac{MAB}{S} = 0 \quad (4)$$

With orthogonal collocation method, the collocation equation made an  $A_i, B_i$ , explicit to be solved by successive approximation method

For component A

$$A_i = \frac{\sum_{j=1}^{N+2} D_{ij} A_j - D_{ii} A_i}{(MB_i - D_{ii})} \quad (5)$$

For component B

$$B_i = \frac{\sum_{j=1}^{N+2} D_{ij} B_j - D_{ii} B_i}{\frac{MA_i}{S} - D_{ii}} \quad (6)$$

### The Development of Column Model

The develop meet of model is begun by forming mass balance for component A ( $H_2S$ ) in gas phase and B  $Fe_2(SO_4)_3$  in liquid phase, which following by the equations:

$$\frac{dY_A}{dz} = \frac{Ek_L a}{G_m} (C_{Ai} - C_A^0) \quad (7)$$

$$\frac{dC_B^0}{dz} = -2 \frac{Ek_L a}{U} (C_{Ai} - C_A^0) \quad (8)$$

The system of non linear differential equations was solved using orthogonal collocation method and collocated equations described as non linear algebraic equations was solved using orthogonal collocation method. Then, the isothermal enhancement factor can be predicted in equation (9), where the value of  $[dC_A/dx]_{x=0}$  can be estimated using orthogonal collocation method. [6]

$$E = \frac{\bar{R}}{k_L C_{Ai}} = \frac{-D_A [dC_A/dx]_{x=0}}{k_L C_{Ai}} \quad (9)$$

Sherwood and Holloway (1940) in Danckwerts (1970) give the following expression for  $k_L$  and  $a$  [6]

$$k_L = 0.42 \left( \frac{g\mu}{\rho} \right)^{\frac{1}{3}} \left( \frac{D_{AB}\rho}{\mu_L} \right)^{\frac{1}{2}} \quad (10)$$

$$a = 0.38 \left( \frac{u}{u_t} \right)^{0.775} \left( \frac{u\rho}{nd\mu_L} \right)^{0.125} \left( \frac{g\rho}{d\sigma} \right)^{\frac{1}{3}} \quad (11)$$

Here  $u$  is the velocity of rise of the bubbles in the froth (taken to be 26.5cm/s under most conditions),  $n$  the number of holes per unit area of plate.

For sieve trays, Chan and Fair (1983) give the following expression for gas-phase mass-transfer coefficient  $k_G a$  [7].

$$k_G a = \frac{316 D_G^{1/2} (1030 f + 867 f^2)}{h_L^{1/2}} \quad (12)$$

Where:  $f$  = approach to flood, fractional

The interfacial Concentration of  $H_2S$  gas dissolved at interface estimated from solubility data following Henry's law and by considering gas side resistance that is,

$$C_{Ai} = \frac{k_G P_A + E.k_L C_A^0}{E.k_L + k_G H_e} \quad (13)$$

### III. RESULT AND DISCUSSION

In this study steady state and isothermal condition are assumed and this study of simulation comprises sieve trays column 70 cm in diameter filled with sieve trays 0.5 m spacing to the height of 450 cm. Simulation the absorption of  $H_2S$  from sour gas available influence, the liquid flow rate was varied 5000-10000  $cm^3/s$ , temperature was varied 30-50°C, and column is operated at atmospheric pressure, the feed sour gas flow rate is 2401 kg/h with mole fraction of  $H_2S$  in inlet sour gas is 0.28887, the concentration of  $Fe_2(SO_4)_3$  in inlet absorbent was varied 0.002 – 0.003  $mol/cm^3$ . The simulation result plot graphically influence various process variables versus % recovery  $H_2S$  showed at Figure. (1) to Figure. (6).

*Variation of the Enhancement Factor with Hatta Number for Different value of  $E_i$*

Figure.1 shows numerical simulation results for the enhancement factor  $E$  as a function of Hatta number  $\sqrt{M}$  according to the film theory, calculated according to Eq. 9 with  $E_i$  parameter. For a given value of  $E_i$  an increase in  $\sqrt{M}$  brings about an increase in  $E$  until a limiting value is approached where  $E = E_i$ . The value of  $E_i = 50$  shows the highest  $E$  value compared to the value  $E_i = 4$  and  $E_i = 20$ . Increasing the value of  $E_i$  will decrease the amount of gas A absorbed and value of  $E$  will increase proportionally. The similarity between this figure and the familiar van Krevelen Hoftijzer plot for isothermal absorption of  $H_2S$  is apparent; one can find a remarkable similarity between Fig .1 and the traditional  $E$  versus  $\sqrt{M}$  plots. For a given  $E_i$ , the enhancement factor tends to reach an asymptotic value which is determined by the instantaneous reaction regime. Increasing the value of  $E_i$  will increase the amount of  $H_2S$  absorbed and value of  $E$  will increase proportionally.

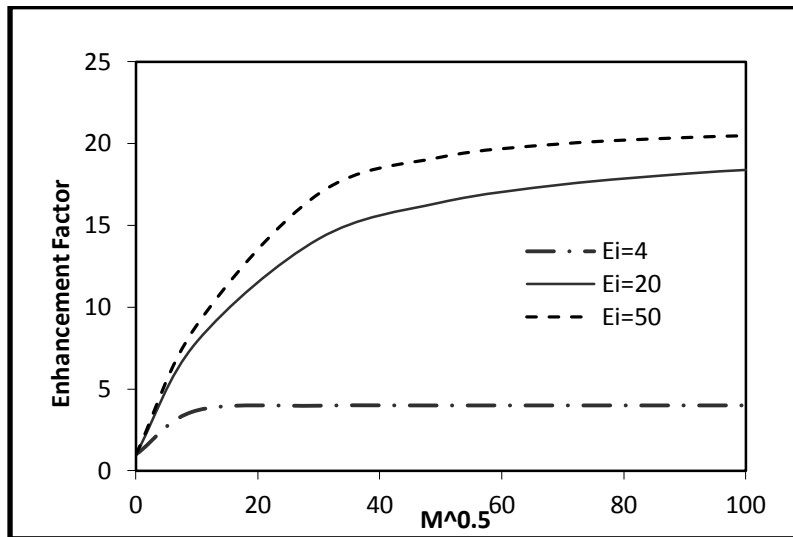


Figure. 1: Variation of the Enhancement Factor with Hatta Number for different values of  $E_i$

*Effect of Temperature and Concentration of  $Fe_2(SO_4)_3$  Solution on  $H_2S$  Removal Efficiency*

Figure.2 shows; An increase in the value of the temperature also produces an increase on the %removal of  $H_2S$ . According to the principle of molecular dynamics, the rate constant of reaction and the diffusion coefficient increase with the increase in the temperature, and this is beneficial to improve the absorption rate .In an absorber, the transfer of  $H_2S$  from sour gas into  $Fe_2(SO_4)_3$  liquid brings about a heating effect.

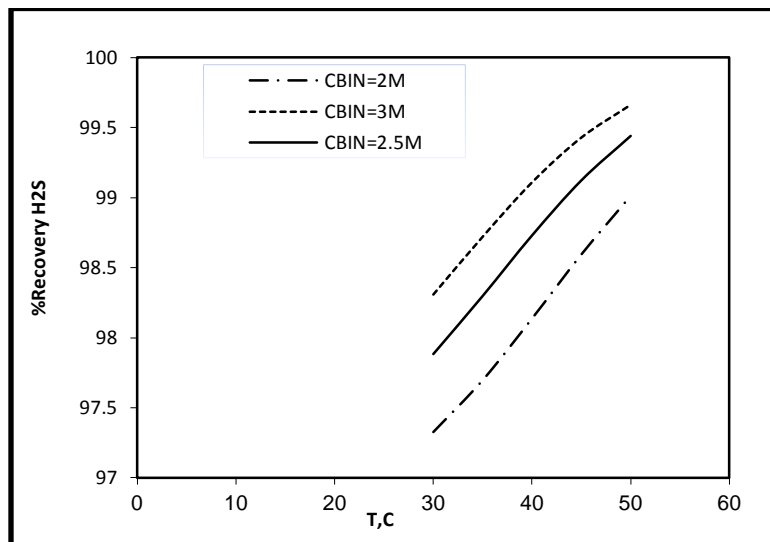


Figure 2: Temperature Influence on the % Removal with different solvent concentration of  $(Fe_2SO_4)_3$

Also Figure.2 shows indicates that the effect of temperature but with difference concentration of  $Fe_2(SO_4)_3$  (0.002, 0.0025, and 0.003mol/cm<sup>3</sup>). For temperature the %removal of  $H_2S$  is given the same result in Figure.2 For that the increase in the value of

$\text{Fe}_2(\text{SO}_4)_3$  concentration is still give influence to increase of  $\text{H}_2\text{S}$  removal efficiency. This is because when the concentration of  $\text{Fe}_2(\text{SO}_4)_3$  is high, more  $\text{H}_2\text{S}$  must be introduced into the system to react with  $\text{Fe}_2(\text{SO}_4)_3$ , and this thing of course is caused because at higher concentration of  $\text{Fe}_2(\text{SO}_4)_3$  in solution, the ferric ion would be more reactive with sulphur ion, so that will increase absorption rate of  $\text{H}_2\text{S}$  from sour gas.

*The Effect of Flow Rate of  $\text{Fe}_2(\text{SO}_4)_3$  Solution on  $\text{H}_2\text{S}$  Removal Efficiency:*

Figure.3; shows indicates that the increase in the value of  $\text{Fe}_2(\text{SO}_4)_3$  flow rate is still give influence to increase of  $\text{H}_2\text{S}$  removal efficiency. Liquid flow rate determines how readily Component  $\text{H}_2\text{S}$  will absorb into the liquid phase. When the liquid flow rate is large, component  $\text{H}_2\text{S}$  will be absorbed more readily into the liquid phase.

This increase of  $\text{H}_2\text{S}$  removal efficiency occurred because the increasing of absorbent flow rate the liquid disturbance is enhanced, increase of driving force concentration that caused as result of decrease of concentration of  $\text{H}_2\text{S}$  in liquid bulk, which results in a higher speed of  $\text{H}_2\text{S}$  diffusing into the liquid. The consumed absorbents at the boundary layer could diffuse into the liquid phase at a higher speed due to the increase of liquid flow rate.

Also Figure3. Shows indicates that the effect of  $\text{Fe}_2(\text{SO}_4)_3$  flow rate but with difference temperature (30 and 40°C). For %removal of  $\text{H}_2\text{S}$  is given the same result in Figure .3 In addition, as the increase of liquid flow rate, the thicknesses of gaseous and liquid-phase boundary layers decrease, leading to enhancement of the mass transfer rate, also it can be explained when the flow rate increased, the interfacial area between gas-liquid places increased. Therefore, the result is to enhance gas-liquid mass transfer rate and improving the  $\text{H}_2\text{S}$  absorption efficiency.

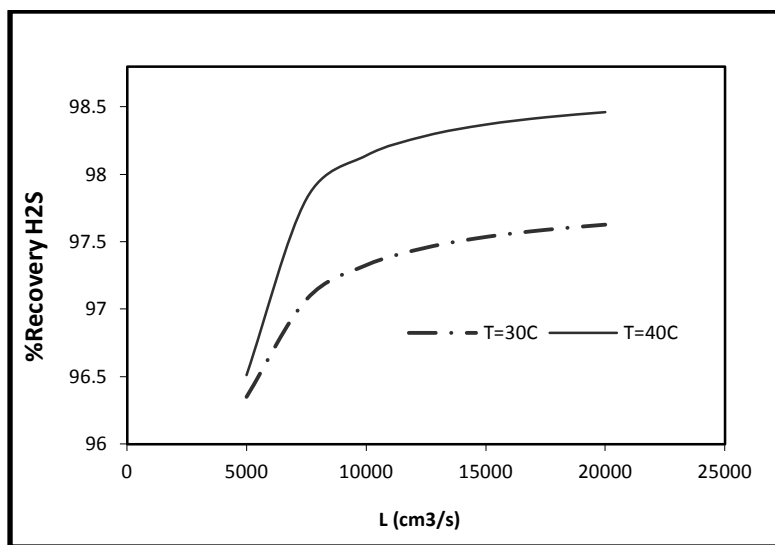


Figure .3: Flow Rate of  $(\text{Fe}_2\text{SO}_4)_3$  Influence on the % Removal with different Temperature

*The Effect of gas Flow Rate of Sour gas on  $\text{H}_2\text{S}$  Removal Efficiency:*

Figures 4, Figures 5 and Figure 6; shows the measurements of  $\text{H}_2\text{S}$  absorption removal into  $\text{Fe}_2(\text{SO}_4)_3$  solution under different flow rate of sour gas in the sieve tray column. In these cases, simulation conditions:  $\text{H}_2\text{S}$  inlet mole fraction was 0.28875, pressure 1 atm, temperatures 30 °C,  $C_{(\text{Fe-EDTA})} = 0.002\text{mol}/\text{cm}^3$ ,  $L = 10000\text{ cm}^3/\text{s}$ , and sour gas flow rate was varied (700-950 liter/s).

Figure 4; shows indicates that the increase in the value of inlet sour gas flow rate is give to declines and main negative effects on removal efficiency  $\text{H}_2\text{S}$  removal efficiency. This is because when the flow rate of sour gas is high would a decrease the gas - liquid two phase contact time in the absorption column so the reaction rate of  $\text{H}_2\text{S}$  absorption slowed down. It was also that the increasing sour gas flow rate carried spray absorbent out from the tower, and led to the loss of the absorbent. Therefore, be concluded that the gas flow rate condition tends to become unfavorable to  $\text{H}_2\text{S}$  absorption when the gas flow rate increases within the operation range investigated.

Also Figure. 5 and Figure.6, shows indicates that the effect of sour gas flow rate but with difference concentration 0.002-0.004  $\text{mol}/\text{cm}^3$  in Figure.5 and difference temperature (30-50°C) in Figures 4.13. For %removal of  $\text{H}_2\text{S}$  is given the same result in Figure.4

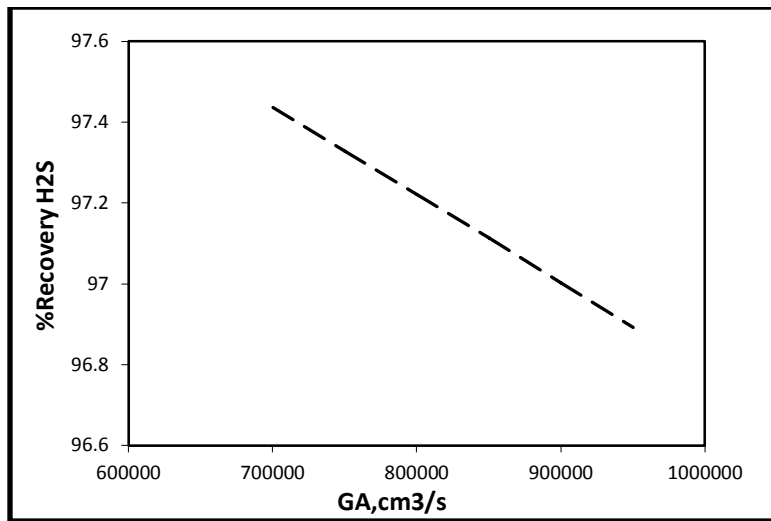


Figure.4: Flow Rate of sour gas Influence on the % Removal

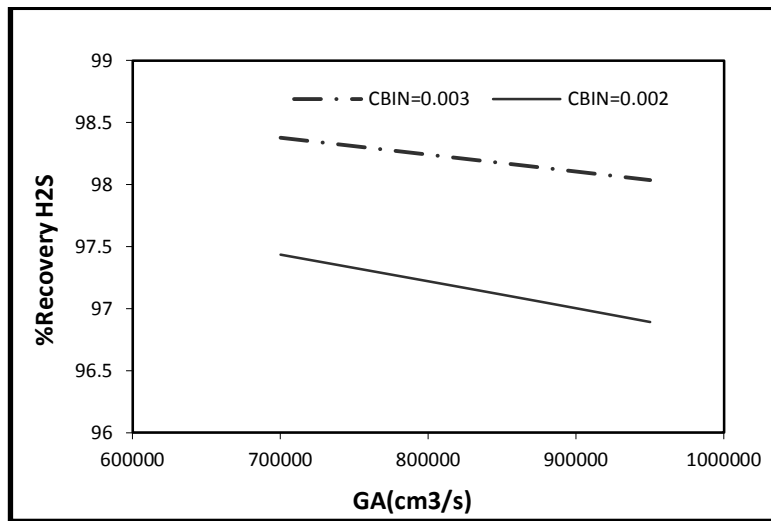


Figure.5: Flow Rate of sour gas Influence on the % Removal with different concentrations of Fe<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub>

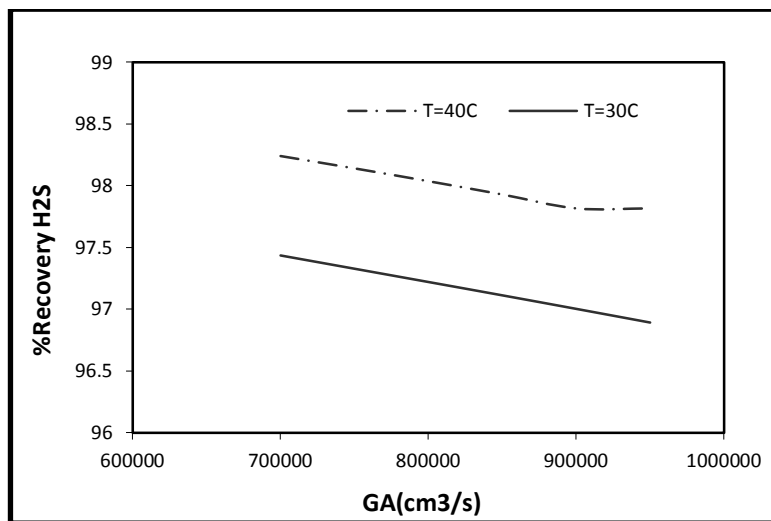


Figure 6: Flow Rate of sour gas Influence on the % Removal with different Temperatures

#### IV. CONCLUSION

H<sub>2</sub>S removal from sour gas using aqueous ferric solution Fe<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub> needs an advanced air pollution control device to reduce greenhouse gas emissions. In this paper, a description of mathematical modeling and simulating for the isothermal gas absorption with chemical reaction in the sieve trays with the sample calculation of H<sub>2</sub>S with Fe<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub> solution was studied by means of numerical simulations

Absorption of H<sub>2</sub>S by Fe<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub> solutions was performed in this study to clarify the H<sub>2</sub>S absorption efficiency. The absorption of H<sub>2</sub>S into aqueous solutions of Fe<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub> as encountered in sour gas was carried out using sieve plate column.

The simulation results showed that the percentage of absorbed H<sub>2</sub>S can be enhanced and should have higher efficiency by increasing temperature, liquid flow rate, and Fe<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub> concentration and decreasing flow rate of sour gas.

The methodology proposed, whereby only one parameter in each column is used to be employed to develop simulation models of industrial plants where measurements of operating variables are available and possible.

It is hoped that with the continuous studies conducted worldwide currently, the challenges related to the absorption process can be overcome, and that H<sub>2</sub>S capture projects can be integrated and materialized in the industrial process.

#### ACKNOWLEDGMENT

The authors wish to thank Sudan University of Science and Technology, Chemical Engineering Department for their help and support during the period for the work of ph,D thesis from which the paper is generated.

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