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Modeling of Reactor Furnace of Sulfur Recovery Units from Acidic Gases

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Abstract. Reaction furnace of Claus Sulfur recovery unit is modeled using Claus reaction equilibrium relation and Sames &Paskall's experimental equations. Concentration of components in outlet stream, H_2S and S_2 conversion and furnace temperature are calculated. Computer program is provided based on the model.

Keywords: Modelling, Claus, Furnace, Acidic Gas, Experimental and equilibrium relations

1. Introduction

The Claus process is the most current process for sulphur production from acidic gases that contents H_2S and CO_2. Claus process was introduced to industry for producing sulphur from H_2S and air before 100 years ago (1883). Modified Claus method was started for improvement previous method by I.B.Farbenindustrie (1937)[4].

2. Claus Process

Claus reaction is based on oxidation of H_2S with air in presence catalyst (Bauxite) in a one stage reactor.

$$2H_2S + \frac{1}{2}O_2 \rightarrow S_2 + H_2O \qquad \Delta H_{rxn}@25\ °C = -520000\ Kj/Kgmole$$

Controlling of exothermic reaction is very hard and the setting of sulfur removing efficiency is in a range of 80-90 %. Modified Claus method contents two stages[7]:

- Burning 1/3 of acidic gas with total necessary air for reaction.

$$H_2S + \frac{3}{2}O_2 \rightarrow SO_2 + H_2O \qquad \Delta H_{rxn}\ @\ 25\ °C = -223100\ Btu/lbmole$$

- Blending remaining acidic gas with production CS2 from first stage.

$$2H_2S + SO_2 \leftrightarrow \frac{3}{x} S_x + 2H_2O \qquad \Delta H_{rxn}\ @\ 25\ °C = -41300\ Btu/lbmole$$

2.1. Straight Through

At first, in this method acidic gas feed stream enter to reaction furnace. Acidic gas blend with stoichiometry air for burning 1/3 of total existent H_2S i.e. it converts to SO_2 and all of hydrocarbons convert to CO_2. Therefore remaining of H_2S will react with the formed SO2 and product sulphur. [9]

2.2. Reaction Furnace:

Reaction furnace is a main part of sulfur recovery unit. Reaction furnace has two primal targets.

First: Burning 1/3 of existent H_2S in feed and product SO_2 for Claus equilibrium process, Catalytic process and preparation $\frac{H_2S}{SO_2} = \frac{2}{1}$ relation for doing Claus equilibrium process with predicting conversion.

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Second: Destruction and burning any type of component that may be damaged downstream equipments operation. [2, 5].

2.3. Reaction Furnace Ovservations

All of reaction is evented in furnace and reaction rates don't specify. Therefore Sames&Paskall 's experimental equations and Claus equilibrium reaction for modeling is used.

1	$R(CO)= 0.002A^{0.0345} \exp(4.534 A)$	2	$R(H_2) = 0.056\ (\pm 0.024)$
3	$R(CS_2) = 2.6\, A^{0.971} \exp(-0.965 A)$	4	$R(S) = 1.58A^{1.099} \exp(-0.73A)$
5	$R(C0S) = 0.01 \tan(100A)$ for $0 \le A \le 0.86$ or $R(C0S) = 0.143$ for $A > 0.86$		

where *R(CO)* is Fraction of initial carbon to format CO, $R(H_2)$ *is* Fraction of initial H_2S to format H_2, *R(COS) is* fraction of initial carbon to format CO*S,* $R(CS_2)$ is fraction of initial carbon to format CS_2, , *R(S) is f*raction of initial carbon to format S, *A* is mol fraction of H_2S in acidic gas in dry state, respectively [3,8,9]. Available method in relation furnace is Straight state, reaction furnace pressure: 120-160 KPa , pressure drop: 10 KPa , Steady state and heat transfer rate is considered negligible.

Table 1: Chemical Reaction

1	$H_2S + \frac{3}{2} O_2 \rightarrow SO_2 + H_2O$
2	$2H_2S + SO_2 \leftrightarrow \frac{3}{2} S_2 + 2\, H_2O$
3	$CH_4 + 2O_2 \rightarrow CO_2 + 2\, H_2O$
4	$CO_2 \rightarrow CO + \frac{1}{2} O_2$
5	$H_2S \rightarrow \frac{1}{2} S_2 + H_2$
6	$CH_4 + 2\, S_2 \rightarrow CS_2 + 2H_2S$
7	$CO + \frac{1}{2} S_2 \rightarrow COS$

$$K_P = \frac{[H_2O]^2 [S_2]^{\frac{3}{2}}}{[H_2S]^2 [SO_2]} \left[\frac{\pi}{totalmoles}\right]^{\frac{3}{2}-1}$$

where Kp is pressure equilibrium Constant, π is pressure, [ ]is Mol rate of component and X is H2S consumption mol rate in Claus equilibrium reaction, respectively. After writing sum of existent components mol rate in reaction[6,7]:

$$Total = f_{i(CH_4)}(3 - 2R(CS_2) + \frac{1}{2} R(CO)) + f_{i(CO_2)}(1 - R(CS_2) + \frac{1}{2} R(CO))$$
$$+ f_{i(H_2S)}(\frac{4}{3} + \frac{1}{2} R(H_2)) + f_{i(N_2)} + f_{i(H_2O)} + \frac{1}{4} X$$

Relation between K_p and react furnace temperature is coming in a graph of GPSA[1]. Interpolation different value of graph can help for getting a straight equation between temperature and equilibrium constant [1-5].

$K_p = 0.621T\text{-}420.49$ T (°C) , K_p (kPa$^{0.5}$)

$$T(^\circ K) = ((\frac{(A + X)^2 (B + 0.75X)^{1.5} \pi^{0.5}}{(C - X)^2 (1/3 f_{i(H_2S)} - 0.5X)(D + 0.25)^{0.5}} + 420.49) / 0.6021) + 273$$

$$A = f_{i(H_2O)} + \frac{1}{3} f_{i(H_2S)} + 2 f_{i(CH_4)}(1 - R(CS_2))$$
$$B = \frac{1}{2} f_{i(H_2S)} R(H_2) - 2 f_{i(CH_4)} R(CS_2) - 0.5 R(COS)(f_{i(CH_4)} + f_{i(CO_2)})$$
$$C = 2R(CS_2) f_{i(CH_4)} - f_{i(H_2S)}(R(H_2) - \frac{2}{3})$$
$$D = f_{i(CH_4)}(3 - 2R(CS_2) + \frac{1}{2} R(CO)) + f_{i(CO_2)}(1 - R(CS_2) + \frac{1}{2} R(CO))$$
$$+ f_{i(H_2S)}(\frac{4}{3} + \frac{1}{2} R(H_2)) + f_{i(N_2)} + f_{i(H_2O)}$$

2.4. Reactor Furnace Energy Balance:

Energy Consumption- Production Energy + Initial Energy = Outlet Energy

Initial Stream Energy :

$$H_{in(i)}(T_1) = (a_i T_1 + \frac{b_i}{2} T_1^2 + \frac{c_i}{3} T_1^3 + \frac{d_i}{4} T_1^4) - (a_i T_0 + \frac{b_i}{2} T_0^2 + \frac{c_i}{3} T_0^3 + \frac{d_i}{4} T_0^4) + H_i(T_0)$$

$$H_{in(i)}(T_2) = (a_i T_2 + \frac{b_i}{2} T_2^2 + \frac{c_i}{3} T_2^3 + \frac{d_i}{4} T_2^4) - (a_i T_0 + \frac{b_i}{2} T_0^2 + \frac{c_i}{3} T_0^3 + \frac{d_i}{4} T_0^4) + H_i(T_0)$$

$$E_{in} = H_1 f_{i(CH_4)} + H_2 f_{i(CO_2)} + H_3 f_{i(H_2S)} + H_4 f_{i(H_2O)} + H_5 f_{i(O_2)} + H_6 f_{i(N_2)}$$

Outlet Stream Energy:

$$H_{out(j)}(T) = (a_j T + \frac{b_j}{2} T^2 + \frac{c_j}{3} T^3 + \frac{d_j}{4} T^4) - (a_j T_0 + \frac{b_j}{2} T_0^2 + \frac{c_j}{3} T_0^3 + \frac{d_j}{4} T_0^4) + H_j(T_0)$$

$$E_{out} = H_7 f_{O(CH4)} + H_8 f_{O(CO2)} + H_9 f_{O(H2S)} + H_{10} f_{O(H2O)} + H_{11} f_{O(O2)} + H_{12} f_{O(N2)}$$
$$+ H_{13} f_{O(SO2)} + H_{14} f_{O(S2)} + H_{15} f_{O(CO)} + H_{16} f_{O(CS2)} + H_{17} f_{O(COS)} + H_{18} f_{O(H2)}$$

E_{in} *is a function of* x and numerical form *and* E_{out} *is function of* x *&,* T. Writing and simplification equation can help to get below equation:

$$X = \frac{A_0 + A_4 T + B_4 T^2 + C_4 T^3 + D_4 T^4}{B_0 + A_5 T + B_5 T^2 + C_5 T^3 + D_5 T^4}$$

$$T = ((\frac{(A + X)^2 (B + 0.75X)^{1.5} \pi^{0.5}}{(C - X)^2 (1/3 f_{i(H2S)} - 0.5X)(D + 0.25)^{0.5}} + 420.49) / 0.6021) + 273$$

Using these equations and trial and error methods, temperature (T) and conversion (x) can be calculated. A_0 ، A_4 ، A_5 ، B_0 ، B_4 ، B_5 ، C_4، C_5 ،D_4 ، D_5 are constant parameters that specified with initial stream conditions and computate numeral form..

3. Results and Discussion

In this project, H_2S Concentration change in feed stream will change furnace temperature, H_2S & S_2 conversion and H_2S, S_2 , H_2,, COS, CS_2 concentration in outlet stream. Increasing H_2S concentration in feed stream will increase furnace temperature , H_2S total & equilibrium conversion , S_2 & H_2 concentration in outlet stream but H_2S concentration decreases and SO_2 concentration at first will decrease and next increase (Fig. 1, 2, 3, 4, 5, 6). Increasing initial feed and air streams temperature occur to furnace temperature, H_2S & S_2 concentration (Fig. 7, 8, 9). Furnace pressure is affected in H_2S & S_2 conversion. Pressure increase will increase furnace temperature but H_2S & S_2 conversion decrease (Fig. 10, 11, 12).

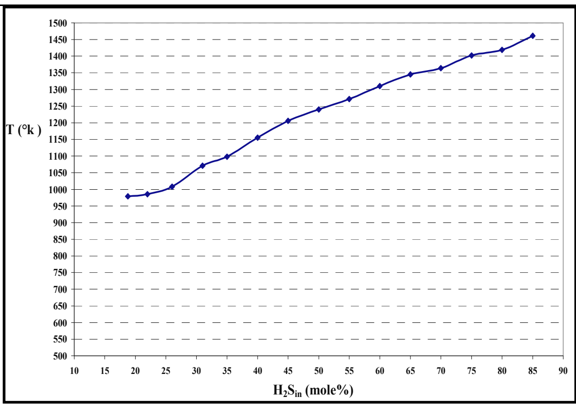

Fig. 1: Predicting reaction furnace temperature against H_2S concentration

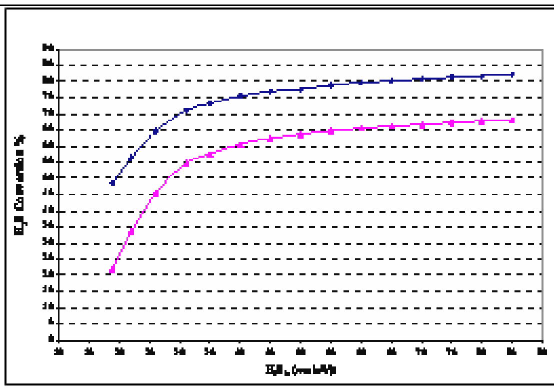

Fig. 2: Predicting reaction furnace H_2S total conversion (blue) and equilibrium conversion(red) against H_2S concentration

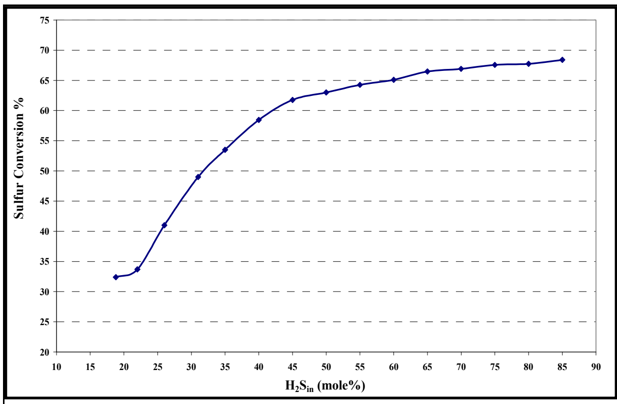

Fig. 3: Predicting reaction furnace S_2 conversion against H_2S concentration

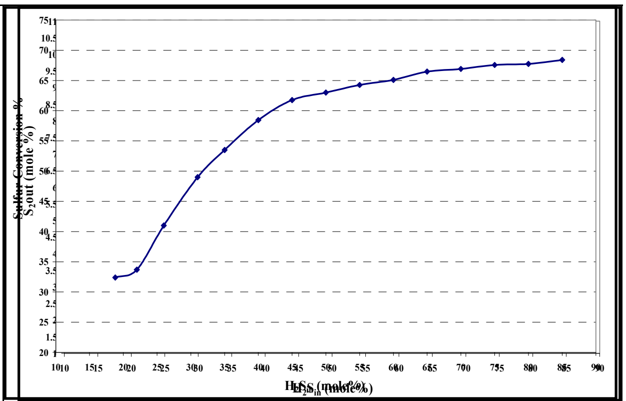

Fig. 4: Predicting reaction furnace S_2 concentration against H_2S concentration

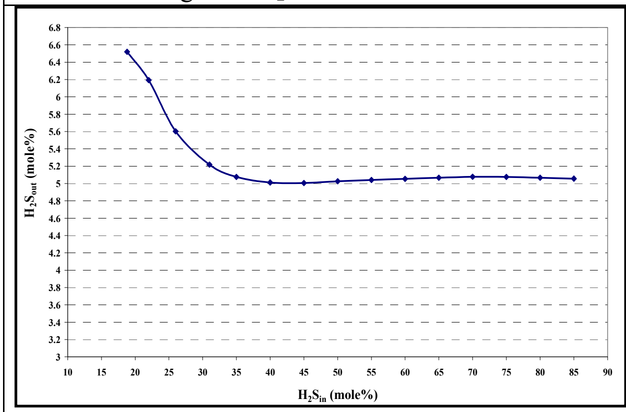

Fig. 5: Predicting reaction furnace H_2S concentration in outlet stream against H_2S concentration

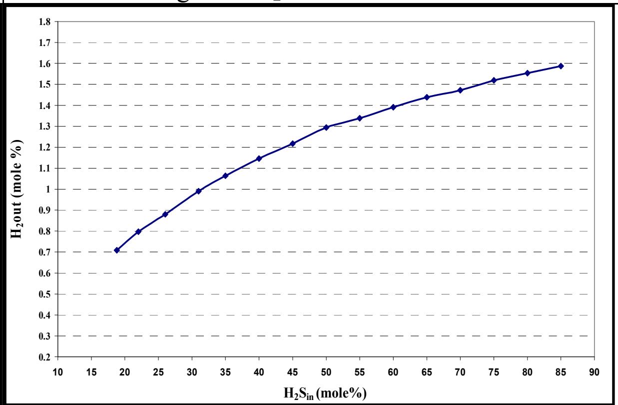

Fig. 6: Predicting reaction furnace H_2 concentration in outlet stream against H_2S concentration

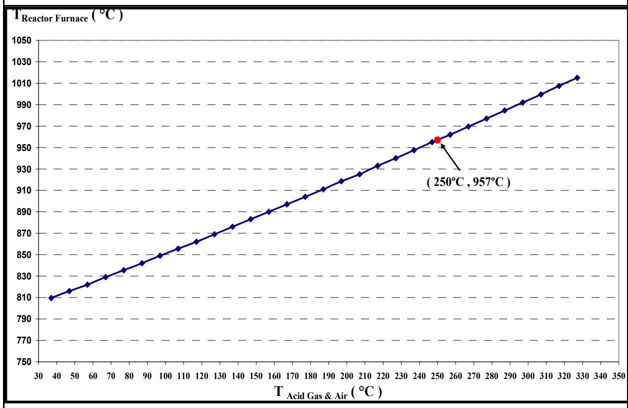

Fig. 7: Predicting reaction furnace temperature against air and feed initial streams temperature

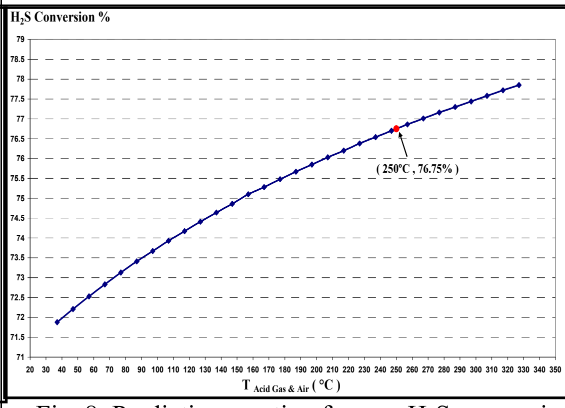

Fig. 8: Predicting reaction furnace H_2S conversion against air and feed initial streams temperature

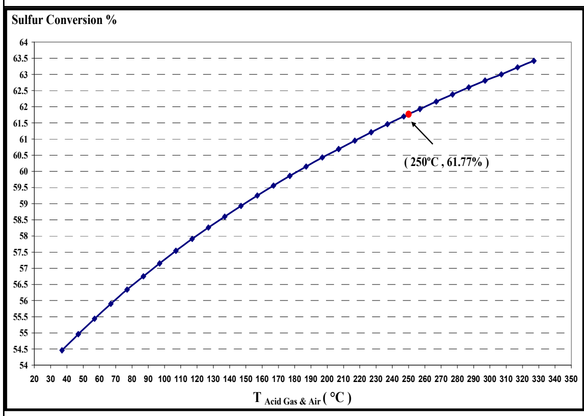

Fig. 9: Predicting reaction furnace S_2 conversion against air and feed initial streams temperature

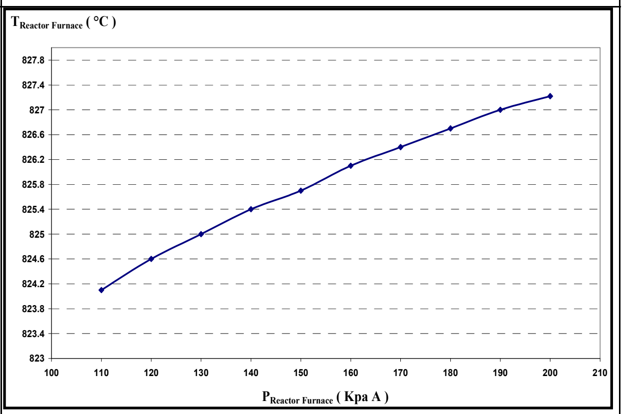

Fig. 10: Predicting reaction furnace temperature against pressure change

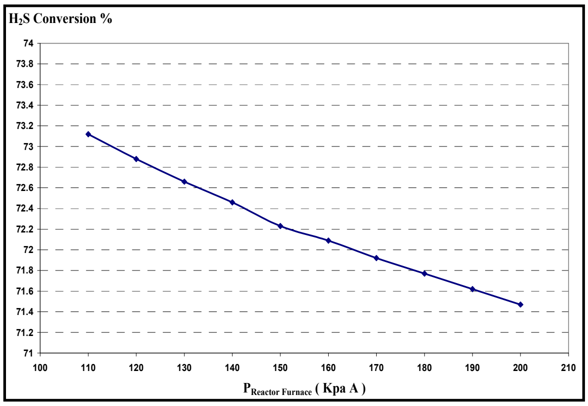

Fig. 11: Predicting reaction furnace H_2S conversion against pressure change

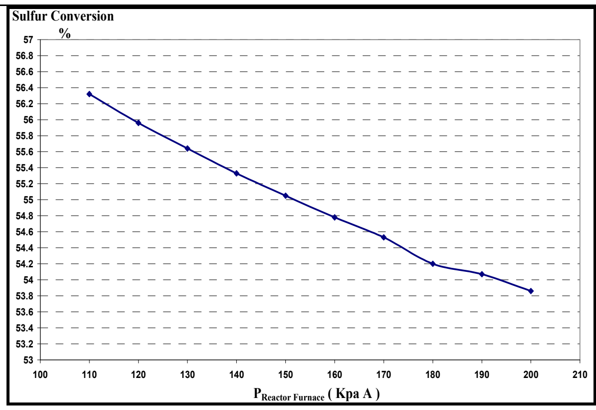

Fig. 12: Predicting reaction furnace S_2 conversion against pressure change

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