MATHEMATICAL MODELING OF THE INSTANTENOUS REACTION OF H_2S –MEA IN A FALLING FILM REACTOR

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ABSTRACT

A mathematical model was formulated using the absorption of carbon dioxide by monoethanolamine amine as an absorbent in a falling film reactor. A program wrote in Fortran language was used to obtain these profiles via using of multi grid method through programming of kinetic and thermodynamic equation and physical properties of the studied system. Through the formulated model film thickness, surface temperature, velocity, concentration and temperature profiles were obtained.

The mathematical analysis validated by a test run in a Baiji refinery through intrusion of liquid flow rate, liquid concentration and gas fraction. In this study we have four factors as independent variables ,they are mole fraction of hydrogen sulfide in gaseous mixture (Y) (0.05, 0.75 and 0.1), molar concentration of absorbent (monoethanolamine) (C_{MEA}) (0.05, 0.075 and 1 M), volumetric flow rate of liquor MEA (Q_{MEA}) (5, 10, 15, and 20), and its temperature (T) (30, 35, 40, 45, 50 and 55◦ C).

It is found that the entrance effect of the falling film absorber can be related to the axial distance from the reactor entrance exponentially:-

$$E = B_0 \exp(-B_1 y)$$

The constants B_0 and B_1 were calculated by optimization technique.

The mathematical model describes the effect of the process variables, through the following profiles:

$$T_S = \frac{h_G.T_G + T_{(NGX-1)}\cdot\frac{k_L}{h_x} + \left(-\Delta H_S\right).\left[\frac{k_G k_L}{R_G.T_S(k_L + H_1 k_G)}\left(P^G_{H_2S} - G\right)\right]}{\left[h_G + \frac{k_L}{h_x}\right]}$$

$$U_y = -\frac{\Omega x^2}{2\mu_L} + \left[\frac{R_i}{\mu_L} + \frac{\Omega \delta}{\mu_L}\right] x$$

The highest concentration of MEA used in this study (3 M) solution is more efficient in absorption than the lower one (1 M) , this is consistent with the recent researchers trend line in using high concentration of MEA solution in the range (2- 5) M .

The optimum operating condition for the highest H_2S conversion (92.84%) was found to be : C_{MEA}: 3 M , Y: 0.1 , Q_{MEA}: 20 L/hr ,and T: 55°C.

KEY WORDS: Falling film reactor, kinetic, H_2S-MEA , modeling.

INTRODUCTION

Due to presence of sulfur in the petroleum crude, oil refining inherently involves sour gas treating to remove hydrogen sulfide formed during oil processing.

The principle amines used in amine sweetening plants are MEA, DEA, DGA, DIPA and MDEA. The rate of reaction between the amine molecule and sour gas species are similar for MEA, DEA and DGA. MDEA and DIPA are known as selective amines, because there is a significant difference in the reaction rate between the amine and H_2S and CO_2. The reaction rate with H_2S is fast (instantaneous) with alkanolamine molecules. In comparison, the reaction rate with CO_2 is slow due to the intermediate zwitterionic reaction mechanism through a carbonic acid intermediate[1]. Falling film gas absorption, in particular, is a very common phenomenon to be encountered in industrial operations specifically in exothermic gas-liquid reactions such as chlorination, sulphonation, nitration, detergent and wetting/dispersing agent industries, polymerization units, fermentation processes and waste disposal systems. Absorption of a gas in a falling liquid film may take place with or without reaction[2]. The reactant gas absorbs at the liquid interface due to diffusion perpendicular to the direction of liquid flow. Previous mathematical models for falling film reactors in the field of sulphonation reaction have been proposed by Johnson and Crynes[3], Davis et al. [4], Mann et al. [5], Gutierrez et al. [6] and Dabir et al. [7]. Bhattacharya et al. [8] and Nielsen and Villadsen et al. [9] studied the gas absorption for chlorination reactions. All these studies predict chemical conversion and interfacial temperatures as the most important variable in product yield and product quality. The aim of the present work is to develop mathematical models for the falling film reactor, which can be used for laminar and turbulent films. The coupled partial differential equations, which describe the mass and heat transfer in the liquid for first and second order reactions are solved by finite difference backward implicit scheme. Many other researchers [10-16] enabled the designer to simplify his work by performing their kinetic studies on H_2S- MEA reactions.

MATHEMATICAL MODELING

The mathematical model consist of differential balance equations in the liquid phase with their corresponding boundary conditions. Through these equations, velocity, concentration, and temperature profiles are obtained. The equations are for steady state operation, common in industrial and laboratory reactors.

1-The Principle Assumptions

Modeling of the liquid phase was based on the following assumptions:-

1) the liquid circulates in a laminar flow, and the gas circulates co-currently in a turbulent flow.
2) The liquid film is symmetric with respect to the reactor axis.
3) The film thickness is small compared to the column radius.
4) Liquid reactant and liquid product are assumed to be nonvolatile at working temperatures.
5) The solubility of the reactant gas in the liquid reactant and in the reaction product is ideal according to Henry's law.

2-Equations of Mathematical Model

The column is divided into N number of annular segments figure (1), so we have N number of equations for the liquid reactant and another system with the same number of equations for the dissolved gas.

To formulate a comprehensive model, it must include the effect of hydrodynamic, mass transfer, kinetics, and heat transfer.

2.1 Hydrodynamics

the liquid shear and velocity profiles are obtained using Navier-Stockes equations, which states that for an element volume of moving fluid, the rate of change of momentum equals the net of the forces acting on the element volume[17] mathematically expressed with respect to fig (1) as:

Rate of change viscous force
pressure force gravity force
of momentum = on element per +
on element + on element
Per unit volume unit volume
per unit volume per unit volume

$$\rho_l \frac{\partial U_y}{\partial t} = \mu_L \left[\frac{\partial U_y}{\partial x^2} + \frac{\partial^2 U_y}{\partial y^2} + \frac{\partial^2 U}{\partial z^2} \right] - \frac{\partial P}{\partial y} + \rho_L g_g$$

……………(1)

Which is for steady state one-dimensional flow reduces to :

$$\rho_L g_y - \frac{\partial P}{\partial y} + \mu_L \frac{\partial^2 U_y}{\partial x^2} = 0 \qquad …….(2)$$

Or in the form of shear stress:-

$$\rho_L g_y - \frac{\partial P}{\partial y} - \frac{\partial R}{\partial x} = 0 \qquad ………..(3)$$

For a constant axial pressure gradient equation (2) becomes:

$$\frac{\partial^2 U_y}{\partial x^2} = -\frac{\Omega}{\mu_L} \qquad ……………..(4)$$

Where, $\Omega = \rho_L g_y - \frac{\partial P}{\partial y}$ = constant

The gas phase exerts an interfacial shear R_i on the liquid film, and the velocity varnishes at the solid boundary, so according to figure (1), we can write the boundary conditions as:

At x= δ, $\frac{\partial U_y}{\partial x} = \frac{R_i}{\mu_L}$ …………..(5)

x = 0 , U_y=0

Hanaratty and Engen[18], Cohen and Hanaratty [19], and others have measured interfacial shear in two phase gas-liquid flows, reporting the interfacial friction factor φ_i defined by:

$$\varphi_i = \frac{R_i}{\rho_{G.} . U^2{}_G} \qquad ……………..(6\ )$$

Integrating equation (4) twice, and applying boundary conditions, we obtain:

$$\frac{dU_y}{dx} = -\frac{\Omega}{\mu_L} x + C_1 \qquad ……..…….(7)$$

$$U_y = -\frac{\Omega}{2\mu_L} x^2 + C_1 x + C_2 \qquad ……..(8)$$

Substitute equation (5) into (7), to get , C_2=0

Substitute equation (6) into (8), to get:

$$C_1=\frac{R_i}{\mu_L}+\frac{\Omega\delta}{\mu_L} \qquad \text{……….(9)}$$

Substitute equation (9) into (3-8) :

$$U_y=-\frac{\Omega x^2}{2\mu_L}+\left[\frac{R_i}{\mu_L}+\frac{\Omega\delta}{\mu_L}\right]x$$

$$U_y=\frac{a.x}{\delta}-\frac{b.x^2}{\delta^2} \qquad \text{……………..(10)}$$

Where :

$$a=\frac{R_i\delta+\Omega\delta^2}{\mu_L} \qquad \text{……………..(11)}$$

$$b=\frac{\Omega\delta^2}{2\mu_L} \qquad \text{……………..(12)}$$

Equation (10) describes the velocity profile in the liquid film.

To develop the equation which describes the shear profile through the liquid film; from equations (7) and (9):

$$\frac{dU_y}{dx}=-\frac{\Omega x}{\mu_L}+\frac{R_i}{\mu_L}+\frac{\Omega\delta}{\mu_L}$$

$$\mu_L\frac{\partial U_y}{dx}=\Omega(\delta-x)+R_i \qquad \text{…………..(13)}$$

$$R=\Omega(\delta-x)+R_i \qquad \text{……………..(14)}$$

At the wall, equation (14) becomes,

$R_w=\Omega\delta+R_i$ ……………..(15)

From equation (6)

$$R_{\circ}=\phi_i.\rho_G.U^2{}_G \qquad \text{……………..(16)}$$

The film thickness is obtained from the volumetric flow rate per unit length of wetted perimeter, (Q_L) which is related to the velocity distribution by:

$$Q_L=\int_0^\delta U_y(x).dx \qquad \text{……………..(17)}$$

Substitute equation (10) into (17);

$$Q_L=\int_0^\delta \frac{a.x}{\delta}-\frac{b.x^2}{\delta^2}.dx$$

$$Q_L=\delta.\left[\frac{a}{2}-\frac{b}{3}\right] \qquad \text{……………..(18)}$$

Substitute equations (11) and (12) into (18);

$$Q_L=\left[\frac{R_i\delta^2}{2\mu_L}+\frac{\Omega\delta^3}{3\mu_L}\right] \qquad \text{…………..(19)}$$

Equation (19) is cubic equation in (δ) which is readily solved by means of Q_L, R_i, Ω and μ_L.

To evaluate the interfacial friction factor (φ_i), due to turbulent gas, Blasius equation [20] is used;

$$\phi_i=E.(04).\mathrm{Re}_G^{-0.25} \qquad \text{…...(20)}$$

E is a correction factor introduced by our model for account of the gas entrance effect, since the gas flow in our experimental work is not fully developed turbulent flow. we assumed further that E decreases exponentially with the axial distance from the reactor entrance:

$E= B_0\exp(-B_1y)$ …………..(21)

2.2 Mass Transfer

There is zone of reaction between gaseous solute H_2S and liquid reactant MEA, which moves a way from the gas – liquid interface taking up some position towards the bulk of the liquid. The final position of this reaction zone will be such that the rate of diffusion of H_2S from the gas – liquid interface equal the rate of diffusion of MEA from the main body of the liquid.

Figure (2) represents the paths of solute (i.e., H_2S), liquid reactant (i.e., MEA), and liquid product in the liquid form, so H_2S diffuses through the gas film as a result of driving force (P_G-P_i) and diffuses to the reaction zone as a result of driving force (C_i) in the liquid phase. The MEA diffuse from the main body of liquid to the reaction zone under a driving force q, and non volatile product diffuses back to the main bulk of liquid under a driving force (m-n).

2.2.1 Concentration Profile

For H_2S (i.e, A component) and MEA (i.e., B component) ,

$$-U_y \frac{\partial C_A}{\partial y} + D_1 \frac{\partial^2 C_A}{\partial x^2} + r_A = 0 \qquad …….(22)$$

Similarly for liquid reactant (B), the differential balance equation is :

$$-U_y \frac{\partial C_B}{\partial y} + D_2 \frac{\partial^2 C_B}{\partial x^2} + r_B = 0 \qquad ……….(23)$$

$$\left.\begin{array}{l} D_1 = D_A \\ D_2 = D_B \end{array}\right\} \qquad ……….(24)$$

$$U_y \frac{\partial C_A}{\partial y} = \frac{\partial}{\partial x}\left[(D_A).\frac{\partial C_A}{\partial x}\right] + r_A \qquad …….(25)$$

$$U_y \frac{\partial C_B}{\partial y} = \frac{\partial}{\partial x}\left[(D_B).\frac{\partial C_B}{\partial x}\right] + r_B \qquad …….(26)$$

2.2.2 Boundary Conditions

The boundary conditions required to integrate equation (25) and (26) are:

(a) On y=0, $C_B = C_B^0$, $C_A = 0$ ……. (27)

(b) On x=0, $\frac{\partial C_B}{\partial x} = 0$, $\frac{\partial C_A}{\partial x} = 0$ ...(28)

(c) On x=δ, $\frac{\partial C_B}{\partial x} = 0$,

$$N_A = K_G\left(C_A^G - C_A^{IG}\right) \qquad ……….(29)$$

Where $N_A = -D_A \frac{\partial C_A}{\partial x}$

The condition (b) indicates that the components mathematically and in fact, can not pass through the wall.

2.2.3 Equilibrium Conditions

(a) Rate of absorption

In the steady state process of absorption, the rate of transfer of material through the gas film will be the same as that through the liquid film, and the general equation of mass transfer[21] may be written as:

$$N_{H_2S} = \frac{K_{OG}}{R_g T_S}\left[P^G_{H_2S} - P^*_{CO_2}\right] \quad \text{……….(30)}$$

Where:

N_{H_2S} : molar flux of gaseous reactant (H_2S), kmol/m^2.s

K_{OG} : overall gas phase mass transfer coefficient, m/s

Rg: gas-liquid interface temperature, K^0.

$P^G_{H_2S}$: partial pressure of H_2S in gas phase, N/m^2.

$P^*_{H_2S}$: partial pressure of H_2S in gas phase which is in equilibrium with bulk liquid phase, N/m^2.

(b) Henry's Constant

Dankwerts [21] mentioned that in many cases, so long as the concentration of dissolved gas is small and the temperature and pressure are far removed from the critical temperature and pressure of the gas, Henry's law is obeyed and the concentration [H_2S] of dissolved gas in equilibrium with a partial pressure Pi of the gas is given by

$$P^*{}_{H_2S} = H_e\left[H_2S\right] \quad \text{……….(31)}$$

[H_2S] : concentration of unreacted H_2S in solution, kmol/m^3

Where He is the Henry's law constant, (N/m^2), m^3/kmol)

If the gas reacts in solution, Henry's law does not apply to the total concentration of unreacted gas.

For the H_2S -MEA system, at the temperature range of (0-100) °C and (0.5-3 M) MEA Bendall[22] reported a relation given by:

$$H_e = 2.3486 e^{-0.0793 T_S} \quad \text{……….(32)}$$

Where T_S is the gas –liquid interface temperature K.

c) Conversion of gaseous H₂S

When H_2S is absorbed in MEA solution it reacts according to the following overall reaction ;

$$H_2S + RNH_2 \Leftrightarrow RNH_2H^+ + HS^- \quad \text{….(33)}$$

The equilibrium condition is given by:

$$K = \frac{\left[RNH_2H^+\right]\left[HS^-\right]}{\left[H_2S\right]\left[RNH_2\right]} \quad \text{……….(34)}$$

$$P^* = \frac{H_e}{K} m \frac{Z^2}{1-Z} \; {}^{[156]} \quad \text{……….(35)}$$

Where:

m: total H_2S concentration, kmol/m^3

Astarita [23] proposed a simplification by replacing $\frac{H_e}{K}$ with constant

$$P^* = 2.4571*10^6 m^{0.25}\frac{Z^2}{1-Z}\exp\left(\frac{-7545}{T_S}\right)$$

………(36)

Substitute equation (36) into (30);

$$N_{H_2S} = \frac{K_{OG}}{R_g T_S}\left[P^G_{H_2S} - 2.4571*10^6 m^{0.25}\frac{Z^2}{1-Z}\exp\left(\frac{-7545}{T_S}\right)\right]$$

…..(37)

$$Conversion = \frac{N_{H_2S} \times A_S}{M_{H_2S}} \quad ………(38)$$

Where :

A_S: total area of mass transfer, m^2

M_{H_2S}: Initial molar rate of H_2S, kmol/s.

2.2.4 Mass Transfer Coefficients

a) Gas-Side Mass Transfer Coefficient

$$K_G = I\sqrt{\phi_i}\,U_G (Sc_G)^{-0.0704} \quad ……….(39)$$

b) Liquid side mass transfer coefficient

To estimate the liquid side mass transfer coefficient, the correlation of Wilkes[24] is used. They investigated the characteristics of H_2S-H_2O system in a wetted wall column and suggested the following equation:

$$K_L = 0.523\left[\frac{3\mu_L D_L}{\rho_L}\right]^{1/2}\left[\frac{L}{g_y \mu_L^2}\right]^{1/3} \quad …(40)$$

Where :

D_L: diffusion coefficient of solute in liquid, m^2/s

g_y: gravitational constant=9.8 m/sec^2.

L: length of wetted wall, m.

μ_L: viscosity of liquid, N.s/m^2.

ρ_L: density of liquid, kg/m^2

K_L: liquid-side mass transfer coefficient, m/s

c) Overall mass transfer coefficient

The overall mass transfer coefficient for the absorbed component CO_2 consist of the gas, and liquid side mass transfer coefficients and is expressed as:

$$\frac{1}{K_{OG}} = \frac{1}{K_G} + \frac{H_1}{K_L} \quad …………(41)$$

$$H_1 = \frac{H_e}{R_G.T_S} \quad ……………..(42)$$

Substitute equation (41) into equation (37) :

$$N_{H_2S} = \frac{K_G K_L}{R_G T_S (K_L + H_1 K_G)}\left[P^G_{H_2S} - 2.4571*10^6 m^{0.25}\frac{Z^2}{1-Z}\exp\left(\frac{-7545}{T_S}\right)\right]$$

…………(43)

2.3 Heat Transfer

$$U_y.\frac{\partial}{\partial y}\left(\rho_L C_{P_L} T\right) = -\frac{\partial}{\partial x}\left(-k_L\frac{\partial T}{\partial x}\right) - \Delta H_R.r_A \quad ..(44)$$

Equation (44) is used to formulate the temperature profile through the column. With the same boundary conditions of item (2.4.1) and gas side mass transfer coefficient of item (2.4.2). Applying Newton- Raphson method on the resultant equation (44) through the main program (NAG Library Software) to estimate the interfacial H_2S –MEA temperature.

3. Solution of the mathematical model

Equations (25), (26) and (44) are two dimensional second order non linear partial differential equation include:

$C_A = f(x, y)$

$C_B = F(x, y)$

$T = S(x, y)$

Through the liquid film, where f , F and S are functions of two independent variables (i.e., x and y). the above equations can not be solved analytically. So this is done numerically. Concentration and velocity profiles will be obtained by means of the same techniques in sections (2.1) and (2.2).

RESULTS AND DISCUSSION

Results of the Present Model

The present model is formulated to predict velocity, concentration, and temperature profiles through the liquid falling-film radially and axially along the reactor. The axial conversion of the solute in the gas phase and the axial interfacial temperature can be also predicted.

Figures (3 to 7) show the output results of the present model, taking a test run of a refinery as an example.

1-Interfacial Temperature Profile

Figure (3) shows the model prediction for the interfacial temperature along the reactor. Analyzing the behavior of the curve indicates an average increase of interfacial temperature (= 8°K) through the first meter of the reactor while through the rest of the reactor the cooling effect of the gas stream begins to diminish the interfacial temperature lower than the initial input temperature of liquid.

2-Concentration Distribution

The present model has the capability to predict concentration profile of the reactants through the liquid film, axially and radially. These are shown in figures (4-6).

Figure (4) shows a linear surface distribution of free hydrogen sulfide concentration in the liquid film. Studying the concentration profiles of figures (4) indicates that the reaction between hydrogen sulfide and monoetanolamine is instantaneous and this is consistent with Davis [4].

3-Temperature Distribution

Figure (5) represents the linear surface distribution of liquid temperature along the reactor. From the mentioned figures we can observe that:

1- The liquid temperature distribution presents a typical bulge shape. This is due to the fact that the exothermic reaction produces heat and the heat is absorbed by the liquid and gas streams.. This means that the liquid absorbs most of the heat in the top of the reactor

2- At constant H_2S content in gas stream, the liquid flow in the column is relatively small, thus the liquid heat capacity is small. As a consequence the liquid temperature gradient at the top of the absorber is very steep. Even though the reaction occurs throughout the column, the temperature starts to decrease in the middle of the column, because the liquid is cooled by the flue gas flowing up the column till a constant value of temperature.

3- The average increase of liquid temperature along the first meter of the reactor length is within (6 °K).

4-Velocity Distribution

Figure (6) represents the linear surface distribution of liquid velocity along the reactor. It can be seen from equation (3) that the maximum liquid velocity occurred at the gas-liquid interface and the minimum value (i.e., $U_y=0$) occurred at tube wall, equation (3) is used by the present model to predict the velocity profile in the liquid along the reactor. The parameters influences the velocity profile are gas flow rate, liquid flow rate, liquid viscosity, and tube wall roughness. Liquid velocity is proportional to gas and liquid flow rate while it is inversely proportional to liquid viscosity and tube wall roughness.

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NOMENCLUTURE

Symbol	Definition	Unit (SI System)
C_A	Molar concentration of H_2S in liquid	kmol/m^3
C_A^G	Molar concentration of H_2S in gas	kmol/m^3
C_A^{IG}	Molar concentration of H_2S at gas-liquid interface	kmol/m^3
C_B	Molar concentration of unreacted H_2S in liquid	kmol/m^3
C_B^0	Initial molar concentration of MEA in liquid	kmol/m^3
$[H_2S]$	Molar concentration of MEA in liquid	kmol/m^3
C_{PG}	Specific heat of gas	J/kg.K
C_{PL}	Specific heat of solution	J/kg.K
D_A	Molecular diffusivity of H_2S in liquid	m^2/s
D_B	Molecular diffusivity of MEA in liquid	m^2/s
D_E	Eddy diffusivity	m^2/s
g_C	Conversion factor	kg.m/N.s^2
g_y	Gravitational acceleration	m/s^2
h_G	Gas- side heat transfer coefficient	W/m^2.K
h_x	Grid spacing in x-direction	m
H	Henry's law constant	N/m^2.m^3/kmol
ΔH_L	Heat of absorption and reaction of H_2S with MEA solution	kJ/kmol
ΔH_R	Heat of reaction of H_2S with MEA	kJ/kmol

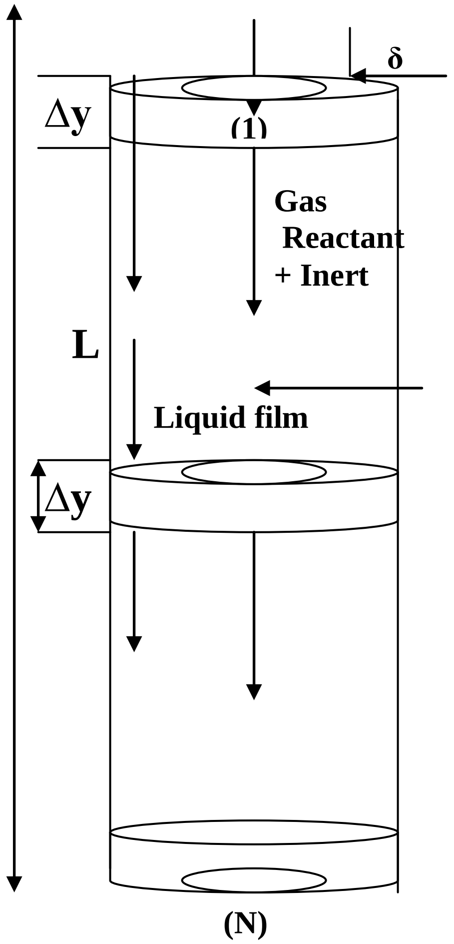

Figure (1) Falling film reactor divided into N annular segments each of length Δy and thickness δ.

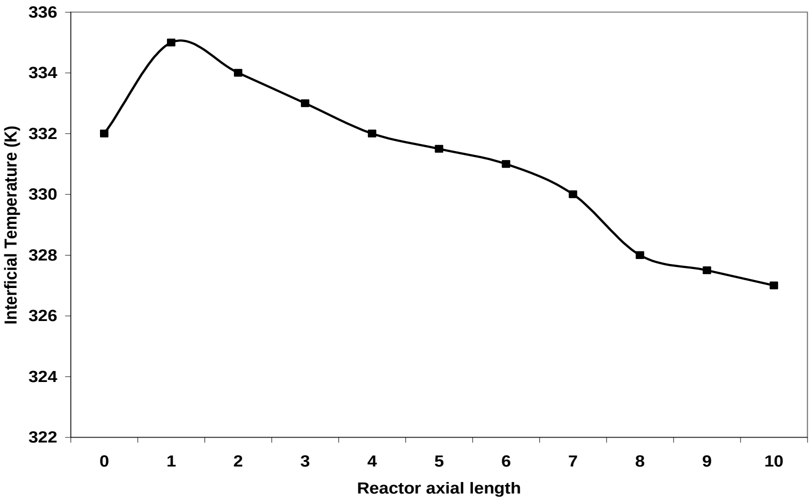

Figure (3) Interfacial temperature profile along the reactor length as predicted by present model for operating condition refinery test run

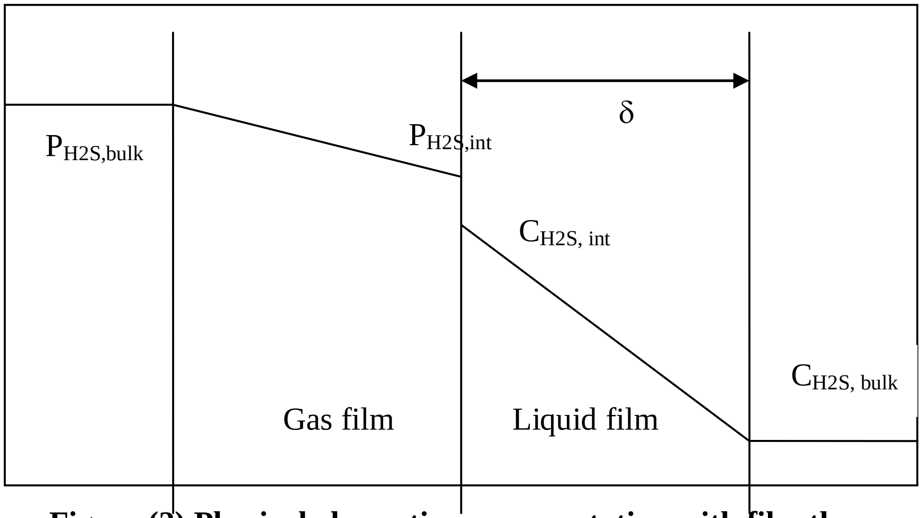

Figure (2) Physical absorption representation with film theory

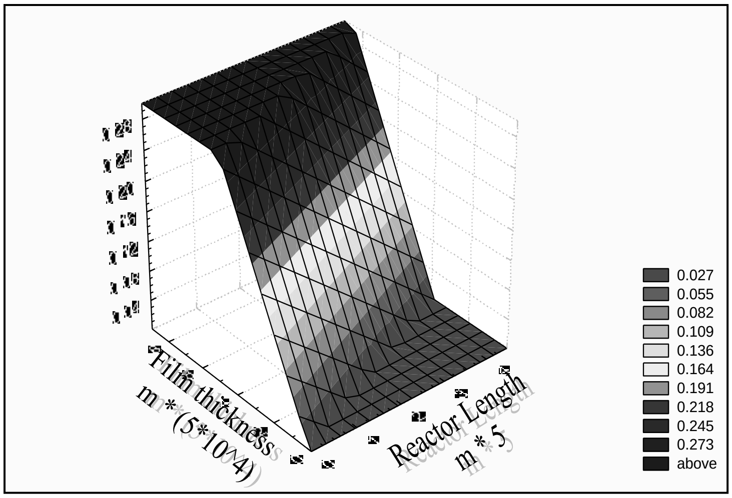

Figure (4) Surface distribution of free H_2S concentration in the liquid film for operating condition of Baiji Refiner as predicted by present model

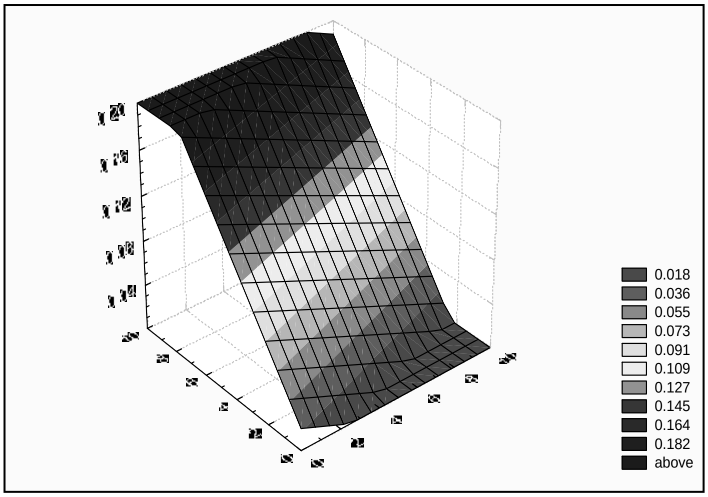

Figure (6) Surface distribution of liquid velocity for operating condition of Baiji Refinery

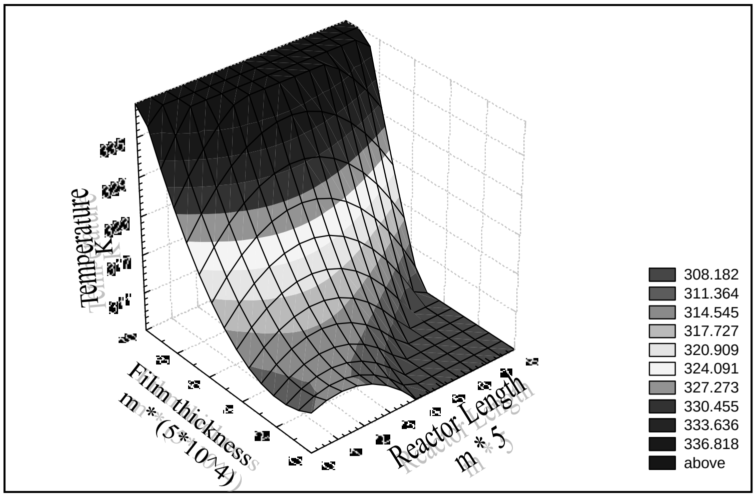

Figure (5)Surface distribution of Temperature through the liquid along the reactor length for operating conditions of Baiji Refinery

إعداد موديل رياضي للتفاعل اللحظي لغاز ثاني كبريتيد الهيدروجين في مفاعل الطبقة المتساقطة

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الخلاصة

ان الهدف من العمل المقدم هو دراسة تأثير عدة عوامل التي تلعب دوراً معروفاً في امتزاز غاز ثاني كبريتيد الهيدروجين و هي معدل جريان السائل، تركيز المادة المازة، درجة حرارة السائل و الكسر المولي لغاز ثاني كبريتيد الهيدروجين في المزيج الغازي.

تم تكوين موديل رياضي و تجريبي لنظام امتزاز ثاني كبريتيد الهيدروجين باستخدام احادي ايثانول الأمين كمادة مازة في مفاعل الطبقة المتساقطة.

و هذه أهم المعادلات التي تم التوصل إليها:

$$T_S = \frac{h_G.T_G + T_{(NGX-1)}.\frac{k_L}{h_x} + \left(-\Delta H_S\right).\left[\frac{k_G k_L}{R_G.T_S\left(k_L + H_1 k_G\right)}\left(P^G_{H_2S} - G\right)\right]}{\left[h_G + \frac{k_L}{h_x}\right]}$$

$$U_y = -\frac{\Omega x^2}{2\mu_L} + \left[\frac{R_i}{\mu_L} + \frac{\Omega\delta}{\mu_L}\right]x$$

تم تصميم التجارب على نظام العوامل المتعددة و تم دراسة العوامل المؤثرة على تحول غاز ثاني اوكسيد الكاربون ضمن المديات التالية: الكسر المولي لغاز ثاني كبريتيد الهيدروجين (0.05 ,0.075, 0.1) و تركيز السائل الماز (2,1 , 3 مولاري) و معدل جريان الحجمي (5، 10، 15، 20) لتر/ساعة و درجة حرارته (35، 40، 45، 50 و 55 م).

تم إعداد برنامج بلغة فورتران للحصول الدوال الخاصة بالسرعة و درجة الحرارة و التركيز باستخدام تقنية الشبكات المتعددة من خلال برمجة المعادلات الحركية و الثرموديناميكية للنظام و بالاستعانة ايضاً بالخواص الفيزيائية لمكونات النظام.

و تم الحصول على دوال التركيز و درجة الحرارة و السرعة من خلال ذلك البرنامج و كذلك عدة دوال بعدية اخرى ذات اهمية.

و تم ادخال مجموعة من البيانات الخاصة بظروف التشغيل لذلك البرنامج من خلال التشغيل الموقعي لمصفى الشمال /مصافي بيجي (بالنسبة لنظام ثاني كبيرتيد الهيدروجين). و إن مدى انطباق الموديل الرياضي له علاقة وثيقة بمدى دقة النتائج.

ε_n

ε_{cr} ⌋

$$\frac{\alpha_1-\varepsilon_n/\varepsilon_{cr})}{(\alpha_1-1.0)}$$

و قد تبين أن تأثير المدخل لمفاعل الطبقة المتساقطة يمكن ان يرتبط بعلاقة اسية مع المسافة المحورية تبعاً للمعادلة :

$$E = B_0 \exp(-B_1 y)$$

و قد تم استخراج قيم الثوابت B0و B1 من النتائج التجريبية

و قد تبين ان التفاعل في هذا النظام هو تفاعل وري و التفاعل يحدث عند السطح البيني.

ان نسبة تحول ثاني كبريتيد الهيدروجين في الطور الغاز تتناسب اسياً مع طول المفاعل.

ان الموديل الرياضي وصف تأثير متغيرات العملية، و هي معدل جريان السائل، درجة حرارته ، تركيزه و الكسر المولي لثاني اوكسيد الكاربون على معدل الامتزاز.

ان هذا الوصف دلّ على ان العملية تكون اكثر كفاءة عندما يتم تبريد المفاعل.كما ان التركيز الأعلى للامين (3 مولاري) يزيد من معدل الامتزاز و هذا يتوافق مع توجه الباحثين حالياً نحو استخدام التراكيز العالية من الامين في عمليات امتزاز و ثنائي كبريتيد الهيدروجين (2-5) مولاري.

الكلمات الدالة

مفاعل الطبقة المتساقطة، حركية ، نظام غاز ثنائي كبريتيد الهيدروجين-احادي ايثانول الامين، نمذجة