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MATHEMATICAL MODELING OF JET BUBBLING REACTOR

by

Fred Jyh-Woei Cheng

Thesis submitted to the Faculty of the Graduate School
of the New Jersey Institute of Technology in partial
fulfillment of the requirement for the degree of
Master of Science in Chemical Engineering

1981

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Reactor

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ABSTRACT

Title of Thesis: Mathematical Modeling of Jet Bubbling
Reactor

Fred Jyh-Woei Cheng, Master of Science, 1981

Thesis directed by: Dr. C. R. HUANG
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A jet bubbling reactor for flue gas desulfurization is described by a mathematical model with the concept of two-stages mass transfer with chemical reactions. The model consists of two coupling differential equations which are solved simultaneously. The result from the theoretical model is agreeable SO_2 removal data obtained from a pilot plant reactor.

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I. INTRODUCTION

Gas absorption accompanied by chemical reaction is of great industrial importance. A lime and limestone based system for the flue gas desulfurization process, falls into this category. All the usual types of gas-liquid reactors, such as bubble columns; plate columns; packed columns; mechanically agitated contactors; etc., are employed in industry for carrying out gas-liquid reactions. Bubble columns are widely used in industry due to the simple design, the absence of moving parts eliminating the need for seals and large liquid hold-up time. However, bubble columns do suffer from the disadvantage of high pressure drop due to the hydrostatic head of the liquid. The gas dispersion in plate columns and packed columns are coarse and there some tendency for channels of gas to be formed which will reduce the effective interfacial area. The effective interfacial area is a very important variable when the reactor design is based on mass transfer considerations. Also, when a soluble gas is to be absorbed in slurry or a clear liquid with solid deposition in the absorption device which could create unreliability and unscheduled shutdown problem.

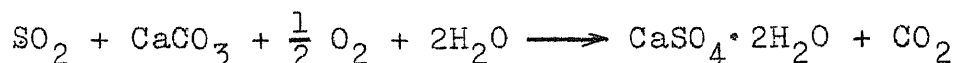
In general, industry desires the following of an absorption device in a flue gas desulfurization system for the following reasons: operational reliability; high

liquid-to-gas ratio; low pressure drop characteristics; high absorption efficiency potential; high specific surface area; good byproduct utilization; low investment and operating costs; and easy operation without scaling and plugging condition.

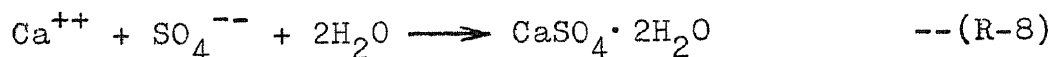
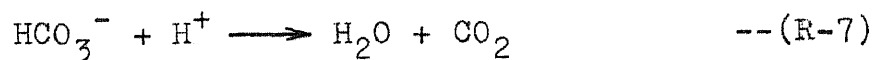
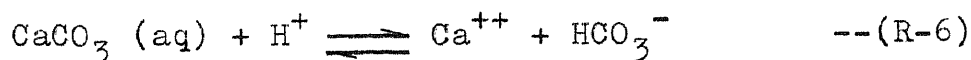
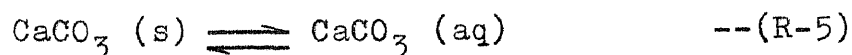
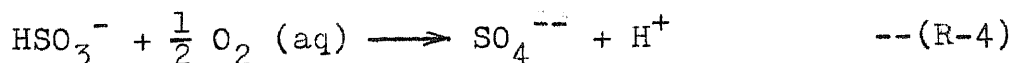
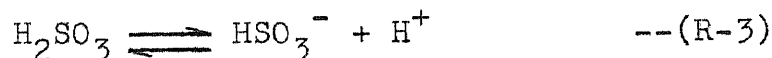
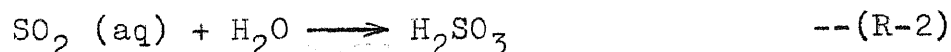
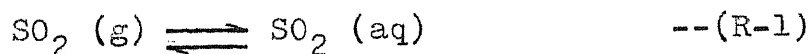
In Japan, Chiyoda Chemical Engineering and construction Co. Ltd. has developed a jet bubbling reactor which has high specific surface, low pressure drop and high liquid-to-gas ratio capabilities. The reactor is equipped with a gas sparging device to create a jet bubbling layer. In this layer, a large gas-liquid interface area and turbulent motion of liquid provide effective SO_2 removal. This reactor replaced the usual type of scrubber in limestone-based system which uses a solution instead of a slurry to remove both SO_2 and particulates with great efficiency. This system is able to avoid the problem of scaling and plugging and produces a gypsum that may be used for wall-board and as an additive for portland cement. The system was tested over a period of years with minimal process difficulty. This reactor has been analyzed mathematically in the jet bubbling zone with the assumption of plug flow in the gas phase and back mixing in liquid phase. The objective of this research is to focus our attention on the jet bubbling zone with a description of the reactor of jet bubbling type by a mathematical model with the concept of two-stages mass transfer with chemical reactions.

II. DESCRIPTION OF CHEMICAL PROCESS

The jet bubbling flue gas desulfurization process uses a solution instead of a slurry to absorb SO_2 . The principal absorption reaction for this system is given by:



The essential reactions governing this system in the jet bubbling zone are:



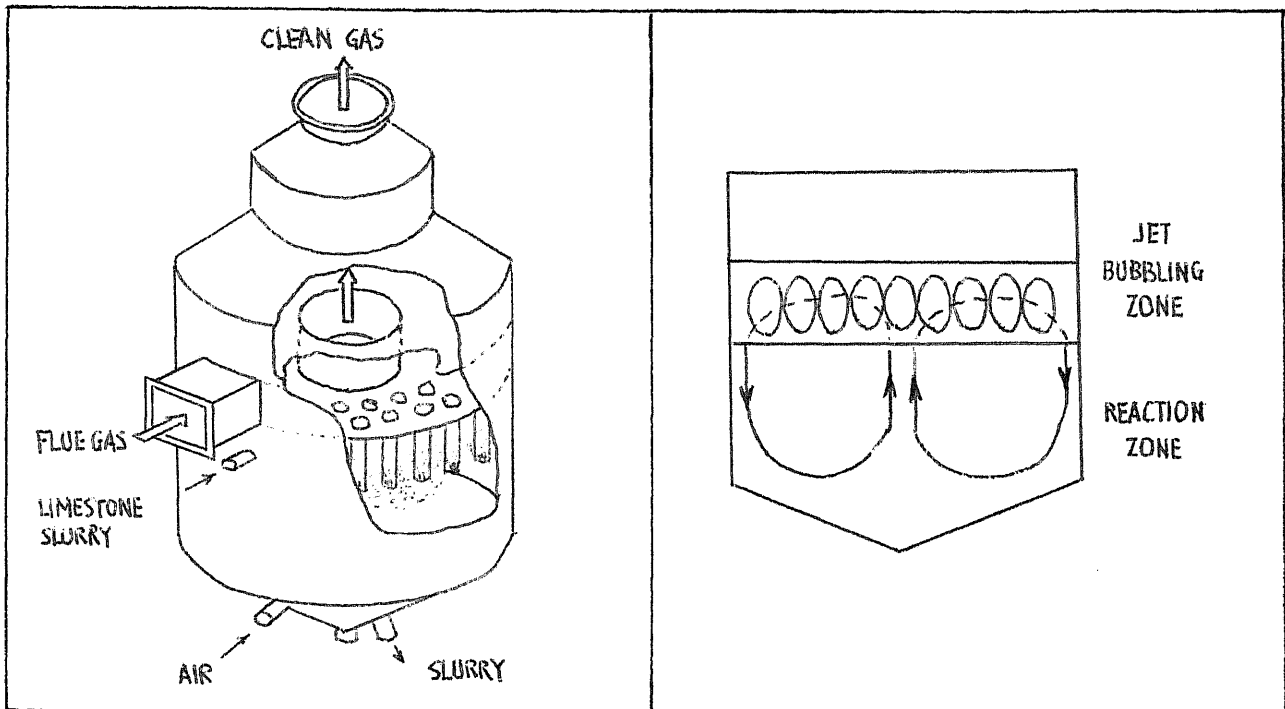
In this zone, gas-phase mass transfer of SO_2 and dissolution of CaCO_3 are the controlling steps (Ref. (1)).

Control of scaling in the reactor walls is achieved by keeping gypsum crystal concentration in the range of 10 to 20 wt.% and having sufficient liquid volume in the reactor. The utilization of limestone is governed by the pH value of the slurry. Therefore, weak sulfuric acid of 2 wt.% is charged to the reactor continuously to give the desired pH value. Gypsum byproduct from this system is chemically stable and is of high quality and can be used in many categories.

III. DESCRIPTION OF THE REACTOR

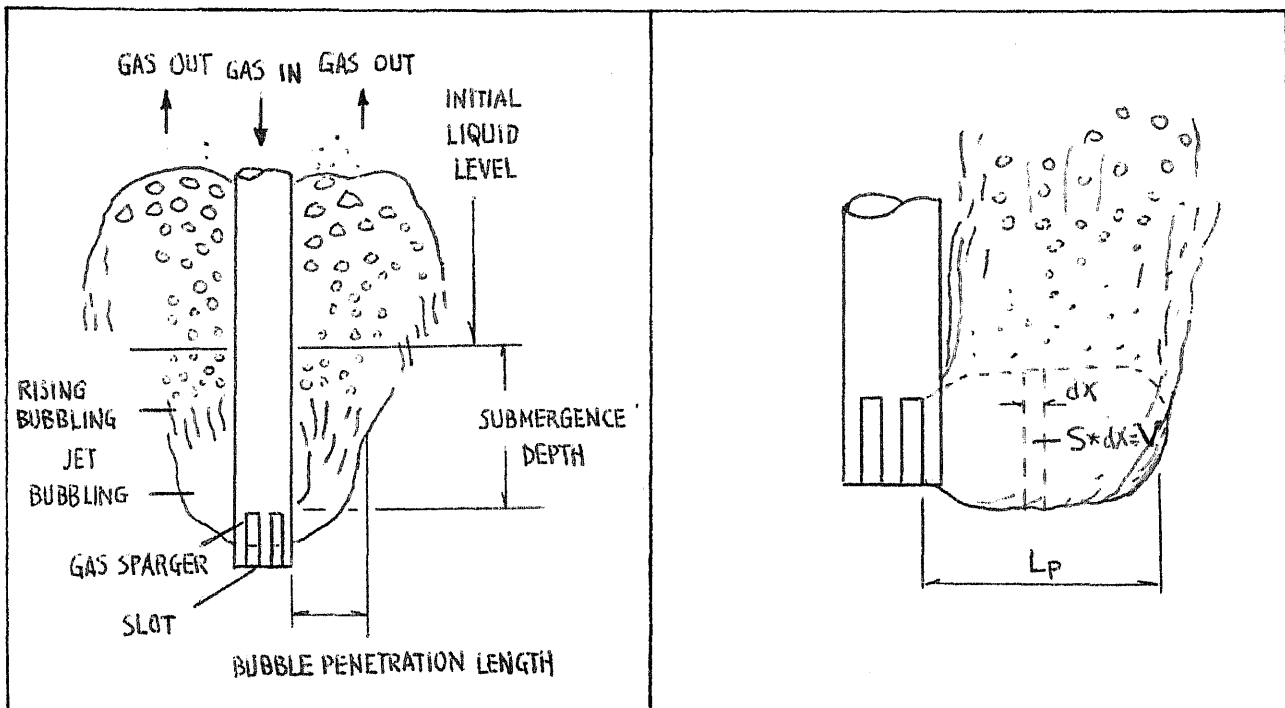
A sketch of a jet bubbling reactor is shown in Fig. 1. The reactor consists of two zones: jet bubbling zone and reaction zone. The reactor is equipped with a gas sparging device which has slot open ends 100 mm. to 400 mm. (refer to Fig. 1) below the liquid surface. Flue gas was injected horizontally through the slots into the liquid-phase with a velocity of 5 m./sec. to 20 m./sec.. Then, the gas was split into bubbles by the turbulent motion of liquid. A gas jet of bubbles was formed horizontally near the slots and then deflected upward due to the buoyant force. In this zone, the gas bubbles are finely broken by liquid motion and a large gas-liquid interface area is created to provide for effective SO₂ removal. Residence time for the gas-phase is very short (0.5 sec. to 1.5 sec.) in this zone.

In the reaction zone, air is pumped into the reactor from the bottom and a mechanical agitator is stirred to keep proper liquid circulation. In this zone, air is dissolved into the liquid as the source of oxygen and a proper amount of suspending solid and sufficient residence time permit the gypsum to grow to the desired size.



Cutaway view of the jet bubbling reactor

Liquid flow pattern in the jet bubbling reactor



Schematic of the gas sparger in operation

Schematic of jet bubbling zone

Figure 1. Sketch of the jet bubbling reactor (reference (1))

IV. MATHEMATICAL MODEL OF THE REACTOR

The gas bubble reactor in which flue gas is bubbled through a gas sparging device generates a jet bubbling layer near the device. This region of gas is dominated by gas momentum. Beyond this region, the dispersed gas bubbles rise up by buoyant force. Therefore, the mathematical modeling of this reactor will be divided into two portions: A). modeling of the jet bubbling zone, and B). modeling of the rising bubble zone.

A). Modeling of the Jet Bubbling Zone:

The rate of SO₂ transfer between phase is

$$W = K_G A (P_{SO_2} - P_{SO_2}^*) \quad \text{---(1)}$$

where K_G is the gas-side mass transfer coefficient, A is the interphase area, P_{SO_2} is the gas phase partial pressure of SO₂, and $P_{SO_2}^*$ is the equilibrium vapor pressure of SO₂ with respect to the liquid SO₂ concentration. The interphase area A is defined as $A = NaV$, where N is the number of slots, a is the specific interface area, V is the volume of jet bubbling zone per slot (refer to Fig. 1). Then, equation (1) becomes:

$$dW = K_G aN (P_{SO_2} - P_{SO_2}^*) dV \quad \text{---(2)}$$

The mass balance of SO_2 in the gas phase is

$$dW = M_g' d\left(\frac{y}{1-y}\right) = M_g \frac{dy}{1-y} \quad \text{---(3)}$$

where M_g' is molar flow rate of carrier gas, y is the mole fraction of SO_2 in flue gas, and M_g is the molar flow rate of flue gas. Using equation (3), equation (2) becomes:

$$M_g \frac{dy}{1-y} = K_G aN(P_{\text{SO}_2} - P_{\text{SO}_2}^*)dV \quad \text{---(4)}$$

The volume of jet bubbling zone is assumed as:

$$V = L_p * S \quad \text{---(5)}$$

where S is the average cross-sectional area of jet bubbling zone, L_p is the bubble penetration length. Since the penetration length of bubble is linear with respect to the volumetric flow rate of gas :

$$L_p = b_0 + b\left(\frac{V_g}{N}\right) \quad \text{---(6)}$$

where b_0 and b are the intercept and slope of the curve respectively which can be obtained from Fig. 2, V_g is the volumetric flow rate of flue gas. Using equation (5) and (6) and applying the ideal gas law, $P_{\text{tot}}V_g = GA_S NRT$, equation (4) becomes

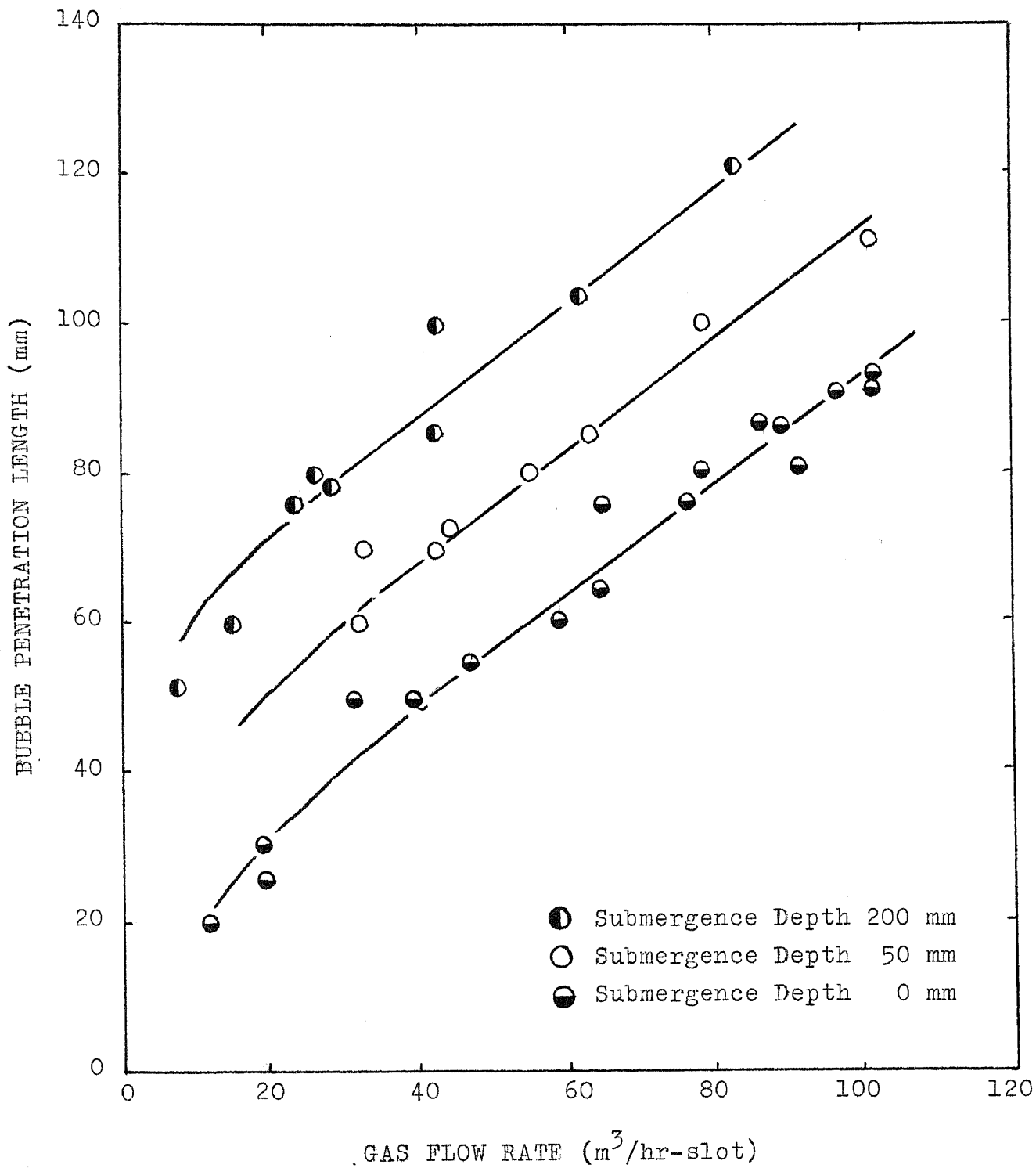


Figure 2. Effect of gas flow rate on bubble penetration length. (reference (1))

$$M_g \frac{dy}{1-y} = K_G a_N (P_{SO_2} - P_{SO_2}^*) \frac{bRT}{P_{tot}} A_s S_d G \quad \text{--- (7)}$$

where A_s is the slot cross-sectional area, R is the gas law constant, T is the flue gas temperature, P_{tot} is the total pressure of the reactor and G is the molar velocity of gas based on the slot cross-sectional area. Since gas phase mass transfer of SO_2 is the controlling step, when we apply Henry's law to the liquid phase, $P_{SO_2}^* = K_H C_{SO_2}(aq)$, we find that the concentration of SO_2 in the liquid phase $C_{SO_2}(aq)$ is affected by the concentration of O_2 in the liquid phase C_{O_2} ; the pH value of the liquid phase C_{H^+} ; and the concentration of Ca^{++} in the liquid phase $C_{Ca^{++}}$. Here, the concentration of SO_2 in the liquid phase is obtained from the following:

Refer to Section II (R-2) and (R-3), we have $C_{SO_2}(aq) = K_1 (C_{HSO_3^-})(C_{H^+})$. From (R-4), $C_{HSO_3^-}$ can be expressed as $(C_{SO_4^{--}})(C_{H^+}) / (C_{O_2}^{1/2})$, and from (R-8), $C_{SO_4^{--}}$ can be replaced by $1/C_{Ca^{++}}$, where $C_{HSO_3^-}$ is the concentration of HSO_3^- in the liquid phase, $C_{SO_4^{++}}$ is the concentration of SO_4^{++} in the liquid phase, and K_1 is the reaction rate constant. Therefore, we get $C_{SO_2}(aq) = K_3 (C_{H^+}^2) / (C_{Ca^{++}})(C_{O_2}^{1/2})$ and then:

$$P_{SO_2}^* = K_H K_3 \frac{C_{H^+}^2}{(C_{Ca^{++}})(C_{O_2}^{1/2})} \quad \text{--- (8)}$$

Therefore, equation (7) becomes:

$$M_g \frac{dy}{1-y} = K_G a N (P_{tot} \cdot y - \frac{K_H \cdot K_3 \cdot C_H^2}{(C_{Ca^{++}})(C_{O_2}^{\frac{1}{2}})}) \frac{bRT}{P_{tot}} A_s S_d G \quad - - - - (9)$$

where K_H is the Henry's law constant, K_3 is the reaction rate constant. For the calculation of $K_G a$, the data in reference (2) and (3) indicates that the following relationship is likely to hold:

$$K_G a \propto D_g^{0.5} U^{0.75} H^{-0.67} \quad - - - - - (10)$$

where D_g is the diffusion coefficient for the SO_2 -Air system, U is the flue gas flow rate, and H is the submergence depth. ZABBAN and DODGE (4) have found that at a given mass flow rate of the gas, the gas-side mass transfer coefficient is inversely proportional to the total pressure, i.e.: $K_G a \propto 1/P_{tot}$. Therefore, the gas-side mass transfer coefficient becomes:

$$K_G a = B_0 (Sc)^{-\frac{1}{2}} (Re)^{\frac{3}{4}} (Hi)^{-\frac{2}{3}} = A_0 G^{\frac{3}{4}} \quad - - - (11)$$

$$\text{where } A_0 = B_0 (Sc)^{-\frac{1}{2}} \left(\frac{D_b}{\mu} \right)^{\frac{3}{4}} (Hi)^{-\frac{2}{3}}$$

$$B_0 = \text{constant}$$

$$Sc = \text{Schmidt Number} = \frac{\mu}{\rho D_g}$$

$$Re = \text{Reynolds Number} = \frac{GD_b}{\mu}$$

$$H_i = \text{constant} = \frac{H \rho_L g}{P_{\text{tot}} \cdot g_c}$$

D_b = gas bubble diameter

μ = viscosity of gas

ρ = density of gas

ρ_L = density of liquid

g = gravitational acceleration

g_c = gravitational conversion factor

Substitute equation (11) into equation (9), we have:

$$M_g \frac{dy}{1-y} = A_o G^{\frac{3}{4}} N \left(P_{\text{tot}} \cdot y - \frac{K_H \cdot K_3 \cdot C_{H^+}^2}{(C_{Ca^{++}})(C_{O_2}^{\frac{1}{2}})} \right) \frac{bRT}{P_{\text{tot}}} A_s S_d G \quad \text{--- (12)}$$

Since $M_g = N A_s G$, therefore:

$$\frac{dy}{(y-y^*)(1-y)} = A_o bRTSG^{-\frac{1}{4}} dG \quad \text{--- (13)}$$

$$\text{where } y^* = \frac{K_H \cdot K_3 \cdot C_{H^+}^2}{(C_{Ca^{++}})(C_{O_2}^{\frac{1}{2}})(P_{\text{tot}})}$$

Equation (13) integrate from $y=y_i$ to $y=y_f$ at $X=0$ to $X=L_p$ and $G=G_i$ to $G=G_f$, where $G_i=G|_{X=L_p=0}$ and $G_f=G|_{X=L_p}$, we have:

$$\frac{1}{1-y^*} \ln\left(\frac{y-y^*}{1-y}\right) \Big|_{y=y_i}^{y=y_f} = \frac{4}{3} A_o bRTSG^{\frac{3}{4}} \Big|_{G=G_i}^{G=G_f} \quad \text{--- (14)}$$

and then:

$$\frac{1}{1-y^*} \ln\left(\frac{y_f - y^*}{1-y_f} * \frac{1-y_i}{y_i - y^*}\right) = \frac{4}{3} A_o bRTS (G_f^{\frac{3}{4}} - G_i^{\frac{3}{4}}) \quad \text{--- (15)}$$

If we let $Y_c = \frac{1-y_i}{y_i - y^*}$

$$G_c = (1 - y^*) \frac{4}{3} A_o bRTS (G_f^{\frac{3}{4}} - G_i^{\frac{3}{4}})$$

where $G_i = G|_{X=L_p=0} = - \frac{P_{tot}}{bRTA_s} b_o$

$$G_f = G|_{X=L_p} = \frac{P_{tot}}{bRTA_s} (L_p - b_o)$$

equation (15) can be expressed as follows:

$$\ln\left(\frac{y_f - y^*}{1 - y_f} * Y_c\right) = G_c \quad \text{--- (16)}$$

Finally, we can get the mole fraction of SO_2 in the flue gas at jet bubbling zone:

$$y_f = \frac{y^* \cdot Y_c + e^{G_c}}{Y_c + e^{G_c}} \quad \text{--- (17)}$$

Since the pressure drop in the reactor for a given gas rate may be calculated by simply multiplying the submergence depth H by the holdup of liquid Z_L (Ref. (6)):

$$\Delta P = H * Z_L \quad \text{--- (18)}$$

G_c can be expressed as:

$$G_c = \frac{4}{3} bRTSB_0 (G_f^{\frac{3}{4}} - G_i^{\frac{3}{4}}) (Sc)^{-\frac{1}{2}} \left(\frac{D_b}{\mu}\right)^{\frac{3}{4}} \left(\frac{P_L \cdot g}{P_{tot} \cdot g_c \cdot Z_L}\right)^{-\frac{2}{3}} (1 - A_1 C_{H^+}^2) (\Delta P)^{-\frac{2}{3}}$$

$$= A_2 (1 - A_1 C_{H^+}^2) (\Delta P)^{-\frac{2}{3}} \text{----- (19)}$$

where $A_1 = \frac{K_H \cdot K_3}{(C_{Ca^{++}})(C_{O_2}^{\frac{1}{2}})(P_{tot})}$

$$A_2 = \frac{4}{3} bRTSB_0 (G_f^{\frac{3}{4}} - G_i^{\frac{3}{4}}) (Sc)^{-\frac{1}{2}} \left(\frac{D_b}{\mu}\right)^{\frac{3}{4}} \left(\frac{P_L \cdot g}{P_{tot} \cdot g_c \cdot Z_L}\right)^{-\frac{2}{3}}$$

Substitute equation (19) into equation (17), y_f can be expressed as function of concentration of H^+ in the liquid phase C_{H^+} , and pressure drop across the reactor ΔP :

$$y_f = \frac{A_1 C_{H^+}^2 (1 - y_i) + (y_i - A_1 C_{H^+}^2) e^{A_2 (1 - A_1 C_{H^+}^2) (\Delta P)^{-\frac{2}{3}}}}{(1 - y_i) + (y_i - A_1 C_{H^+}^2) e^{A_2 (1 - A_1 C_{H^+}^2) (\Delta P)^{-\frac{2}{3}}}} \text{--- (20)}$$

B). Modeling of the Rising Bubble Zone:

In this model it is assumed that the change in volume due to the absorption of the SO_2 is small because the bubble is predominantly inserts, the change of hydrostatic head during the bubble rise is also small, and to some extent the two effects offset one another.

A mass balance on a spherical shell leads to

$$-\frac{d}{dr}(r^2 \cdot N_{\text{SO}_2, r}) = r^2 \frac{\partial c_{\text{SO}_2}}{\partial t} \quad \text{--- (21)}$$

since the molar flux $N_{\text{SO}_2, r} = -D_g \frac{\partial c_{\text{SO}_2}}{\partial r}$, therefore

$$D_g \frac{d}{dr} \left(r^2 \frac{\partial c_{\text{SO}_2}}{\partial r} \right) = r^2 \frac{\partial c_{\text{SO}_2}}{\partial t} \quad \text{--- (22)}$$

This equation is to be solved with the following initial and boundary conditions:

I.C. : at $t=0$, $c_{\text{SO}_2} = c_f$ for all r

B.C.1.: at $r=0$, $c_{\text{SO}_2} = \text{finite}$, or $\frac{\partial c_{\text{SO}_2}}{\partial r} = 0$

B.C.2.: at $r=R$, $N_{\text{SO}_2, r}|_{r=R} = k_G (c_{\text{SO}_2}|_r - c_{\text{SO}_2}^*)$

where c_f = concentration of SO_2 in the bubble before it rises

$C_{SO_2}^*$ = concentration of gas SO_2 at the interphase
in equilibrium with liquid concentration of
 SO_2

Now, we introduce the following dimensionless quantities:

$$\theta = \frac{C_{SO_2} - C_{SO_2}^*}{C_f - C_{SO_2}^*} = \text{dimensionless concentration}$$

$$\xi = \frac{r}{R} = \text{dimensionless radial coordinate}$$

$$\tau = \frac{D_g \cdot t}{R^2} = \text{dimensionless time}$$

Then, equation (22) may be restated as:

$$\frac{1}{\xi^2} \frac{\partial}{\partial \xi} \left(\xi^2 \frac{\partial \theta}{\partial \xi} \right) = \frac{\partial \theta}{\partial \tau} \quad \text{--- (23)}$$

this equation is to be solved with the condition that

I.C. : at $\tau=0$, $\theta = 1$

B.C.1.: at $\xi=0$, $\theta = \text{finite}$, or $\frac{\partial \theta}{\partial \xi} = 0$

B.C.2.: at $\xi=1$, $\frac{\partial \theta}{\partial \xi} \Big|_{\xi=1} = - \frac{k_G R}{D_g} \cdot \theta \Big|_{\xi=1}$

Let $f(\xi, \tau) = \xi \cdot \theta(\xi, \tau)$, then equation (23) becomes:

$$\frac{\partial^2 f}{\partial \xi^2} = \frac{\partial f}{\partial \tau} \quad \text{--- (24)}$$

with I.C. : at $\tau=0, f=1 \quad \xi=\xi$

B.C.1.: at $\xi=0, f=0 \quad \xi=0$

B.C.2.: at $\xi=1, \frac{\partial f}{\partial \xi} \Big|_{\xi=1} + (Sh - 1)f \Big|_{\xi=1} = 0$

The above partial differential equation can be solved by separation of variables:

$$f = \sum_{n=1}^{\infty} C_n \cdot e^{-\alpha_n^2 \tau} \cdot \sin \alpha_n \xi \quad \text{--- (25)}$$

Then, we have to find C_n by using orthogonal properties

$$C_n = \frac{2 \cdot Sh \cdot \cos \alpha_n}{\alpha_n (\sin^2 \alpha_n - Sh)}$$

Since $\theta = \frac{f}{\xi} = \frac{C_{SO_2} - C_{SO_2}^*}{C_f - C_{SO_2}^*}$, then we can find the con-

centration of SO_2 in the gas at the outlet of the reactor C_{SO_2} , assuming the average concentration of SO_2 in the gas is close to the SO_2 concentration on the spherical surface, i.e. at $\xi=1$:

$$\frac{C_{SO_2} - C_{SO_2}^*}{C_f - C_{SO_2}^*} = \frac{2 \cdot Sh}{\xi} \sum_{n=1}^{\infty} \frac{\cos \alpha_n}{\alpha_n (\sin^2 \alpha_n - Sh)} e^{-\alpha_n^2 \tau} \cdot \sin \alpha_n \xi \quad \text{--- (26)}$$

where α_n = eigen value ($n= 1,2,3,4,5, \dots$)

Sh = Sherwood Number = $k_G R/D_g$

If we let " F " equal to right-hand-side of equation (26),

i.e.: $\frac{C_{SO_2} - C_{SO_2}^*}{C_f - C_{SO_2}^*} = " F "$, the fraction of SO_2 in the

outlet of the flue gas will be written:

$$\frac{C_{SO_2}}{C} = F * y_f + E \quad \text{--- (27)}$$

where $E = (1 - F) \frac{C_{SO_2}^*}{C}$

C = total concentration of SO_2 in the flue gas

Then, SO_2 removal is:

$$\eta_{SO_2} = 1 - \left(\frac{C_{SO_2}}{C} \right) \left(\frac{1}{y_i} \right) = 1 - (F * y_f + E) \left(\frac{1}{y_i} \right) \quad \text{--- (28)}$$

Combine equation (20) with equation (28), then the SO_2 removal is obtained by:

$$\eta_{SO_2} = 1 - \frac{A_3 C_{H^+}^2 + A_4 + A_5 (y_i - A_1 C_{H^+}^2) e^{A_2 (1 - A_1 C_{H^+}^2) (\Delta P)}^{-\frac{2}{3}}}{y_i (1 - y_i) + y_i (y_i - A_1 C_{H^+}^2) e^{A_2 (1 - A_1 C_{H^+}^2) (\Delta P)}^{-\frac{2}{3}}} \quad \text{--- (29)}$$

$$\text{where } A_3 = F(1 - y_i)A_1 = F(1 - y_i) \frac{K_H \cdot K_3}{(C_{Ca^{++}})(C_{O_2}^{\frac{1}{2}})(P_{tot})}$$

$$A_4 = E(1 - y_i) = (1 - y_i)(1 - F) \frac{C_{SO_2}^*}{C}$$

$$A_5 = F + E = F + (1 - F) \frac{C_{SO_2}^*}{C}$$

V. DESCRIPTION OF QUANTITIES
IN
THE DIFFERENTIAL EQUATION

A. The Interfacial Area and The Gas-Side Mass Transfer Coefficient in both Jet Bubbling Zone and Rising Bubble Zone

SO₂ absorption in limestone solution is a very fast irreversible reaction and therefore the mass transfer in the gas phase is most probably the rate determining step. For the calculation of K_Ga in the jet bubbling zone, much information available literatures (2), (3) shows that K_Ga varies as 0.5 power of the diffusivity D_g, it also shows that the gas-side mass transfer coefficient varies as -0.67 power of the submergence H, and as 0.75 power of the gas flow rate U. Therefore, the following relationship is likely to be hold:

$$K_G a \propto D_g^{0.50} U^{0.75} H^{-0.67}$$

VIDWANS and SHARMA (5) have found that when the pressure is increased for a particular system the diffusivity varies inversely as the pressure and therefore the mass transfer coefficient should decrease with increase in pressure at a given superficial velocity of gas. i.e.: $K_G a \propto 1/P_{tot}^{1.1}$ While according to ZABBAN and DODGE (4) K_Ga is proportional to 1/P_{tot}. Therefore, the mass transfer coefficient may be calculated from the following equation:

$$K_G a = B_0 (Sc)^{-\frac{1}{2}} (Re)^{\frac{3}{4}} (Hi)^{-\frac{2}{3}}$$

For the calculation of gas-side mass transfer coefficient $k_G a'$ in the rising bubble zone, the liquid-side resistance can be eliminated by absorbing the gas into a solution of a reagent with which it reacts instantaneously. It is necessary to base on the analysis of the outgoing gas stream. VIDWANS and SHARMA (5) have shown that an insignificant error in the analysis can affect the value of the gas-side mass transfer coefficient very significantly. The gas-side mass transfer coefficient $k_G a'$ for the air-sulfuric dioxide system is about $6.54 \times 10^{-5} \frac{\text{g-mole}}{\text{cm}^3 \text{-atm-sec}}$.

B. The Submergence depth and Bubble Penetration Length

IDEMURA, KANAI, and YANAGIOKA (1) have shown that at a given gas sparging velocity an increase in the submergence depth results in an increase in bubble penetration length. The liquid submergence depth varies from 0 mm to 200 mm (0 to 0.2 m.). When flue gas was injected horizontally into the liquid-phase through the slots with the velocity of 5 m/sec to 20 m/sec (1.8×10^4 to 7.2×10^4 m/hr), the bubble penetration length varies from 10 mm to 80 mm (0.01 to 0.08 m) depends on different submergence depth. From Fig. 2, the penetration length of bubble is linear with respect to the volumetric rate of flue gas:

$$L_p = b_o + b\left(\frac{V_g}{N}\right)$$

where b_o = intercept of the curve in Fig. 2

b = slope of the curve in Fig. 2

V_g = volumetric flow rate of flue gas

N = number of slots in the gas spargers

Since $P_{tot} \cdot V_g = M_g RT$, therefore

$$L_p = b_o + \frac{bRT}{P_{tot}} \left(\frac{M_g}{N}\right)$$

Let $G = M_g / NA_s$ = molar velocity of gas based on slot cross-sectional area

where A_s = slot cross-sectional area

M_g = molar flow rate of flue gas

then:

$$L_p = b_o + \frac{bRT}{P_{tot}} \cdot A_s \cdot G$$

The penetration length of bubble is a function of molar velocity of gas, b_o and b are constants to be determined from Fig. 2, while the submergence depth is determined in a reactor and A_s is the slot cross-sectional area which can be measured in the reactor system. The reactor temperature and pressure are known. G is calculated from the gas velocity through the slot and then the penetration length L_p can be calculated.

C. The Physical Properties of The Reactor System

The diffusion coefficient for the Air-SO₂ system and the density of flue gas were calculated according to the following equations (Perry--Chemical Engineers' Handbook--5th edition, Ref.(7)).

Diffusion coefficient for the Air-SO₂ system:

$$D_g = \frac{B \cdot T \cdot \sqrt{\frac{1}{M_1} + \frac{1}{M_2}}}{P \cdot r_{1,2}^2 \cdot I_D}$$

where D_g = gas diffusivity, cm²/sec

$$B = (1.0 - 2.46 \sqrt{\frac{1}{M_1} + \frac{1}{M_2}}) * 10^{-4}$$

T = absolute temperature, °K

M_1 , M_2 = molecular weights of component 1 and 2

P = absolute pressure, atm

$$r_{1,2} = \text{collision diameter, } \text{\AA} = \frac{(r_o)_1 + (r_o)_2}{2}$$

$$r_o = 1.18V_b^{\frac{1}{3}}$$

V_b = molal volume of liquid at normal boiling point, cc/g-mole

I_D = collision integral for diffusion, function of $kT/\epsilon_{1,2}$

$$\epsilon_{1,2}/k = (\epsilon_1/k)(\epsilon_2/k)$$

k = Boltzmann constant = $1.38 * 10^{-6}$, erg/°K

$\epsilon_{1,2}$ = energy of molecular interaction, ergs

The value of D_g increases as the flue gas temperature is increased, but, when the system pressure is increased, the diffusivity coefficient varies inversely as the pressure.

Density of flue gas:

$$\rho = \frac{MP_{\text{tot}}}{10.72ZT}$$

where ρ = density of flue gas, lb/ft³

M = molecular weight

Z = compressibility

T = temperature, °R

P_{tot} = total pressure, psia

D. Pressure Drop

The pressure drop across the reactor was found to be expressed as feet of liquid per foot of submergence depth. This means the pressure drop due to the liquid is equal to the liquid holdup expressed as cubic feet of liquid per cubic foot of reactor volume. SHULMAN and MOLSTAD (6) have found that the pressure drop, due to the liquid, for a given gas rate may be calculated by simply multiplying the submergence depth by the holdup of liquid, in which the units of ΔP , H, and Z_L are mm(aq), mm, and m³ of liquid/m³ of reactor volume, respectively.

$$\Delta P = H * Z_L$$

VI. RESULTS AND DISCUSSION

Using equation (26), a concentration profile across the gas bubble was plotted as a function of two dimensionless terms of ξ -radial coordinate and τ -time. It shows in Fig. 3 that the concentration of SO_2 at the outlet of the reactor may be calculated once we know the concentration of SO_2 at the jet bubbling zone and the time of bubble rising at the rising bubble zone. Fig. 3 shows that when the bubble rising time is up to 3.0 sec. ($\tau=2.0$), the SO_2 concentration gradient within the bubble is very small. We have found that the mole fraction of SO_2 at the jet bubbling zone can be expressed as function of both pH value of the system and pressure drop due to the passage of gas through the liquid phase. Therefore, SO_2 removal is dependent on pH value of the system and pressure drop across the reactor.

The present model was predicted based on the following reported or estimated values from IDEMURA, KANAI, and YANAGIOKA (1): The volumetric flow rate of flue gas is $1000 \text{ N m}^3/\text{hr}$, the flue gas was injected into the liquid phase through the slots with the velocity of 5 to 20 m/sec or 1.8×10^4 to $7.2 \times 10^4 \text{ m/hr}$, the slot cross-sectional area was estimated as $A_s = 1.0 \times 10^{-5} \text{ m}^2$, a gas jet of bubbles zone were formed horizontally near the slots, assuming, S , the cross-sectional area of this zone, is about ten times of A_s

The submergence depth H varies from 0 mm to 200 mm, or 0 m to 0.2 m, gas bubble diameter D_b equivalent to spheres ranged from 3 mm to 20 mm, or 0.003 m to 0.02 m. From Fig. 1 the slope of the curve was estimated as $b=0.776 \times 10^{-3}$ hr/m², and the intercept of the curves b_0 varies from 15 mm to 55 mm. The incoming gas is considered at $T=300$ °F, or 149 °C, or 422 °K, and $P_{tot}=1$ atm, the diffusivity of SO₂ and the density of flue gas were estimated as 0.238 cm²/sec or 0.08568 m²/hr, and 0.86 Kg/m³, respectively, and then Sc-Schmidt Number was obtained as 1.124 based upon the value of $\mu=8.28 \times 10^{-2}$ Kg/m-hr.

The concentration of SO₂ in the incoming flue gas is 1000 p.p.m., or 4.1×10^{-5} Kg-mole/m³, and the initial mole fraction of SO₂ y_i is equal to 0.053. Therefore, the mole fraction of SO₂ in the flue gas at jet bubbling zone was calculated from equation (20) with the conditions of $\Delta P=370$ mm aq., and $pH=5$, or $C_{H^+}=10^{-5}$. The results show that y_f is equal to 0.00636, the prediction of SO₂ removal at this stage is about 88%. Then, the total SO₂ removal can be calculated from equation (29), and we have $y_f=0.002652$, or $\eta_{SO_2}=95\%$. (see Appendix A for detailed calculation)

The comparison of predictions of the present model and those of the model proposed by IDEMURA, KANAI, and YANAGIOKA (1) are presented in Fig. 4 and 5. It is seen that there are a good agreement between the predicted curves and experiment data points.

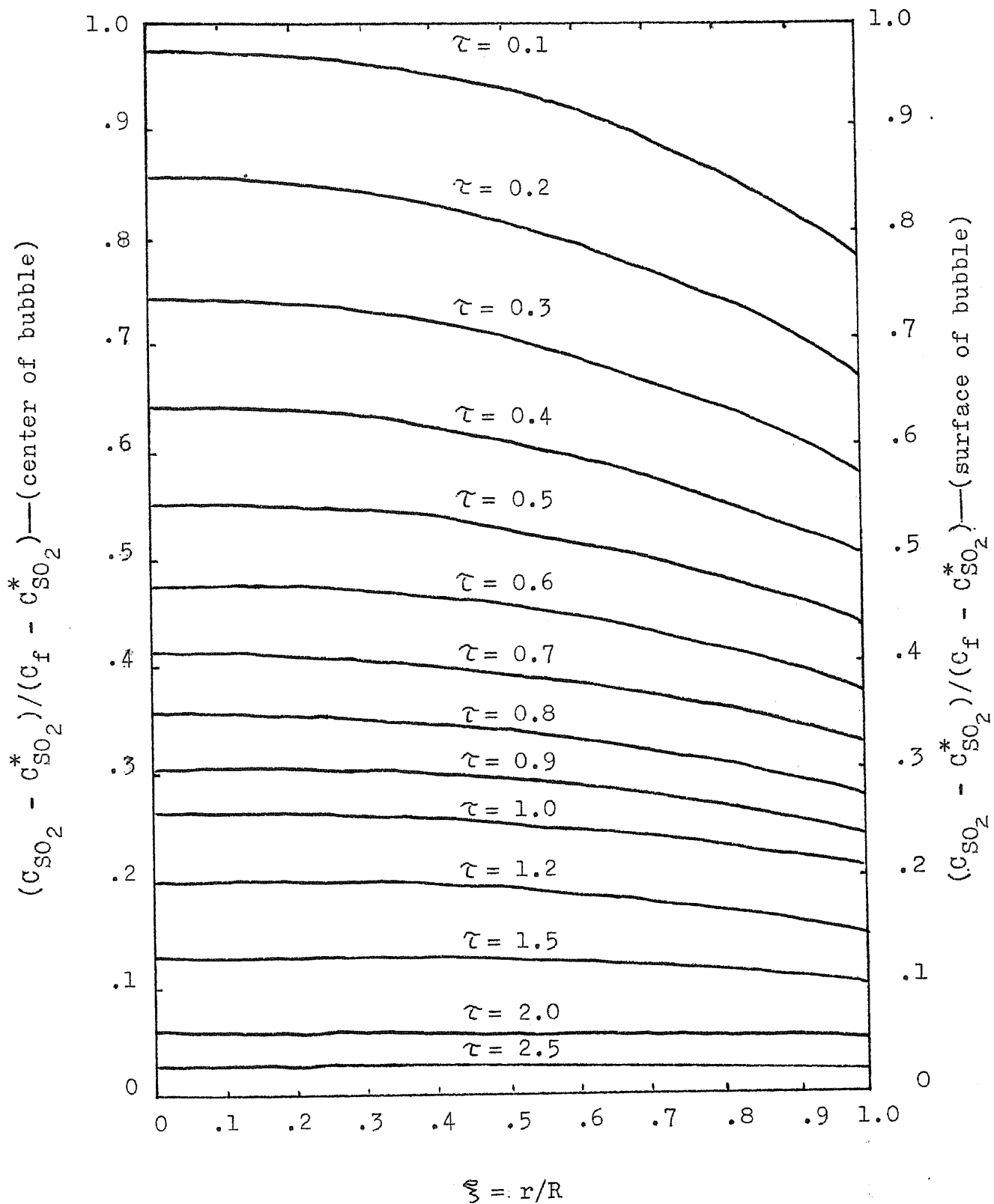


Figure 3. SO₂ concentration profile across the gas bubble (refer to equation (26))

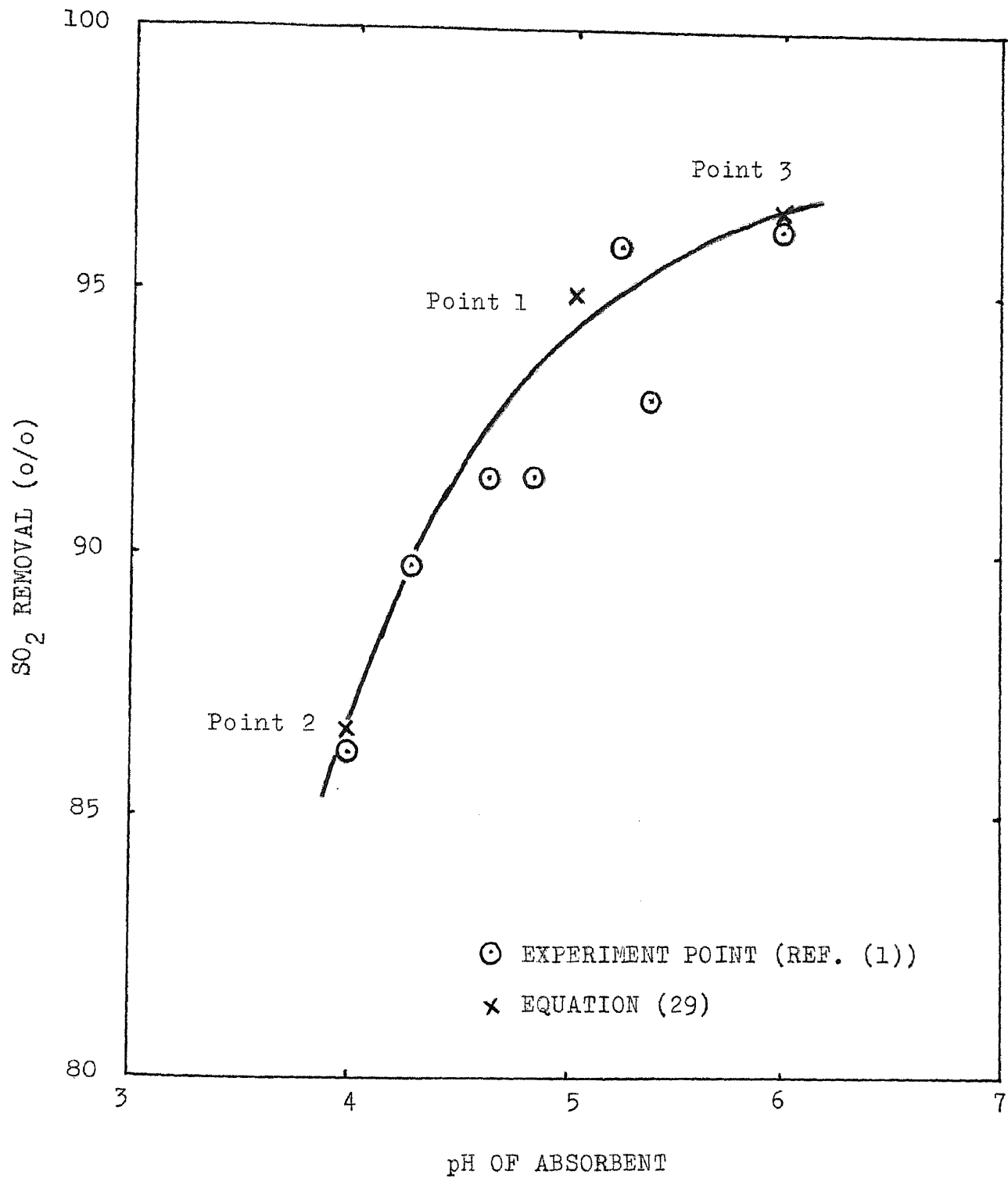


Figure 4. Sulfur dioxide removal vs. pH of absorbent.

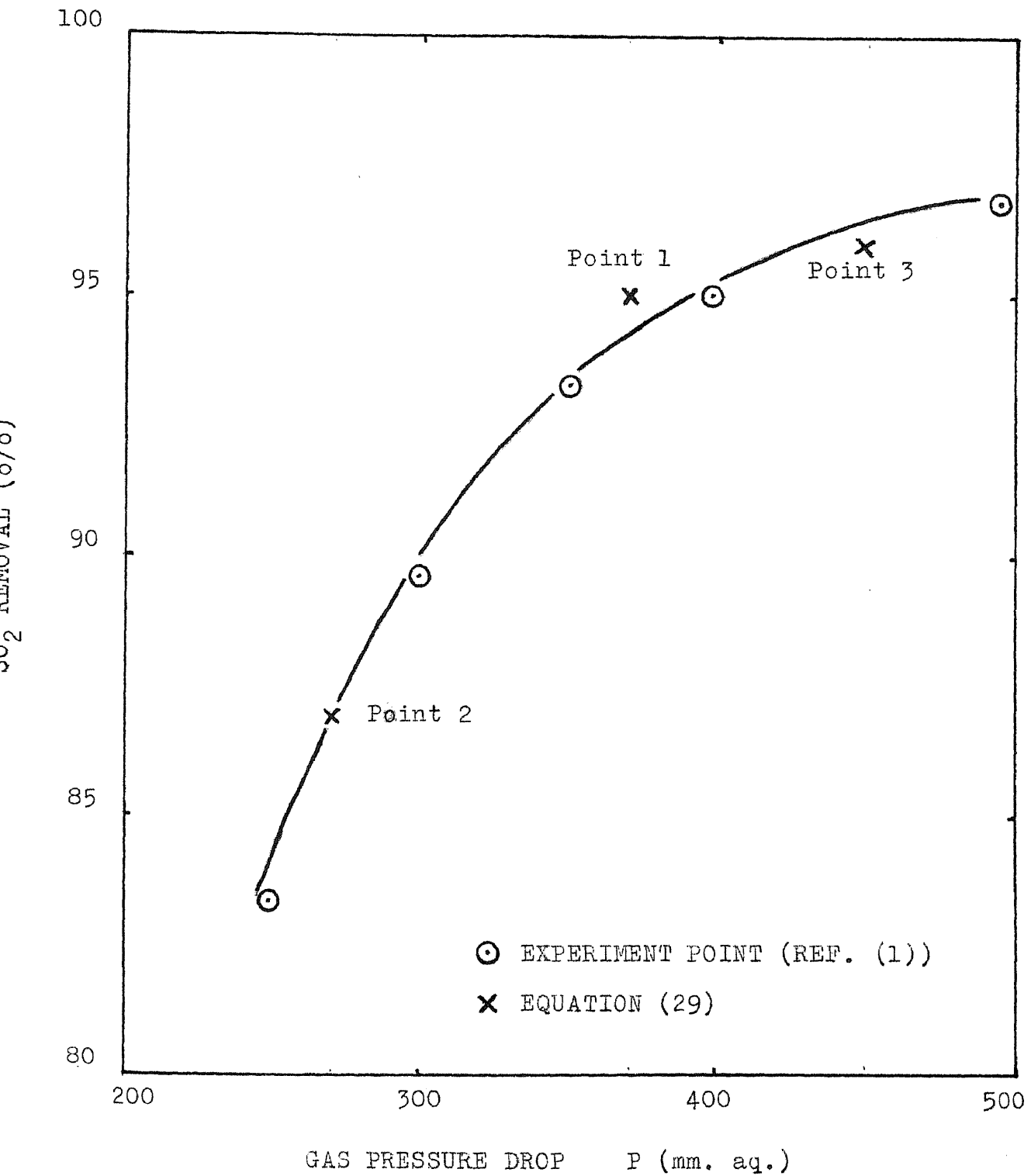


Figure 5. Sulfur dioxide removal vs. gas pressure drop.

VII. SYMBOLS USED

A	= interphase area, m^2
A_s	= slot cross-sectional area, m^2
a	= specific interface area in jet bubbling zone, m^2/m^3
a'	= specific interface area in rising bubble zone, m^2/m^3
b	= slope of the curve, hr/m^2
b_0	= intercept of the curve, m
C	= total conc. of SO_2 in the flue gas, $Kg\text{-mole}/m^3$
C_{SO_2}	= conc. of SO_2 in the outgoing gas stream, $Kg\text{-mole}/m^3$
$C_{SO_2(aq)}$	= conc. of SO_2 in the liquid phase, $Kg\text{-mole}/m^3$
C_{O_2}	= conc. of O_2 in the liquid phase, $Kg\text{-mole}/m^3$
C_{H^+}	= conc. of H^+ in the liquid phase, $Kg\text{-mole}/m^3$
$C_{Ca^{++}}$	= conc. of Ca^{++} in the liquid phase, $Kg\text{-mole}/m^3$
$C_{SO_2}^*$	= conc. of gas SO_2 at the interphase in equilibrium with liquid conc. of SO_2 , $Kg\text{-mole}/m^3$
$C_{HSO_3^-}$	= conc. of HSO_3^- in the liquid phase, $Kg\text{-mole}/m^3$
$C_{SO_4^{=}}$	= conc. of $SO_4^{=}$ in the liquid phase, $Kg\text{-mole}/m^3$
C_f	= conc. of SO_2 in the bubble before it rises, $Kg\text{-mole}/m^3$
D_g	= diffusivity of SO_2 in the gas phase, m^2/hr
D_b	= diameter of gas bubble, m
G	= molar velocity of gas based on the slot cross-sectional area, $Kg\text{-mole}/m^2\text{-hr}$
g	= gravitational acceleration, m/hr^2

\mathcal{E}_c	= gravitational conversion factor,
H	= the slot submergence depth, m
K_1, K_3	= reaction rate constant, $m^3/Kg\text{-mole-hr}$
K_H	= Henry's Law constant,
K_G	= gas-side mass transfer coefficient in jet bubbling zone, $Kg\text{-mole}/m^2\text{-hr-atm}$
k_G	= gas-side mass transfer coefficient in rising bubble zone, $Kg\text{-mole}/m^2\text{-hr-atm}$
L_p	= bubble penetration length, m
M_g	= molar flow rate of flue gas, $Kg\text{-mole/hr}$
M_g	= molar flow rate of carrier gas, $Kg\text{-mole/hr}$
N	= number of slots in the gas sparger,
$N_{SO_2,r}$	= molar flux of SO_2 with respect to stationary coordinates, $Kg\text{-mole}/m^2\text{-hr}$
P_{tot}	= total pressure of the flue gas, atm
$P_{SO_2}^*$	= the equilibrium vapor pressure of SO_2 with respect to the liquid SO_2 conc., atm
R	= gas law constant,
R,r	= radial distance in both cylindrical & spherical coordinates, m
S	= average cross-sectional area of jet bubbling zone, m^2
T	= flue gas temperature, $^{\circ}K$
t	= time, hr
U	= gas flow rate, m^3/hr
V	= volume of the jet bubbling zone per slot, $m^3/slot$
V_g	= volumetric flow rate of flue gas, m^3/hr

W	= mass transfer rate of SO_2 between phase, Kg-mole/hr
X	= rectangular coordinates,
y	= mole fraction of SO_2 in the flue gas,
y_i	= initial mole fraction of SO_2 in the flue gas,
y_f	= final mole fraction of SO_2 in the flue gas at jet bubbling zone,
Z_L	= liquid holdup,
η_{SO_2}	= SO_2 removal fraction,
μ	= viscosity of gas, Kg/m-hr
ρ	= density of gas, Kg/m ³
ρ_L	= density of liquid, Kg/m ³

APPENDIX A

The procedures of calculation are shown below:

1. Reported or calculated values from Ref. (1), (6), & (7):

volumetric flow rate of flue gas: $1000 \text{ N m}^3/\text{hr}$

flue gas velocity through the slot: 5 m/sec to 20 m/sec
 or $1.8 \times 10^4 \text{ m/hr}$ to $7.2 \times 10^4 \text{ m/hr}$

concentration of SO_2 in the incoming flue gas: 1000 ppm
 or $4.1 \times 10^{-5} \text{ Kg-mole/m}^3$

bubble diameter D_b : 3 mm to 20 mm , or 0.003 m to 0.02 m

submergence depth H : 0 mm to 200 mm , or 0 m to 0.2 m

estimated: gas velocity = $7.2 \times 10^4 \text{ m/hr}$

$$D_b = 1.2 \times 10^{-2} \text{ m}$$

$$H = 200 \text{ mm, or } 0.2 \text{ m}$$

$$A_s = 10^{-5} \text{ m}^2$$

$$S = 10^{-4} \text{ m}^2$$

$$Z_L = 0.6-0.7$$

$$T = 300 \text{ }^\circ\text{F, or } 149 \text{ }^\circ\text{C} = 422 \text{ }^\circ\text{K}$$

$$P_{\text{tot}} = 1 \text{ atm}$$

$$C_{\text{SO}_2}^* = 1.73 \times 10^{-6} \text{ Kg-mole/m}^3$$

calculated: $b_o = 0.057 \text{ m}$

$$b = 0.776 \times 10^{-3} \text{ hr/m}^2$$

$$P = 0.86 \text{ Kg/m}^3$$

$$\mu = 8.28 \times 10^{-2} \text{ Kg/m-hr}$$

$$D_g = 0.238 \text{ cm}^2/\text{sec} = 0.08568 \text{ m}^2/\text{hr}$$

$$B_o (P_L g / P_{\text{tot}} g_c Z_L)^{-\frac{2}{3}} = 2.5 \times 10^{-4} \text{ g-mole/cm}^3\text{-atm-sec}$$

$$= 9.0 \times 10^2 \text{ Kg-mole/m}^3\text{-atm-hr}$$

$$C = 7.736 \times 10^{-4} \text{ Kg-mole/m}^3$$

$$G = 2120 \text{ Kg-mole/m}^2\text{-hr}$$

$$L_p = 0.0575696 \text{ m}$$

$$G_i = - 2.12 \times 10^5 \text{ Kg-mole/m}^2\text{-hr}$$

$$G_f = 2120 \text{ Kg-mole/m}^2\text{-hr}$$

$$A_2 = - 4.866$$

$$A_4 = 1.909 \times 10^{-3}$$

$$A_5 = 0.102016$$

2. Calculation of Point 1:

Point 1 is calculated with the following conditions:

$$\Delta P = 370 \text{ mm aq.}$$

$$C_{H^+} = 10^{-\text{pH}} = 10^{-5}$$

$$A_1 = 6.36 \times 10^7$$

$$A_3 = 6.023 \times 10^6$$

mole fraction of SO_2 in the flue gas at jet bubbling zone is obtained from equation (20):

$$\begin{aligned} y_f &= \frac{6.023 \times 10^{-3} + (0.04664)e^{-4.866(0.99364)(9.2043)}}{0.947 + (0.04664)e^{-4.866(0.99364)(9.2043)}} \\ &= \frac{0.006023 + 2.194 \times 10^{-21}}{0.947 + 2.194 \times 10^{-21}} \\ &= 0.00636 \end{aligned}$$

and SO_2 removal at this stage is: $\frac{0.053 - 0.00636}{0.053}$

$$= 0.88, \text{ or } 88\%$$

Then, the final SO₂ removal is calculated from equation (29):

$$\begin{aligned}
 \eta_{\text{SO}_2} &= 1 - \left(\frac{1}{0.053} \right) \left(\frac{6.023 \cdot 10^{-4} + 1.909 \cdot 10^{-3} + 2.238 \cdot 10^{-22}}{0.947 + 2.194 \cdot 10^{-21}} \right) \\
 &= 1 - \left(\frac{1}{0.053} \right) \left(\frac{0.002511}{0.947} \right) \\
 &= 1 - \left(\frac{2.652 \cdot 10^{-3}}{0.053} \right) \\
 &= 1 - 0.05 \\
 &= 0.95, \text{ or } 95\%
 \end{aligned}$$

3. Calculation of Point 2 & 3:

The procedures of calculation of Point 2 and 3 are similar to step 2.

Point 2: $\Delta P = 270 \text{ mm aq.}$

$$C_{\text{H}^+} = 10^{-4}$$

$$A_1 = 5.14 \cdot 10^6$$

$$A_3 = 4.87 \cdot 10^5$$

Then, we have: $y_f = 0.0159$

SO₂ removal at this stage = 70%

final SO₂ removal $\eta_{\text{SO}_2} = 86.5\%$

Point 3: $\Delta P = 450 \text{ mm aq.}$

$$C_{\text{H}^+} = 10^{-6}$$

$$A_1 = 3.69 \cdot 10^9$$

$$A_3 = 3.49 \cdot 10^8$$

Then, we have: $y_f = 0.00369$

SO₂ removal at this stage = 93%

final SO₂ removal $\eta_{\text{SO}_2} = 95.7\%$

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