ENCH 501 Transport Phenomena University of Calgary Name________________________________

<u>**Quiz #6**</u> / **Time Allowed**: 50 minutes Use of cheat sheet allowed. December 6, 2016 aj

Alkaline solutions such as amines and hydroxides are used to remove acid gases such as H_2S, CO_2 and Cl_2 from streams of gases such as air and natural gas in either purification operations or recovery processes. The acid gases both dissolve in and react with components of the solvent. Reactive absorption is usually more effective and efficient than physical absorption.

A stagnant pool of aqueous alkaline solution is contained in a vessel. The solution is initially free of chlorine. At time t = 0, a gentle stream of air containing chlorine is blown over the surface. The chlorine (A) dissolves in the liquid at the interface and then diffuses into the bulk of the stagnant solution (B). In the solution, the chlorine also reacts with the hydroxide by a first order reaction – the rate of removal of chlorine is proportional to the local concentration of dissolved chlorine. The reaction rate constant is 9 (10^{-4}) s^{-1}. The diffusion coefficient for chlorine in the solution is 1.79 (10^{-7}) m^2/s, the molar concentration of the solution is assumed constant at 58 kmols/m^3, and the mole fraction of chlorine at the liquid-gas interface is assumed constant at 0.117.

(i) (10 pts) Use the ***integral method*** to determine the distance to which chlorine would have penetrated into the solution in 10 minutes. Assume that the profile for y_A in the solution is given by

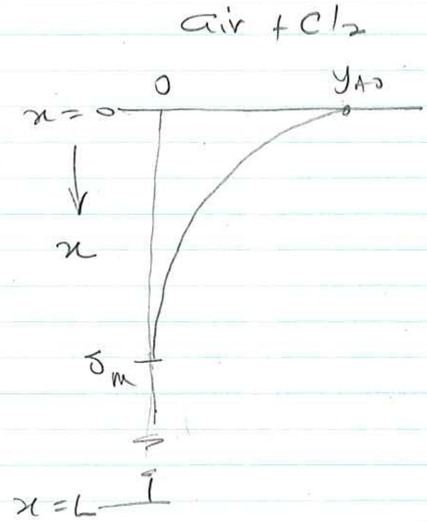
$$y_A = \mathbf{a} + \mathbf{b}\sin(\mathbf{d}x),$$

where x is distance into the solution from the gas-liquid interface. Do necessary derivations.

(ii) (Bonus 2 pts) How much total chlorine (kg) would have been removed by the solution per m^2 of the interface area in 10 minutes? The molar mass of chlorine is 70.9 g/mol.

[Some useful relationships: $d \sin u/dx = \cos u \, du/dx$ and $d \cos u/dx = -\sin u \, du/dx$; $\cos 0 = 1$, $\cos \pi/2 = 0$ and $\sin 0 = 0$, $\sin \pi/2 = 1$; $\int \sin ax \, dx = -\frac{\cos ax}{a}$ and $\int \cos ax \, dx = \frac{\sin ax}{a}$]

ENCH 501 Quiz 6 Solution Dec. 6, 2016



This is a reactive absorption problem in a semi-infinite domain. The medium is stagnant. Material balance on chlorine (A) is given by

Input + Generation = Accum.

$$N_A\Big|_{x=0} - \int_0^L k_1 c y_A \, dx = \frac{d}{dt}\left[\int_0^L c y_A \, dx\right]$$

The molar flux of A within the solution B is given by

$$N_A = -c D_{AB} \frac{dy_A}{dx} + y_A(N_A + \cancelto{0}{N_B})$$

$$N_A = -\frac{c D_{AB}}{1-y_A} \frac{dy_A}{dx}$$

The integral mass balance equation on A is

$$(1) \quad -\left[\frac{c D_{AB}}{1-y_A} \frac{dy_A}{dx}\right]_{x=0} - \int_0^{\delta_m} k_1 c y_A \, dx = \frac{d}{dt}\left[\int_0^{\delta_m} c y_A \, dx\right]$$

where the upper limits of the integrals have been changed to $\delta_m(t)$.

The conditions are

$$x=0 \quad y_A = y_{A0} \, ; \quad x = \delta_m , \quad y_A = 0 \quad \text{and} \quad \frac{dy_A}{dx} = 0$$

Assume $y = a + b\sin(dx)$

apply the conditions to get

$$\frac{y_A}{y_{A0}} = 1 - \sin\left(\frac{\pi}{2}\frac{x}{\delta_m}\right)$$

$$\left.\frac{dy_A}{dx}\right|_{x=0} = \left. bd\cos(dx)\right|_{x=0} = bd = -y_{A0}\frac{\pi}{2}\frac{1}{\delta_m}$$

Substitute into integral eq.

$$+\frac{c D_{AB}}{1-y_{A0}} y_{A0}\frac{\pi}{2}\frac{1}{\delta_m} - \int_0^{\delta_m} k_1 c\, y_{A0}\left(1 - \sin\frac{\pi}{2}\frac{x}{\delta_m}\right)dx$$

$$+ \frac{d}{dt}\left[\int_0^{\delta_m} c\, y_{A0}\left(1 - \sin\frac{\pi}{2}\frac{x}{\delta_m}\right) dx\right.$$

Let $\eta = x/\delta_m$ and $\beta = \frac{D_{AB}}{1-y_{A0}}\frac{\pi}{2}$

$$c\, y_{A0}\,\beta/\delta_m - k_1 c\, y_{A0}\,\delta_m \int_0^1 \left(1 - \sin\frac{\pi}{2}\eta\right)d\eta =$$

$$\frac{d}{dt}\left[c\, y_{A0}\,\delta_m \int_0^1 \left(1 - \sin\frac{\pi}{2}\eta\right. d\eta\right]$$

Cancel out $c\, y_{A\infty}$

$$\frac{\beta}{\delta_m} - k_1 \delta_m \left[\eta + \frac{\cos \frac{\pi}{2}\eta}{\pi/2} \right]_0^1 =$$

$$\frac{d}{dt}\left[\delta_m \left[\eta + \frac{\cos \frac{\pi}{2}\eta}{\pi/2} \right]_0^1 \right]$$

$$\frac{\beta}{\delta_m} - k_1 \delta_m \left(1 - \frac{2}{\pi}\right) = \frac{d}{dt}\left[\delta_m \left(1 - \frac{2}{\pi}\right)\right]$$

$$\frac{\beta}{1 - 2/\pi} - k_1 \delta_m^2 = \delta_m \frac{d\delta_m}{dt} = \frac{1}{2}\frac{d\delta_m^2}{dt}$$

$$\frac{d\delta_m^2}{dt} = \frac{2\beta}{1 - 2/\pi} - 2k_1 \delta_m^2 = \varepsilon - \lambda \delta_m^2$$

This is an ODE with the condition that

$t = 0 \,,\ \delta_m = 0$

$$\left(-\frac{1}{\lambda}\right) \frac{d(\varepsilon - \lambda \delta_m^2)}{\varepsilon - \lambda \delta_m^2} = dt$$

$$\int_0^{\delta_m} d\ln\left(\varepsilon - \lambda\delta_m^2\right) = -\int_0^t \lambda\, dt$$

$$\ln\left[1 - \frac{\lambda}{\varepsilon}\delta_m^2\right] = -\lambda t$$

or

$$\delta_m^2 = \frac{\varepsilon}{\lambda}\left(1 - e^{-\lambda t}\right)$$

$$\delta_m = \left(\frac{\varepsilon}{\lambda}\right)^{\frac{1}{2}}\left(1 - e^{-\lambda t}\right)^{\frac{1}{2}}$$

where $\lambda = 2k_1$ and $\varepsilon = \dfrac{\pi D_{AB}}{1 - y_{A0}} \dfrac{1}{\left(1 - \frac{2}{\pi}\right)}$

$$\delta_m = \left(\frac{2.75194\ \pi\ D_{AB}}{2k_1}\right)^{\frac{1}{2}}\left(1 - e^{-2k_1 t}\right)^{\frac{1}{2}}$$

(a) $k_1 = 9(10^{-4})\ s^{-1}$, $D_{AB} = 1.79(10^{-7})\ m^2/s$

and $t = 10\,\text{mins} = 600\,s$

$$\delta_m = 0.02932\,(0.48644) = 0.01426\ m$$

(b) Total chlorine uptake is given by

$$Q = \int_0^{600\,s} N_A\Big|_{x=0}\, dt \quad \text{per } m^2$$

But

$$N_A\Big|_{x=0} = -\frac{c\,D_{AB}}{1-y_{A0}}\left(-y_{A0}\,\frac{\pi}{2}\cdot\frac{1}{\delta_m}\right)$$

Substitute for δ_m

$$N_A\Big|_{x=0} = \gamma\cdot\left(1-e^{-2k_1t}\right)^{-\frac{1}{2}}$$

where $$\gamma = \frac{c\,D_{AB}}{1-y_{A0}}\,y_{A0}\cdot\frac{\pi}{2}\left(\frac{2.75194\,\pi\,D_{AB}}{2k_1}\right)^{-\frac{1}{2}}$$

$$\therefore\quad Q = \gamma\int_0^{600}\left(1-e^{-2k_1t}\right)^{-\frac{1}{2}}dt$$

Let $$u = 1-e^{-2k_1t}\quad;\quad 0\leq u<1$$

$$du = -e^{-2k_1t}(-2k_1)\,dt$$

or $$dt = \frac{du}{2k_1(1-u)}$$

$$Q = \gamma\int\frac{du}{2k_1(1-u)\,u^{\frac{1}{2}}}$$

From integral tables

$$\int\frac{dx}{(px+q)\sqrt{ax+b}} = \frac{2}{\sqrt{aq-bp}\,\sqrt{p}}\tan^{-1}\sqrt{\frac{p(ax+b)}{aq-bp}}$$