ENCH 501 F2017 **Quiz #7** Name:____

December 5, 2017 Time Allowed: 45 minutes aJ

Carbon dioxide (CO_2) is a greenhouse gas that contributes to atmospheric warming. It has been suggested that the gas produced at stationary sources such as coal power plants can be removed by absorption into solutions of sodium hydroxide (NaOH) in water. CO_2 reacts with water in the solution to first produce carbonic acid (H_2CO_3) in dilute solutions ($pH < 8$). The carbonic acid then reacts with the sodium hydroxide to form sodium bicarbonate. Both reactions can be combined to give a reaction with a rate constant k (s^{-1}) for a first order reaction with respect to the concentration of CO_2 present at a location.

Consider a stagnant pool of a caustic solution at 20°C. The solution has no dissolved CO_2 at $t = 0$. Then the surface was suddenly contacted with a gas mixture with CO_2. The mole fraction of CO_2 dissolved at the liquid side of the interface (x_{AO}) was determined to be constant at 0.027. The reaction of CO_2 with the hydroxide solution is first order in the concentration of CO_2 ($k\,C\,x_A$) where k is $3.5\ (10^{-5})\ s^{-1}$.

a) Estimate the depth to which the CO_2 will have penetrated into the solution after 2 hours.
b) After 2 hours, how much molecular (or unreacted) CO_2 in mols/m^2 surface area would be in the solution?
c) How many moles total CO_2 (reacted plus unreacted) would have been absorbed in 2 hours per m^2 of surface area?

Data: Assume that the molar concentration of the caustic solution is constant at 55.4 moles per litre. The diffusivity of CO_2 in the caustic is $1.5\ (10^{-9})\ m^2/s$.

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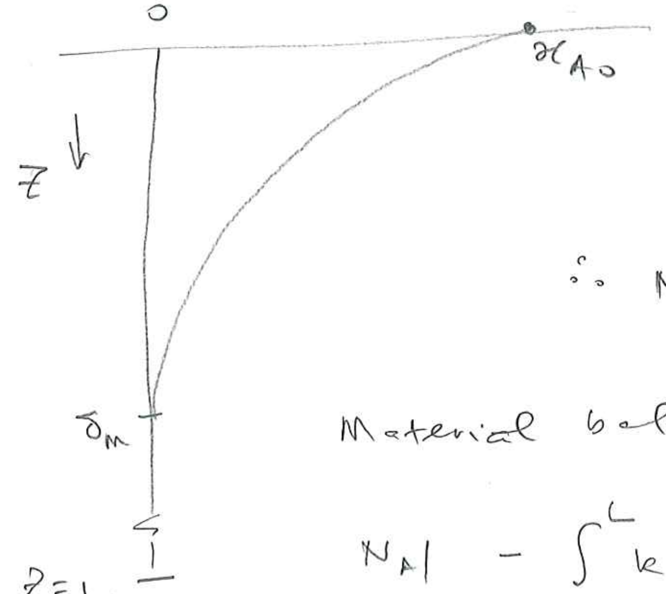
CO_2 in mixture.



Let $A \equiv CO_2$

$B \equiv$ caustic solution

$N_B = 0$

$$\therefore \quad N_A = -\frac{cD_{AB}}{1-x_A}\frac{dy_A}{dz}$$

Material balance on A is

$$N_A\Big|_{z=0} - \int_0^L kCx_A\,dz = \frac{d}{dt}\left[\int_0^L c\,x_A\,dz\right]$$

Since $x_A = 0$ for $z > \delta_M$, the eq. becomes

$$-\frac{D_{AB}}{1-x_A}\frac{dx_A}{dz}\Big|_{z=0} - \int_0^{\delta_M} k\,x_A\,dz = \frac{d}{dt}\left[\int_0^{\delta_M} x_A\,dz\right]$$

since C = constant.

The boundary conditions are

$z = 0$, $x_A = x_{A0}$, $z = \delta_M$, $x_A = 0$ and

$z = \delta_M$, $\frac{dx_A}{dz} = 0$

assume $x_A = a + bz + cz^2$ and use b.c.s

$$\Rightarrow \quad \frac{x_A}{x_{A0}} = \left(1 - \frac{z}{\delta_M}\right)^2$$

Apply profile in the integral equation with

$$\left.\frac{dx_A}{dz}\right|_{z=0} = -\frac{2x_{A0}}{\delta_m}\left(1-\frac{z}{\delta_m}\right)\Bigg|_{z=0} = -\frac{2x_{A0}}{\delta_m}$$

$$\frac{D_{AB}}{1-x_{A0}}\,\frac{2x_{A0}}{\delta_m} - k\,x_{A0}\,\frac{\delta_m}{3} = \frac{d}{dt}\left[\frac{x_{A0}\,\delta_m}{3}\right]$$

$$\frac{6\,D_{AB}}{1-x_{A0}} - k\,\delta_m^2 = \delta_m\frac{d\delta_m}{dt} = \frac{1}{2}\frac{d\delta_m^2}{dt}$$

or

$$\frac{12\,D_{AB}}{1-x_{A0}} - 2k\,\delta_m^2 = \frac{d\delta_m^2}{dt}$$

Subject to the condition $t=0,\ \delta_m=0$

ⓐ The solution is

$$\delta_m = \sqrt{\frac{12\,D_{AB}}{1-x_{A0}}}\left[\frac{1-e^{-2kt}}{2k}\right]^{\frac{1}{2}}$$

Given: $x_{A0} = 0.027$, $t = 2\text{ hrs} = 7200\,s$

$k = 3.5(10^{-5})\ s^{-1}$, $D_{AB} = 1.5(10^{-9})\ m^2/s$

Substitute:

$\delta_m = (0.000136)\,75.2 \quad = \quad 0.0102 \text{ m}$

or $\quad 1.02$ cm $\longrightarrow$

(b) The unreacted amount of CO_2 present at $t = 2$ hrs is given by

$$W = \int_0^{\delta_m} C\, x_A\, dz = \underset{\substack{/ \\ 55.4 \\ \text{moles / litre}}}{C}\, x_{A0} \frac{\delta_m}{3} = \frac{55.4(10^3)(0.027)(0.0102)}{3}$$

$$\frac{\text{moles}}{m^3} \cdot m = \frac{\text{moles}}{m^2}$$

$W = 5.1$ moles / m^2 $\longrightarrow$

(c) The amount of CO_2 that has entered the caustic solution is given by

$$Q = \int_0^{t=7200\,s} N_A\Big|_{z=0}\, dt = \int_0^t \frac{2 C x_{A0} D_{AB}}{1 - x_{A0}} \frac{1}{\delta_m}\, dt$$

where $\delta_m = \beta\left(1 - e^{-2kt}\right)^{\frac{1}{2}}$ and

$$\beta = \left[\frac{12 D_{AB}}{2k(1 - x_{A0})}\right]^{\frac{1}{2}}$$

$$Q = \int_0^t \gamma \frac{dt}{\left(1 - e^{-2kt}\right)^{\frac{1}{2}}} \quad ; \quad \gamma = \frac{2 C x_{A0} D_{AB}}{\beta(1 - x_{A0})}$$

$$Q = \int_0^{Y} \frac{\gamma}{2k} \frac{dY}{Y^{\frac{1}{2}}(1-Y)} \quad \text{where } Y = 1 - e^{-2kt}$$

$$\text{and } \gamma = C x_{A0} \sqrt{\frac{2k D_{AB}}{3(1-x_{A0})}}$$

$$= \frac{\gamma}{2k} \int_0^{\psi} \frac{d\psi^2}{\psi(1-\psi^2)} \quad \text{where } \psi = Y^{\frac{1}{2}}$$

$$= \frac{\gamma}{k} \int_0^{\psi} \frac{d\psi}{1-\psi^2} = \frac{\gamma}{2k} \ln\left|\frac{1+\psi}{1-\psi}\right| = \frac{\gamma}{2k} \tanh^{-1}\psi$$

$$= \frac{\gamma}{2k} \ln\left|\frac{1+(1-e^{-2kt})^{\frac{1}{2}}}{1-(1-e^{-2kt})^{\frac{1}{2}}}\right|$$

$$= C x_{A0} \sqrt{\frac{D_{AB}}{6k(1-x_{A0})}} \ln\left|\frac{1+(1-e^{-2kt})^{\frac{1}{2}}}{1-(1-e^{-2kt})^{\frac{1}{2}}}\right|$$

$$= 55.4(10^3)(0.027)(0.002709)(1.480176)$$

$$Q = 5.9988 \text{ moles}/m^2$$

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