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ENCH 501: Transport Processes Quiz #6 **November 20, 2007**

Time Allowed: 40 mins. **Name:**

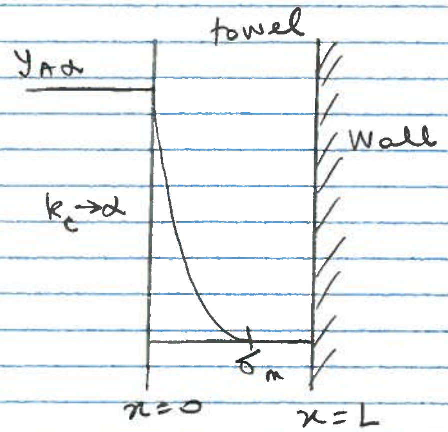
Hydrogen sulphide, H_2S, is a very toxic compound to mammals, even in low concentrations in air. It must, therefore, be removed as quickly as possible, particularly from an enclosed space. When a cannister of the gas accidentally discharged its content into a small, enclosed analytical laboratory, the manager instructed that a thick towel be soaked in an alkali (or amine) solution and the excess liquid squeezed out. The towel then becomes a porous medium with a thin layer of alkali covering the fibers. The towel is then pinned to a wall. As H_2S from the air diffuses into the towel, the gas also reacts with the alkali to form a complex held on the towel fibers.

You are given that the thickness of the towel is L and the towel initially contained no H_2S. Because the towel is mounted on a wall, you may assume that the towel side at the wall is impervious. The gas in the towel occupies a void fraction ε. The reaction in the towel is first order, i.e. the rate of removal of H_2S is proportional to the local concentration of H_2S in the gas. The rate is also proportional to the fraction of the towel occupied by the fibers. Assume the rate constant is $\mathbf{k_1}$. At the ambient air side of the towel, the mole fraction of H_2S in the air, $\mathbf{y_{A\infty}}$, is substantial (about 20%) and the air is rapidly moved around by a fan such that it may be assumed that the mass transfer coefficient ($\mathbf{k_c}$) at the open towel surface is very large. The temperature and pressure in the room are constant at T and P. Assume that the air within the towel is stagnant.

a) Use the ***integral method*** to derive an expression for the concentration profile for H_2S $\mathbf{y_A(x,t)}$ in the towel, up to the instant the compound has just penetrated to the face of the towel at the wall. Show all your steps.

b) How would you estimate the total amount of H_2S removed by the towel at this instant?

ENCH 501 Quiz #6 Solution Nov. 20, 2007



- Because of the air movement outside, $k_c \to \infty$, and therefore the concentration of H_2S (substance A) at $x=0$ is given by

$$c_A = c_{A\infty} = c\, y_{A\infty} \; ; \; c = \frac{P}{RT}$$

- This is a semi-infinite domain problem since $\delta_m \le L$

- The flux of A is given by (within the towel)

$$N_{Ax} = -c D_{AB} \varepsilon \frac{dy_A}{dx} + y_A (N_A + N_B)$$

where B is the air in the pore space of the towel.

The air is stagnant, hence $N_B = 0$

$$\therefore \quad N_{Ax} = \frac{-c D_{AB} \varepsilon}{1-y_A} \frac{dy_A}{dx} \qquad (1)$$

- Let the control volume be the towel, $0 \le x \le L$

$$\text{Input} + \text{Generation} = \underbrace{\text{Output}}_{0} + \text{Accum}$$

$$\underset{\text{per unit area}}{\text{Input}} = N_{Ax}\Big|_{x=0} = \frac{-c D_{AB} \varepsilon}{1-y_A} \frac{dy_A}{dx}\Bigg|_{x=0}$$

$$\underset{\text{per unit towel surface area}}{\text{Generation}} = \int_0^{\delta_m} -k_1 (1-\varepsilon) c\, y_A \, dx$$

$$\text{Accum} = \frac{d}{dt}\left[\int_0^{\delta_m} \varepsilon c\, y_A \, dx\right]$$

The upper limits of both integrals are δ_m because ~~$y_A = 0$ for $\delta_m < x \le L$~~

The integral material balance equation is

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

or

$$-\frac{\mathcal{D}_{AB}}{1-y_{A\alpha}}\left.\frac{dy_A}{dx}\right|_{x=0} - k_1\left(\frac{1-\varepsilon}{\varepsilon}\right)\int_0^{\delta_m} y_A\,dx = \frac{d}{dt}\left[\int_0^{\delta_m} y_A\,dx\right] \qquad (2)$$

□ Identify the b.c.

$x=0 \qquad y_A = y_{A\alpha}$

$x=\delta_m \qquad y_A = 0$

$x=\delta_m \qquad \frac{dy_A}{dx} = 0$

Assume profile $y_A = a + bx + cx^2$

Apply b.c.

$$\frac{y_A}{y_{A\alpha}} = \left(1 - 2\frac{x}{\delta_m} + \frac{x^2}{\delta_m^2}\right) = \left(1 - \frac{x}{\delta_m}\right)^2 \qquad (3)$$

$$\left.\frac{dy_A}{dx}\right|_{x=0} = -\frac{2y_{A\alpha}}{\delta_m} + \cancel{\frac{2x\,y_{A\alpha}}{\delta_m^2}}$$

$$y_{A\alpha}\int_0^{\delta_m}\left(1-2\frac{x}{\delta_m}+\frac{x^2}{\delta_m^2}\right)dx = y_{A\alpha}\left(x - \frac{x^2}{\delta_m} + \frac{1}{3}\frac{x^3}{\delta_m^2}\right)\Bigg|_0^{\delta_m}$$

$$= \frac{y_{A\alpha}\,\delta_m}{3}$$

Substitute these into equation (2)

$$-\frac{D_{AB}}{1-y_{A\alpha}}\left(-\frac{2y_{A\alpha}}{\delta_m}\right) - k_1\left(\frac{1-\varepsilon}{\varepsilon}\right)\frac{y_{A\alpha}\delta_m}{3} = \frac{d}{dt}\left[y_{A\alpha}\frac{\delta_m}{3}\right] \quad (3)$$

or

$$\frac{6D_{AB}}{1-y_{A\alpha}}\frac{1}{\delta_m} - k_1\left(\frac{1-\varepsilon}{\varepsilon}\right)\delta_m = \frac{d\delta_m}{dt}$$

or

$$\alpha - \beta\delta_m^2 = \frac{d\delta_m^2}{dt} \;; \quad \alpha = \frac{12D_{AB}}{1-y_{A\alpha}}$$

$$\beta = 2k_1\left(\frac{1-\varepsilon}{\varepsilon}\right)$$

Subject to the condition:

$$t=0 \;, \quad \delta_m = 0$$

Let $\Upsilon = \alpha - \beta\delta_m^2 \quad \therefore \quad d\Upsilon = -\beta\, d\delta_m^2$

$\therefore$ eq. becomes

$$\frac{d\Upsilon}{\Upsilon} = -\beta dt = d\ln\Upsilon$$

Integrate $\displaystyle\int_{\Upsilon=\alpha}^{\Upsilon} d\ln\Upsilon = -\int_0^t \beta dt$

$$\ln\frac{\Upsilon}{\alpha} = -\beta t \quad \text{or} \quad \Upsilon = \alpha e^{-\beta t}$$

i.e. $\quad \alpha - \beta\delta_m^2 = \alpha e^{-\beta t}$

$$\text{or} \quad \delta_m = \left[\frac{\alpha}{\beta}\left(1-e^{-\beta t}\right)\right]^{\frac{1}{2}} \quad (4)$$

Substitute this into eq. (3) for profile. →

(b) At the instant $\delta_m = L$, equation (4) can be used to estimate the time, τ.

The total uptake of H_2S can be estimated from

$$Q = \int_0^{\tau} N_A\Big|_{x=0} dt$$

$$= \frac{-c\mathcal{D}_{AB}\varepsilon}{1-y_{A\delta}} \int_0^{\tau} \frac{dy_A}{dx}\Bigg|_{x=0} dt$$

or from both amount reacted and still diffusing.

That is:

$$Q = \int_0^L \left[\int_0^{\tau} k_1 (1-\varepsilon) c\, y_A\, dt \right] dx \;+$$

$$\int_0^L c\, y_A\, \varepsilon\, dx$$

$\longrightarrow$