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ENCH 501: Transport Processes Quiz #5 **November 5, 2002**

Time Allowed: 45 mins. **Name:**

Several products are being sold for removing contaminants (foul smelling or toxic substances) from air. A test of one such device to remove benzene vapor from the air in a room is being conducted. The device is a flat board attached to the wall and it consists of thin fibers randomly arranged to form a porous medium. Benzene would diffuse through the medium as part of it is adsorbed on the fibers and converted to another substance which bonds to the fibers.

The following information is provided. The board is assumed to be thick and semi-infinite. Its porosity is 38% and the air within is assumed stagnant. The mole fraction of benzene in the air (y_A) in the room is constant at 0.25. The pressure in the room is 1 atm. And the temperature is 20°C. The currents in the room are significant that the mass transfer coefficient at the boundary between the board and the room air is assumed to be very large. The rate at which benzene reacts in the porous medium, per unit volume of the fibers, is first order with respect to the local concentration of benzene, i.e. k_1C_A where k_1 is $5.2(10^{-4})$ s^{-1}. The diffusivity of benzene in air is $8.82(10^{-6})$ m^2/s.

Use the integral method to answer the following. Assume no benzene was present in the board initially.

(a) Estimate the depth to which the benzene has penetrated into the board after 3 minutes.
(b) Determine the total amount of benzene taken up by the board in 40 minutes. How much of this has been bonded to the fiber?

Hint: $c = P/RT$, Universal Gas Constant, $R = 0.08205$ (m^3.atm)/(kmol.K)

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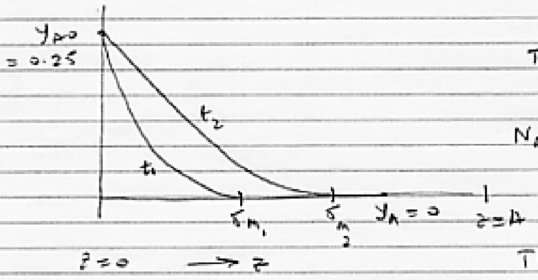

The flux is defined by

$$N_A = -cD_{AB}\frac{\partial y_A}{\partial z} + y_A(N_A + N_B)$$

Air is stagnant ∴ $N_B = 0$

Thus $N_A = -\dfrac{cD_{AB}}{1-y_A}\dfrac{dy_A}{dz}$

Perform a mass balance on species A (benzene) in the porous medium

Input + Generation = Output + Accumulation

$$N_A\Big|_{z=0} + \int_0^H -k_1 C_A(1-\varepsilon)\,dz = \frac{d}{dt}\left[\int_0^H c\,y_A\,\varepsilon\,dz\right] \quad (1)$$

where $N_A\Big|_{z=0} = -\dfrac{cD_{AB}}{1-y_A}\dfrac{dy_A}{dz}\Big|_{z=0}\cdot\varepsilon$; $C_A = c\,y_A$ (2)

Note that eq. (1) is per unit area of board and ε is porosity.

Re-arranging equation (1) with (2) substituted

$$-\varepsilon\frac{D_{AB}}{1-y_A}\frac{dy_A}{dz}\Big|_{z=0} - \int_0^{\delta_m} k_1 y_A(1-\varepsilon)\,dz = \frac{d}{dt}\left[\int_0^{\delta_m} y_A\,\varepsilon\,dz\right] \quad (3)$$

where the parameter ε reflects that the whole unit area of the board is unavailable for mass transfer and $(1-\varepsilon)dz$ is the volume of fibers in a differential element. The upper limit is changed also from H to δ_m.

Re-arranging eq. (3)

$$-\frac{D_{AB}}{1-y_{A0}}\frac{dy_A}{dz}\Big|_{z=0} - \int_0^{\delta_m} k_1\left(\frac{1-\varepsilon}{\varepsilon}\right)y_A\,dz = \frac{d}{dt}\left[\int_0^{\delta_m} y_A\,dz\right] \quad (4)$$

This is the integral mass transfer equation, similar to Equation 5.99 in Notes.
The boundary conditions are

$z = 0 \quad y_A = y_{A0}$; $z = \delta_m$, $y_A = 0$; and $z = \delta_m$, $\frac{dy_A}{dz} = 0$

Assume a profile

$$y_A = a + bz + cz^2 \qquad (5)$$

and substitute conditions to give

$$\frac{y_A}{y_{A0}} = \left(1 - \frac{z}{\delta_m}\right)^2 \qquad (6)$$

substitute (6) into (4) to yield

$$\frac{12 D_{AB}}{1 - y_{A0}} - 2 k_1 \beta \delta_m^2 = \frac{d\delta_m^2}{dt} \quad \text{where } \beta = \frac{1-\varepsilon}{\varepsilon}$$

(7) similar to 5.100 in Notes (with β)

Solve for δ_m

$$\delta_m = \sqrt{\frac{12 D_{AB}}{1 - y_{A0}}} \left[\frac{1 - e^{-2k_1\beta t}}{2k_1\beta} \right]^{\frac{1}{2}}$$

(8) similar to Eq 5.101 in Notes (with β)

(a) $k_1 = 5.2(10^{-4})\ s^{-1}$

$\beta = \frac{1 - 0.38}{0.38} = 1.6316$

$t = 180\ s \quad$ (or 3 min)

$D_{AB} = 8.82(10^{-6})\ m^2/s$

$y_{A0} = 0.25$

$$\delta_m = 1.1879(10^{-2}) \left[\frac{1 - 0.7368}{1.6967(10^{-3})} \right]^{\frac{1}{2}}$$

$= 0.1479\ m \quad$ or $\quad 14.8$ cm $\longrightarrow$

The total amount of benzene taken up is given by

$$\frac{Q}{A} = \int_0^t N_A\Big|_{z=0} dt = \int_0^t \varepsilon\left(-\frac{D_{AB}c}{1-y_{A0}}\frac{dy_A}{dz}\Big|_{z=0}\right) dt \qquad (9)$$

$$\frac{dy_A}{dz}\Big|_{z=0} = 2y_{A0}\left(1-\frac{z}{\delta_m}\right)\left(-\frac{1}{\delta_m}\right)\Big|_{z=0} = -\frac{2y_{A0}}{\delta_m} \qquad (10)$$

where δ_m is given by eq. (8)

$$\frac{Q}{\varepsilon . c . A} = +\frac{D_{AB}}{1-y_{A0}} \cdot 2y_{A0}\int_0^t \frac{1}{\delta_m}\, dt \qquad (11)$$

$$= 2D_{AB}\frac{y_{A0}}{1-y_{A0}}\sqrt{\frac{2k_1\beta(1-y_{A0})}{12 D_{AB}}}\int_0^t \frac{dt}{\left[1-e^{-2k_1\beta t}\right]^{\frac{1}{2}}} \qquad (12)$$

$$= y_{A0}\sqrt{\frac{2k_1\beta D_{AB}}{3(1-y_{A0})}}\int_0^\psi \frac{1}{k_1\beta}\frac{d\psi}{1-\psi^2} \qquad (13)$$

where $\psi = \left[1-e^{-2k_1\beta t}\right]^{\frac{1}{2}}$

$$\frac{Q}{\varepsilon . c . A} = y_{A0}\sqrt{\frac{2D_{AB}}{3k_1\beta(1-y_{A0})}}\int_0^\psi \frac{d\psi}{1-\psi^2}$$

$$= y_{A0}\sqrt{\frac{2D_{AB}}{3k_1\beta(1-y_{A0})}}\left[\frac{1}{2}\ln\left(\frac{1+\psi}{1-\psi}\right)\right]_0^\psi$$

$$\frac{Q}{\varepsilon . c . A} = \frac{y_{A0}}{2}\sqrt{\frac{2D_{AB}}{3k_1\beta(1-y_{A0})}}\ln\left(\frac{1+\psi}{1-\psi}\right) \qquad (14)$$

$\longrightarrow$

For $t = 40$ min or 2400 s,

$$\psi = \left[1 - e^{-2k_1\beta t}\right]^{1/2} = 0.9914$$

$$\therefore \ln\left(\frac{1+\psi}{1-\psi}\right) = 5.45$$

$$\frac{Q}{A} = \frac{0.25}{2} \sqrt{\frac{2 D_{AB}}{3 k_1 \beta (1 - y_{A0})}} \; C \; (5.45017) \, \varepsilon \qquad (15)$$

where $C = P/RT = \frac{1}{(0.08205)(293)} = 0.0416 \; \frac{\text{kmols}}{m^3}$

$$\frac{Q}{A} = \varepsilon(0.002724) \; \frac{\text{kmols}}{m^2} \quad \text{or} \quad 1.0351 \; \frac{\text{mols}}{m^2}$$

The unreacted amount is found by integrating. That is

$$\frac{W}{A} = \int_0^{\delta_m} C \, y_A \varepsilon \, dz \qquad (16)$$

When $t = 40$ min or 2400 s,

$$\delta_m = \sqrt{\frac{12(8.52)(10^{-6})}{(0.75)(2)(5.2)(10^{-4})(1.6316)}} \; (0.9914)$$

$$= 0.2859 \text{ m}$$

$$\frac{W}{A} = \varepsilon C \, y_{A0} \int_0^{\delta_m} \left(1 - \frac{z}{\delta_m}\right)^2 dz$$

$$= \varepsilon C \, y_{A0} \, \delta_m \int_0^1 (1-\eta)^2 \, d\eta \quad ; \quad \eta = \frac{z}{\delta_m} \qquad (17)$$

$$\therefore \quad \frac{W}{A} = \varepsilon\, c\, y_{Ao}\, \delta_m \int_0^1 (1 - 2\eta + \eta^2)\, d\eta \qquad (18)$$

$$= \varepsilon\, c\, y_{Ao}\, \delta_m \left[\eta - \eta^2 + \tfrac{1}{3}\eta^3 \right]_0^1 = c\, y_{Ao} \frac{\delta_m}{3}$$

$$\frac{W}{A} = \varepsilon . (0.0416)\frac{(0.25)}{3}(0.2859) \quad \frac{\text{kmols}}{m^2}$$

$$= \varepsilon \left(9.9113 (10^{-4}) \right) \quad \text{kmols}/m^3 \quad \text{or} \quad 0.377 \frac{\text{mols}}{m^3}$$

$\longrightarrow$

$$\therefore \quad \frac{\text{Fraction of benzene as gas in board}}{\text{total absorbed}} = \frac{W/A}{Q/A} \qquad (19)$$

$$= \frac{\cancel{\varepsilon}\; 9.913 (10^{-4})}{\cancel{\varepsilon}\; 2.724 (10^{-3})} = 0.3638$$

Hence fraction of Benzene absorbed by board and bonded by fiber $= 1 - 0.3637$ or

$63.62\ \% \longrightarrow$