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ENCH 501: Transport Phenomena Quiz #7 November 24, 2009

Time Allowed: 35 mins. **Name:**

Bisphenol A or BPA, an organic monomer for the production of polycarbonate plastics, has been suspected of being hazardous to people since 1930s. The monomer leaches out of clear and nearly shatter-proof plastics used for baby and water bottles, medical and dental devices, dental fillings, eye glasses and electronic goods such as CDs and DVDs. Epoxy resins containing the monomer are also used in coatings on the inside of almost all food and beverage cans. The transfer of BPA into foods and drinks is of interest since BPA can imitate the hormones of the body and cause health problems.

Cans of tomato paste are lined with an epoxy resin containing BPA. The BPA first dissolves at the boundary of the paste and then diffuses into it. It is to be assumed that the molar concentration of the BPA is not low, i.e. y_A is not << 1. Also the concentration of the BPA at the wall-paste interface is constant at y_{AO}. The paste, initially, does not contain BPA. The diffusivity of BPA in tomato paste is D_{AB} and you may assume that the molar concentration (**c**) for the paste and BPA is constant, irrespective of the amount of BPA present. BPA does not react with tomato paste.

Obtain expressions for the ***concentration profiles*** for BPA in the paste as functions of space and time, and for the **flux** of BPA into the paste. Use the integral method. You may assume that the wall is flat and the domain is semi-infinite. State all your assumptions and show all your steps.

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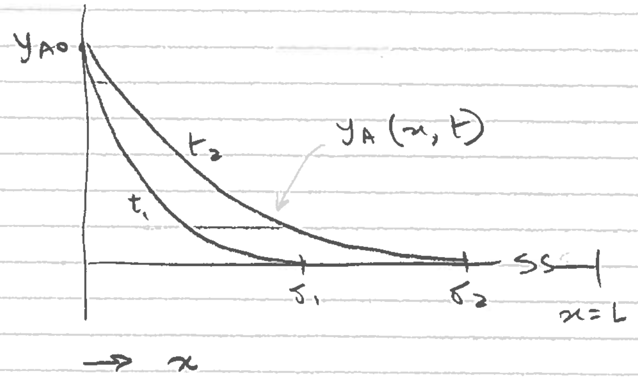

The flux of BPA (substance A) into the paste (substance B) is given by

$$N_A = -cD_{AB}\frac{dy_A}{dx} + y_A(N_A+N_B)$$

where $N_B = 0$ as the paste may be assumed stationary.

$$\therefore \quad N_A = -\frac{cD_{AB}}{1-y_A}\frac{dy_A}{dx}$$

1

Consider the domain $0 \le x < L$; $L >> \delta$

Material balance, unit area of wall

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

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

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

; since $y_A = 0$ for $x > \delta_m$ or conc. penetration depth.

substitute definition

$$-\frac{cD_{AB}}{1-y_{A0}}\frac{dy_A}{dx}\Big|_{x=0} = \frac{d}{dt}\left[\int_0^{\delta_m} c\, y_A \, dx\right]$$

2

The boundary conditions are

$x=0$ $y_A = y_{A0}$

$x=\delta_m$ $y_A = 0$

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

Assume

$\therefore$ $y_A = a + bx + cx^2$

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Apply b.c.

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

$$\frac{dy_A}{dx} = y_{A0}\left(-\frac{2}{\delta_m} + \frac{2x}{\delta_m^2}\right)$$

Substitute into eq. 2

$$-\frac{\cancel{c}D_{AB}}{1-y_{A0}}(\cancel{y_{A0}})\left(-\frac{2}{\delta_m}\right) = \frac{d}{dt}\left[\int_0^{\delta_m} \cancel{c}\,\cancel{y_{A0}}\left(1-\frac{x}{\delta_m}\right)^2 dx\right]$$

$$\frac{2D_{AB}}{(1-y_{A0})\delta_m} = \frac{d}{dt}\left[\int_0^{\delta_m}\left(1 - \frac{2x}{\delta_m} + \frac{x^2}{\delta_m^2}\right)dx\right]$$

$$= \frac{d}{dt}\left[\delta_m\int_0^1 (1 - 2\eta + \eta^2)\,d\eta\right]$$

$$= \frac{d}{dt}\left[\delta_m\left[\eta - \eta^2 + \frac{1}{3}\eta^3\right]_0^1\right]$$

$$= \frac{d}{dt}\left[\delta_m/3\right]$$

$$\therefore \frac{6D_{AB}}{1-y_{A0}} = \delta_m\frac{d\delta_m}{dt} = \frac{1}{2}\frac{d}{dt}\delta_m^2$$

This is subject to the condition

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

Solve

$$\delta_m = \sqrt{\frac{12 D_{AB}}{1-y_{A0}} t}$$

(a) The concentration profile is

$$\frac{y_A}{y_{A0}} = \left(1 - \frac{x}{\delta_m}\right)^2 , \text{ where } \delta_m = \sqrt{\frac{12 D_{AB} t}{1-y_{A0}}}$$

(b) The flux is given by equation $\underline{1}$

At $x = 0$

$$N_A = -\frac{c D_{AB}}{1-y_{A0}} y_{A0} \left(-\frac{2}{\delta_m}\right) \quad \text{as previously shown}$$

$$= \cancel{2} c D_{AB} \frac{y_{A0}}{1-y_{A0}} \frac{(1-y_{A0})^{\frac{1}{2}}}{\cancel{2}\sqrt{3 D_{AB} t}}$$

$$= \frac{c D_{AB}^{\frac{1}{2}}}{(1-y_{A0})^{\frac{1}{2}}} \frac{y_{A0}}{\sqrt{3}} t^{-\frac{1}{2}}$$

$$= c\, y_{A0} \left[\frac{D_{AB}}{3(1-y_{A0})}\right]^{\frac{1}{2}} t^{-\frac{1}{2}}$$

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