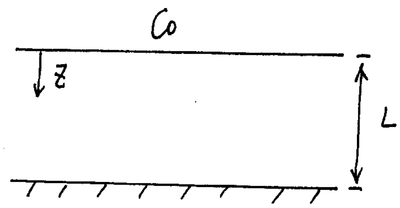
Problems Set 12 Due : 12/08/00

Part A

Problem 1



Zero-Order Reaction

Mass Balance on differential volume to Glucose (A):

$$N_A''|_z - N_A''|_{z+dz} - k''a\,dz = 0$$

$$-\frac{dN_A''}{dz} - k''a = 0$$

$$\mathcal{D}\frac{d^2C_A}{dz^2} - k''a = 0$$

Boundary Conditions:

$$z = 0 \quad C_A = C_o$$

$$z = L \quad \frac{dC_A}{dz} = 0$$

$$\Rightarrow \quad C_A = \frac{1}{2}\frac{k''a}{\mathcal{D}}z^2 - \frac{k''aL}{\mathcal{D}}z + C_o$$

$$\epsilon = \frac{\text{Actual Reaction Rate}}{\text{Maximum Reaction Rate}}$$

$$= \frac{-\mathcal{D}\frac{\partial C_A}{\partial z}\Big|_{z=0}}{k''aL}$$

$$= \frac{-\mathcal{D}\left(-\frac{k''aL}{\mathcal{D}}\right)}{k''aL}$$

$$= 1$$

First-Order Reaction

$$\mathcal{D}\frac{d^2C_A}{dz^2} - k'' C_A a = 0$$

Boundary Conditions:

$$z = 0 \quad C_A = C_0$$

$$z = L \quad \frac{dC_A}{dz} = 0$$

$$\Rightarrow \quad C_A = K_1 \sinh\left(\sqrt{\frac{k''a}{\mathcal{D}}}\, z\right) + K_2 \cosh\left(\sqrt{\frac{k''a}{\mathcal{D}}}\, z\right)$$

$$z = 0 \Rightarrow K_2 = C_0$$

$$z = L \Rightarrow K_1 \cosh\left(\sqrt{\frac{k''a}{\mathcal{D}}}\, L\right) + K_2 \sinh\left(\sqrt{\frac{k''a}{\mathcal{D}}}\, L\right) = 0$$

$$\Rightarrow K_1 = -C_0 \tanh\sqrt{\frac{k''a}{\mathcal{D}}}\, L$$

Therefore

$$C_A = C_0\left[\cosh\left(\sqrt{\frac{k''a}{\mathcal{D}}}\, z\right) - \sinh\sqrt{\frac{k''a}{\mathcal{D}}}\, z \cdot \tanh\sqrt{\frac{k''a}{\mathcal{D}}}\, L\right]$$

$$\epsilon = \frac{-\mathcal{D}\left.\frac{\partial C_A}{\partial z}\right|_{z=0}}{k''a\, C_0 L}$$

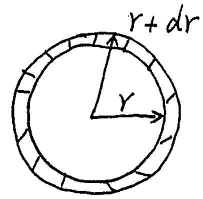
$$= \frac{-\mathcal{D}\left[-\cancel{C_0}\sqrt{\frac{k''a}{\mathcal{D}}}\ \tanh\sqrt{\frac{k''a}{\mathcal{D}}}\, L\right]}{k''a L \cancel{C_0}}$$

$$= \frac{1}{\sqrt{\frac{k''a}{\mathcal{D}}}\, L}\ \tanh\sqrt{\frac{k''a}{\mathcal{D}}}\, L$$

Part A

Problem 2

(a)



Mass Balance on differential shell of normal butane (A):

In - Out + Generation = 0

$$4\pi r^2 \left(-\mathcal{D}_{eff} \frac{dC_A}{dr}\right) - 4\pi (r+dr)^2 \left\{-\mathcal{D}_{eff} \left[\frac{dC_A}{dr} + \frac{d\left(\frac{dC_A}{dr}\right)}{dr} dr\right]\right\}$$

$$+4\pi r^2 dr \left(-k_a C_A\right) = 0 \qquad (1)$$

For the second term

$$= 4\pi \mathcal{D}_{eff} \left(r^2 + dr^2 + 2r \cdot dr\right)\left(\frac{dC_A}{dr} + \frac{d^2C_A}{dr^2} dr\right)$$

$$= 4\pi \mathcal{D}_{eff} \left[r^2 \frac{dC_A}{dr} + r^2 \frac{d^2C_A}{dr^2} dr + \cancelto{0}{dr^2 \frac{dC_A}{dr}} + \cancelto{0}{dr^3 \frac{d^2C_A}{dr^2}}\right.$$

$$\left. +2r \cdot dr \frac{dC_A}{dr} + \cancelto{0}{2r \frac{d^2C_A}{dr^2} dr^2}\right]$$

neglect any term with dr^2 or dr^3 and put into (1)

$$4\pi \mathcal{D}_{eff} \left[r^2 \frac{d^2C_A}{dr^2} \cdot dr + 2r\, dr \frac{dC_A}{dr}\right] + 4\pi r^2 dr \left(-k_a C_A\right) = 0$$

Divided by $4\pi r^2 dr \mathcal{D}_{eff}$

$$\frac{d^2C_A}{dr^2} + \frac{2}{r} \frac{dC_A}{dr} - \frac{k_a C_A}{\mathcal{D}_{eff}} = 0 \qquad (2)$$

Boundary Conditions:

$$r = 0 \qquad \frac{dC_A}{dr} = 0 \qquad (3)$$

$$r = R \qquad C_A = C_s \qquad (4)$$

(b) Define

$$\xi = \frac{C_A r}{C_s R} \Rightarrow C_A = \frac{C_s R \xi}{r} \quad (5)$$

$$\frac{dC_A}{dr} = \frac{C_s R}{r}\frac{d\xi}{dr} - \frac{1}{r^2} C_s R \xi \quad (6)$$

$$\frac{d^2 C_A}{dr^2} = -\frac{1}{r^2} C_s R \frac{d\xi}{dr} + \frac{C_s R}{r}\frac{d^2\xi}{dr^2} + \frac{2}{r^3} C_s R \xi - \frac{1}{r^2} C_s R \frac{d\xi}{dr}$$

$$= \frac{C_s R}{r}\frac{d^2\xi}{dr^2} - \frac{2}{r^2} C_s R \frac{d\xi}{dr} + \frac{2}{r^3} C_s R \xi \quad (7)$$

Put (5)(6)(7) into (2)

$$0 = \frac{C_s R}{r}\frac{d^2\xi}{dr^2} - \cancel{\frac{2}{r^2} C_s R \frac{d\xi}{dr}} + \cancel{\frac{2}{r^3} C_s R \xi} + \frac{2}{r}\left[\cancel{\frac{C_s R}{r}\frac{d\xi}{dr}} - \cancel{\frac{1}{r^2} C_s R \xi}\right] - \frac{k_a}{D_{eff}}\frac{C_s R \xi}{r}$$

$$\frac{C_s R}{r}\frac{d^2\xi}{dr^2} - \frac{k_a}{D_{eff}}\frac{C_s R \xi}{r} = 0$$

$$\frac{d^2\xi}{dr^2} - \frac{k_a}{D_{eff}}\xi = 0 \quad (8)$$

$$\xi = k_1 \sinh\sqrt{\frac{k_a}{D_{eff}}}\, r + k_2 \cosh\sqrt{\frac{k_a}{D_{eff}}}\, r \quad (9)$$

Boundary Condition

$$r = 0 \quad \frac{dC}{dr} = \frac{d\left(\frac{C_s R \xi}{r}\right)}{dr} = C_s R\left[\frac{1}{r}\frac{d\xi}{dr} - \frac{1}{r^2}\xi\right] = 0$$

$$\Rightarrow \frac{d\xi}{dr} = \frac{\xi}{r} \quad \text{at } r = 0$$

from (9)

$$\left(k_1 \cosh\sqrt{\frac{k_a}{D_{eff}}}\, r + k_2 \sinh\sqrt{\frac{k_a}{D_{eff}}}\, r\right)\sqrt{\frac{k_a}{D_{eff}}} =$$

$$\left(k_1 \sinh\sqrt{\frac{k_a}{D_{eff}}}\, r + k_2 \cosh\sqrt{\frac{k_a}{D_{eff}}}\, r\right)/r$$

$$r \to 0 \quad \cosh\epsilon \to 1 \quad \sinh\epsilon \to \epsilon$$

$$\Rightarrow k_1\sqrt{\frac{k_a}{D_{eff}}} = k_1 + \frac{k_2}{r} \longrightarrow \boxed{k_2 = 0}$$

$$r = R \quad C = C_s \quad \xi = 1 \Rightarrow \boxed{k_1 = \frac{1}{\sinh\sqrt{\frac{k_a}{D_{eff}}}\, R}}$$

So,

$$\boxed{C = \frac{C_s R}{r}\sinh\sqrt{\frac{k_a}{D_{eff}}}\, r \Big/ \sinh\sqrt{\frac{k_a}{D_{eff}}}\, R}$$

(c) $$\varepsilon = \frac{\mathcal{D}_{eff} \left.\frac{dc}{dr}\right|_R \cdot 4\pi R^2}{\frac{4}{3}\pi R^3 \, k_a \, C_s}$$

$$= \frac{\mathcal{D}_{eff}}{\frac{R}{3} k_a C_s} \cdot \frac{C_s R}{\sinh \sqrt{\frac{k_a}{\mathcal{D}_{eff}}} R} \left[-\frac{1}{r^2} \sin\sqrt{\frac{k_a}{\mathcal{D}_{eff}}} r + \frac{1}{r}\sqrt{\frac{k_a}{\mathcal{D}_{eff}}} \cosh \sqrt{\frac{k_a}{\mathcal{D}_{eff}}} r \right] \Bigg|_R$$

$$= \frac{\mathcal{D}_{eff}}{\frac{R}{3} k_a C_s} \cdot C_s R \left[-\frac{1}{R^2} + \frac{1}{R}\sqrt{\frac{k_a}{\mathcal{D}_{eff}}} \frac{1}{\tanh \sqrt{\frac{k_a}{\mathcal{D}_{eff}}} R} \right]$$

$$= \frac{3\mathcal{D}_{eff}}{R \, k_a} \left[\sqrt{\frac{k_a}{\mathcal{D}_{eff}}} \frac{1}{\tanh \sqrt{\frac{k_a}{\mathcal{D}_{eff}}} R} - \frac{1}{R} \right]$$

$$= \frac{3}{R}\sqrt{\frac{\mathcal{D}_{eff}}{k_a}} \left[\frac{1}{\tanh \sqrt{\frac{k_a}{\mathcal{D}_{eff}}} R} - \frac{1}{R}\sqrt{\frac{\mathcal{D}_{eff}}{k_a}} \right]$$

define $\phi_s = R\sqrt{\frac{k_a}{\mathcal{D}_{eff}}}$

$$\varepsilon = \frac{3}{\phi_s}\left[\frac{1}{\tanh \phi_s} - \frac{1}{\phi_s} \right]$$

Compare ε when R is different

R (cm)	ϕ_s	ε
0.2	3.46	0.62
0.5	8.66	0.31
0.8	13.86	0.20
1.2	20.78	0.14

Therefore, the smallest pellet size 0.2 cm is recommended.

Part B

Calculate F_o and Bi

$$F_o = \frac{\mathcal{D}t}{L^2} = \frac{10^{-5} \cdot 1000}{(0.15)^2} = 0.44 > 0.2$$

$$Bi = \frac{k_c L}{\mathcal{D}} = \frac{1.5 \times 10^{-4} \cdot 0.15}{10^{-5}} = 2.25 > 0.1$$

$$\frac{C(r, z, t) - C_\infty}{C_i - C_\infty} = \underset{\text{infinite cylinder}}{\underset{\uparrow}{C(r, t)}} \cdot \underset{\text{plane wall}}{\underset{\uparrow}{P(z, t)}}$$

$$C(r, t) = \frac{C(r, t) - C_\infty}{C_i - C_\infty} \quad \text{Infinite Cylinder}$$

$$P(z, t) = \frac{C(z, t) - C_\infty}{C_i - C_\infty} \quad \text{Plane Wall}$$

For infinite cylinder

$$C(r, t) = C_1 \exp(-\zeta_1^2 F_o) J_0(\zeta_1 r^*)$$

For plane wall

$$P(z, t) = C_1 \exp(-\zeta_1^2 F_o) \cos(\zeta_1 x^*)$$

With $Bi = 2.25$

$\zeta_1 = 1.1058 \quad C_1 = 1.1872$ (plane wall)

$\zeta_1 = 1.6468 \quad C_1 = 1.3586$ (infinite cylinder)

Therefore

(r, z)	P(z, t)	C(r, t)	P(z,t)·C(r,t)	C(r,z,t)
(0, 0)	0.6932	0.4119	0.2855	0.7145 C_∞
$(0, \frac{H}{2})$	0.3108	0.4119	0.1280	0.8720 C_∞
$(R, \frac{H}{2})$	0.3108	0.1765	0.0549	0.9451 C_∞

Therefore

$$C(0, 0, t) = 7.145 \times 10^{-6} \text{ g mol/cc}$$
$$C(0, 0.15, t) = 8.720 \times 10^{-6} \text{ g mol/cc}$$
$$C(0.15, 0.15, t) = 9.451 \times 10^{-6} \text{ g mol/cc}$$

Notes:

- $J_0(x)$ Can be got from App. B.4
- Graphical solution is also fine.

Part C

Problem 1

G – Air Phase

L – Water phase

Solubility

Henry's Law

$$P_G = H\,C_L$$

$$\Rightarrow C_L = \frac{P_G}{H} = \frac{X_{SO_2}\,P_T}{H}$$

$$= \frac{1\,atm \cdot 0.36\times10^{-6}}{180\,atm\,cm^3/mol}$$

$$= 2\times10^{-9}\,mol/cm^3$$

$$C_G = \frac{P_G}{RT}$$

$$= \frac{X_{SO_2}\,P_T}{RT}$$

$$= \frac{0.36\times10^{-6}\cdot 1}{82.05\cdot(15.6+273.2)} \qquad (60F = 15.6\,^\circ C)$$

$$= 1.52\times10^{-11}\,mol/cm^3$$

$$S_{G/L} = \frac{C_G}{C_L} = 7.60\times10^{-3}$$

Boundary Conditions

$$-\mathcal{D}_L \frac{\partial c}{\partial r} = h_m\left[C_G(R) - C_G(\infty)\right]$$

$$= h_m S_{G/L}\left[\frac{C_G(R)}{S_{G/L}} - \frac{C_G(\infty)}{S_{G/L}}\right]$$

$$Bi = \frac{h_m S_{G/L} R}{\mathcal{D}_L} = \frac{\mathcal{D}_G}{R}\cdot\frac{S_{G/L} R}{\mathcal{D}_L} = \frac{\mathcal{D}_G}{\mathcal{D}_L}\cdot S_{G/L}$$

$$= \frac{0.2}{2\times10^{-5}} \cdot 7.60\times10^{-3}$$

$$= 76.0 \gg 0.1$$ (lumped method can't be used!)

$$Fo = \frac{\mathcal{D}_L t}{R^2}$$

$$= \frac{(2\times10^{-5})(5)(60)}{(\frac{0.1}{2})^2}$$

$$= 2.4 > 0.2$$

Figure D.7 on Page 873.

θ^* is tiny (off the diagram)

Therefore

$$C_L(0) - C_G(\infty)/S_{G/L} = 0$$

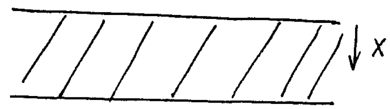
$$C_L(0) = \boxed{2\times10^{-9}\ mol/cm^3}$$ at the center.

Part C

Problem 2

(a) Assume semi-infinite plate solution can be used (case 1),

$$\frac{C(x,t)-C_s}{C_i - C_s} = \operatorname{erf}\left(\frac{x}{2\sqrt{\mathcal{D}t}}\right)$$



$C_i = 0$

$C_s = C_\infty S$ (assume Bi is infinite)

$= 100 \cdot 0.01$

$= 1 mg/ml$

$C(L,t) = 0.01\, C_\infty S = 0.01 \ mg/ml$

Then

$$1 - \frac{C(L,t)}{C_s} = 1 - 0.01 = \operatorname{erf}\left(\frac{L}{2\sqrt{\mathcal{D}t}}\right)$$

$$\Rightarrow \operatorname{erf}\left(\frac{L}{2\sqrt{\mathcal{D}t}}\right) = 0.99$$

$$\frac{L}{2\sqrt{\mathcal{D}t}} = 1.8246 \quad (\text{App. B.2})$$

$$t = \left(\frac{L}{2\sqrt{\mathcal{D}}\ 1.8246}\right)^2$$

$$= \left(\frac{0.1}{2\sqrt{5\times10^{-8}} \cdot 1.8246}\right)^2$$

$$= 1.50 \times 10^4 \ sec$$

$$= 4.17 \ hr$$

Justify Semi-infinite assumption

$$F_o = \frac{\mathcal{D}t}{L^2} = \frac{5\times10^{-8} \cdot 1.50\times10^4}{0.1^2} = 0.075 < 0.2$$

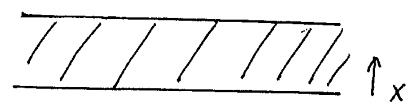
(b)

Assume $Fo > 0.2$, the one-term approximation for plane wall is used,

$$\theta^* = C_1 \exp(-\zeta_1^2 Fo) \cos(\zeta_1 x^*)$$

$Bi = \infty \quad C_1 = 1.2733 \quad \zeta_1 = 1.5707$

$$\theta_0^* = \frac{C(0,t) - C_s}{C_i - C_s} \qquad x^* = 0$$



$$= \frac{0.99\,C_s - C_s}{0 - C_s}$$

$$= 0.01$$

Therefore $\quad 0.01 = 1.2733 \exp(-1.5707^2 Fo) \cos(1.5707 \cdot 0)$

$$\Rightarrow Fo = 1.96$$

$$Fo = \frac{\mathcal{D} t}{L^2} \Rightarrow t = \frac{Fo\,L^2}{\mathcal{D}}$$

$$= \frac{1.96 \cdot 0.1^2}{5 \times 10^{-8}}$$

$$= 3.93 \times 10^5 \text{ sec}$$

$$= 109.1 \text{ hr}$$

$Fo = 1.96 > 0.2$, the assumption is justified.

Part D

$$\mathcal{D} = 10^{-6}\ cm^2/s$$

$$h_m = 10^{-3}\ cm/s$$

(a) Solvent A

$$C_{M,A} = C_{M,P}$$

$$\Rightarrow S_{A/P} = S_{P/A} = 1 \quad (P - \text{Polymer},\ A - \text{Solvent } A,\ M - \text{Monomer})$$

$$Bi = \frac{h_m R}{\mathcal{D}} = \frac{10^{-3} \cdot 0.2}{10^{-6}} = \boxed{200}$$

(b) Boundary Condition

$$-\mathcal{D} \frac{\partial C_{M,P}}{\partial r}\bigg|_R = h_m \left[C_{M,B}(R) - C_{M,B}(\infty) \right]$$

$$C_{M,B} = 0.05\ C_{M,P}$$

$$\Rightarrow S_{P/B} = \frac{C_{M,P}}{C_{M,B}} = 20$$

$$-\mathcal{D} \frac{\partial C_{M,P}}{\partial r}\bigg|_R = \frac{h_m}{S_{P/B}} \left[S_{P/B}\, C_{M,B}(R) - S_{P/B}\, C_{M,B}(\infty) \right]$$

$$Bi = \frac{h_m}{S_{P/B}} \frac{R}{\mathcal{D}}$$

$$= \frac{10^{-3}}{20} \cdot \frac{0.2}{10^{-6}}$$

$$= \boxed{10}$$

(c) $C_{M,A}(\infty) = 0$

$$\theta_0^* = \frac{C_{M,p}(0,t)}{C_i} = 0.1$$

$Bi = 200$

$Fo = 0.5$ (From Figure D.4 on Page 872)

$$t = \frac{Fo\,R^2}{\mathcal{D}} = \frac{0.5\,(0.2)^2}{10^{-6}} = 20,000\ s$$

$$= \boxed{5.56\ hr}$$

(d) $\theta_0^* = 0.1$

$Bi = 10$

$Fo = 0.6$

$$t = \frac{Fo\,R^2}{\mathcal{D}} = \frac{0.6\,(0.2)^2}{10^{-6}} = \boxed{6.67\ hr}$$