1. A first-order reaction A→P, with forward reaction rate, $k_{1,s}$, takes place inside a spherical catalyst. The catalyst is 6×10^{-3} m in diameter and has a surface area per unit volume, a, of 2×10^{8} m^2/m^3 catalyst.
   - (a) Obtain an expression for the concentration profile of A inside the catalyst, and
   - (b) Determine the value of the effectiveness, η

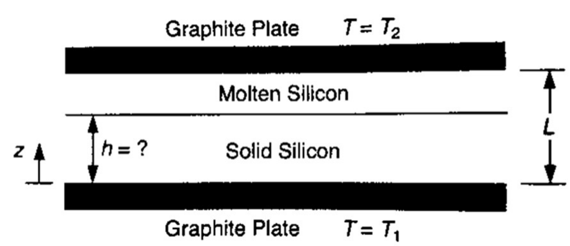
   Provided data/equations: Effective diffusivity $D_{Ae} = 1.26 \times 10^{-4}$ m^2/h
   Surface reaction rate constant: $k_{1s} = 1.728 \times 10^{-7}$ $m^3/h\ m^2$
   Concentration of A at catalyst surface $C_{A,S} = 28$ $kgmol/m^3$
   From handout on Example 3.2-8:

$$C_A = C_{A,S} \frac{R}{r} \frac{\sinh\left(\frac{3\phi r}{R}\right)}{\sinh(3\phi)}$$

$$\eta = \frac{1}{3\phi}(3\phi \coth(3\phi) - 1)$$

2. *3-3 Oxygen Diffusion in Tissues*. Oxygen is consumed in the body tissue, or by cells maintained in vitro, at a rate which is often nearly independent of the O_2 concentration. As a model for a tissue region or aggregate of cells, consider steady-state O_2 diffusion in a sphere of radius, r_o, with zero-order consumption of O_2. Assume that the O_2 concentration at the outer surface ($r=r_o$) is maintained constant at C_o. Determine the O_2 concentration profile, $C(r)$.

3. *3-11 Peltier Effect*. When a melt is an electrical conductor and its solid is a semiconductor, passing a current from the solid to the melt releases heat at the interface, a phenomenon called the Peltier effect. As shown in the figure, suppose that layers of molten and solid silicon are confined between graphite plates separated by a distance L. Both phases occur because the melting temperature of silicon (T_m) is between the temperature of the plates (i.e., $T_1 < T_m < T_2$). Assume that temperature variations in the x and y directions can be neglected and that the system is at steady state.
   - *a.* If there is no electrical current, calculate $T(z)$ in both silicon phases and find the height, h, of the melt-solid interface. The thermal conductivities of the melt and solid are k_m and k_s, $k_m \neq k_s$. The heat of fusion is λ.
   - *b.* With an electrical current present, the rate of energy release at the interface is given by $H_s = \beta \times i_z$, where β is the Peltier coefficient (volts) and i_z is the current density in the z direction (A/m^2). Determine $T(z)$ and h.



Solution to HW3 ChemE 530

1) (a) Determine $C_A(r)$ inside the catalyst
assume homogeneous reaction within catalyst
from lecture:

$$C_A = C_{As} \frac{R}{r} \frac{\sinh(3\phi\, r/R)}{\sinh(3\phi)}$$

$$\phi = \frac{V_p}{S_x}\sqrt{\frac{a\, k_{1s}}{D_{Ae}}} \quad ; \quad \frac{k_{1v}}{k_{1s}} \equiv a$$

$C_{AS} = .28 \text{ kgmol/m}^3$

$R = 3 \times 10^{-3}$ m

$\frac{V_p}{S_x} = \frac{\frac{4}{3}\pi R^3}{4\pi R^2} = 10^{-3}$ m

$a = 2 \times 10^8 \text{ m}^2/\text{m}^3 \text{cat}$

$k_{1s} = \frac{k_{1v}}{a} = 1.728 \times 10^{-7} \frac{1}{h\left(\frac{m^2}{m^3 \text{cat}}\right)}$

$D_{Ae} = 1.26 \times 10^{-4} \text{ m}^2/h$ (h... hour)

Plug the values into equations

$\Rightarrow \phi = 0.5237$

$$\Rightarrow C_A = \frac{0.0365}{r} \sinh(523.7\, r)$$

Solution to HW3 cont. Problem 1 ChemE 530

(b) Determine the effectiveness factor

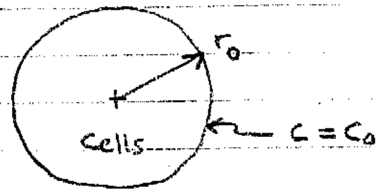
lecture: $\eta = \frac{1}{3\phi^2}\left(3\phi \coth 3\phi - 1\right)$

$\phi = 0.5237$ from (a)

$\Longrightarrow$ $\underline{\underline{\eta = 0.867}}$ this is close to unity, i.e., most of the catalyst volume is reacting at high rate (reactant is able to diffuse quickly)

1/22/11
WMD

3-3. Oxygenation of Cell Aggregates



r_c = radius of anoxic core (if present)

$$R_V = \begin{cases} -k_o, & c>0 \\ 0, & c=0 \end{cases}$$

(a) Determine $C(r)$

Case 1: $C>0$ throughout sphere

$$0 = \frac{D}{r^2}\frac{d}{dr}\left(r^2\frac{dC}{dr}\right) - k_o \qquad \text{(Table 2-4)}$$

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dC}{dr}\right) = \frac{k_o}{D}$$

$$\frac{dC}{dr}(0) = 0, \quad C(r_o) = C_o$$

Integrate DE directly and apply BC's:

$$r^2\frac{dC}{dr} = \frac{k_o}{D}\frac{r^3}{3} + \cancelto{0}{a} \quad \text{from symmetry BC}$$

$$C(r) = \frac{k_o}{D}\frac{r^2}{6} + b$$

$$C(r_o) = C_o = \frac{k_o}{D}\frac{r_o^2}{6} + b \Rightarrow b = C_o - \frac{k_o r_o^2}{6D}$$

$$\boxed{C(r) = C_o - \frac{k_o r_o^2}{6D}\left[1 - \left(\frac{r}{r_o}\right)^2\right]}$$

The minimum O_2 concentration is at $r=0$,

$$C(0) = C_o - \frac{k_o r_o^2}{6D}$$

3-11. Peltier Effect

(a) Temperature and interface location without current

$\frac{d^2T}{dz^2} = 0$ in both phases $\Rightarrow$ $T(z)$ linear in each

$$T(z) = \begin{cases} a_1 + a_2 z & \text{in solid}, \quad 0 \le z \le h \\ b_1 + b_2 z & \text{in melt}, \quad h \le z \le L \end{cases}$$

To be determined: a_1, b_1, a_2, b_2, h. Conditions:

$T(0) = T_1$ (1) bottom temp.

$T(L) = T_2$ (2) top temp.

$T(h^-) = T(h^+) = T_m$ (3),(4) melting temp.

$k_s \frac{dT}{dz}(h^-) = k_m \frac{dT}{dz}(h^+)$ (5) q_z continuous at interface

[q_z is continuous at $z=h$ because there is no flow, no interfacial motion, and no interfacial energy input. See Eq. (2.5-12).]

Using (1) and (3), the solid temp. is

$$\boxed{T(z) = T_1 + (T_m - T_1)\frac{z}{h}} \qquad 0 \le z \le h$$

Using (2) and (4), the melt temp. is

$$\boxed{T(z) = T_2 + (T_m - T_2)\frac{(L-z)}{(L-h)}} \qquad h \le z \le L$$

Applying (5) determines h (see next page).

$$k_s \frac{(T_m - T_1)}{h} = k_m \frac{(T_2 - T_m)}{L-h}$$

$$h\left[k_s(T_m - T_1) + k_m(T_2 - T_m)\right] = k_s L (T_m - T_1)$$

$$h = \frac{k_s L (T_m - T_1)}{k_s(T_m - T_1) + k_m(T_2 - T_m)}$$

$$\boxed{\frac{h}{L} = \frac{1}{1 + \dfrac{k_m(T_2 - T_m)}{k_s(T_m - T_1)}}}$$

(b) Temperature and interface location with current

Same formulation, except (5) must be modified to include heat generation at interface:

$$q_z(h^+) - q_z(h^-) = H_s \qquad (5')$$

$T(z)$ in both phases is unchanged, except for h. Applying (5'),

$$-k_m \frac{(T_2 - T_m)}{L-h} + k_s \frac{(T_m - T_1)}{h} = H_s$$

$$-k_m h (T_2 - T_m) + k_s (L-h)(T_m - T_1) = H_s h (L-h)$$

$$H_s h^2 - \left[k_s(T_m - T_1) + k_m(T_2 - T_m) + H_s L\right] h$$

$$+ k_s L (T_m - T_1) = 0$$

This is a quadratic:

$$H_s h^2 + bh + c = 0$$

$$b \equiv -\left[k_s(T_m - T_1) + k_m(T_2 - T_m) + H_s L\right]$$

$$c \equiv k_s L (T_m - T_1)$$

$$\therefore \quad \frac{h}{L} = \frac{-b \pm \sqrt{b^2 - 4H_s c}}{2H_s L}$$

The correct root is the one which reduces to the result in (a) for $H_s \to 0$. From (a),

$$\frac{h}{L} = \frac{1}{1+A}, \qquad A \equiv \frac{k_m}{k_s}\frac{(T_2 - T_m)}{(T_m - T_1)}$$

For comparison, rearrange the quadratic solution:

$$b = -\frac{c}{L}(1 + A + H), \qquad H \equiv \frac{H_s L^2}{c}$$

$$\frac{h}{L} = \frac{1 + A + H \pm \sqrt{(1+A+H)^2 - 4H}}{2H}$$

The numerator (N) and denominator (D) of h/L both $= 0$ at $H = 0$, so use L'Hopital's rule to find limit:

$$\lim_{H \to 0} \frac{h}{L} = \left.\frac{dN/dH}{dD/dH}\right|_{H=0} = \frac{1}{2}\left.\frac{dN}{dH}\right|_{H=0}$$

$$\frac{dN}{dH} = 1 \pm \frac{1}{2}\left[(1+A+H)^2 - 4H\right]^{-1/2}\left[2(1+A+H) - 4\right]$$

$$\left.\frac{dN}{dH}\right|_{H=0} = 1 \pm \frac{1}{2(1+A)}\left[2(1+A) - 4\right] = 1 \pm \left(1 - \frac{2}{1+A}\right)$$

$$\left.\frac{dN}{dH}\right|_{H=0} = \frac{(A+1) \pm (A-1)}{A+1}$$

$$\lim_{H \to 0} \frac{h}{L} = \frac{(A+1) \pm (A-1)}{2(A+1)}$$

$$= \begin{cases} \dfrac{A}{A+1} & \text{for "+" root} \\[2ex] \dfrac{1}{A+1} & \text{for "−" root} \end{cases}$$

∴ The "−" root is correct and

$$\boxed{\frac{h}{L} = \frac{1+A+H - \sqrt{(1+A+H)^2 - 4H}}{2H}}$$

(A and H defined on p. 3)