ABE370 Test 4

Name:

<u>Problem 1 (20 points)</u>

A. (15 points) For a chemical reaction in which 'ash' layer diffusion controls the overall reaction, a flat plate (total thickness 2L) requires 10 minutes to be completely reacted. Under the same reaction conditions, calculate how long it would take (in min) for a cylinder and a sphere made of the same material to be completely reacted, assuming R = L in both cases.

For 'ash' layer controlled systems

$$tau\_plate := \frac{density \cdot L^2}{2 \cdot b \cdot D \cdot Cg} \qquad tau\_cylinder := \frac{density \cdot R^2}{4 \cdot b \cdot D \cdot Cg} \qquad tau\_sphere := \frac{density \cdot R^2}{6 \cdot b \cdot D \cdot Cg}$$

Assuming R = L and all other parameters are the same

2*tau_plate = 4*tau_cylinder = 6*tau_sphere

If tau_plate = 10 min, then
tau_cylinder =5 min
tau_sphere = 3.33 min

B. (15 points) For a chemical reaction controlled system, a cylinder and sphere made of the same material and of the same radius are reacted under the same conditions. For the same overall conversion of X= 0.80, calculate which shape takes longer to react and how much longer it takes (% slower).

For a chemical reaction controlled system

Cylinder

$$tau := \frac{denstiy \cdot R}{b \cdot k \cdot C}$$

$$\frac{t\_cyl}{tau} = 1 - (1 - X)^{\frac{1}{2}}$$

Sphere

$$tau := \frac{denstiy \cdot R}{b \cdot k \cdot C}$$

$$\frac{t\_sph}{tau} = 1 - (1 - X)^{\frac{1}{3}}$$

In both cases, tau is the same, so given X = 0.80 for both

$X := 0.8$

$$1 - (1 - X)^{\frac{1}{2}} = 0.553 \qquad\qquad 1 - (1 - X)^{\frac{1}{3}} = 0.415$$

$$t\_cyl := 0.553 tau \qquad\qquad t\_sph := 0.415 tau$$

$$\frac{0.415}{0.553} = 0.75$$

So the reaction time for the sphere is 25% faster than for the cylinder

$$\frac{0.553}{0.415} = 1.333$$

Alternatively, the cylinder is 33.4% slower than the sphere

Problem 2 (30 points)

Corn flakes are made by roasting (an oxidation reaction) thin flat plates of corn dough at 450 K in air. The rate of the roasting process is controlled by the oxidation reaction. Lab testing on 4 mm thick flakes shows that 50% of the flake is reacted in 15 minutes in air at 1 atm.

A. (10 points) How long (min) would it take to completely roast the flakes?

B. (10 points) The marketing dept. wants to develop a new product, Corn Stix, using the same basic process, but in the form of sticks (cylinders). They suggest that a radius of 4 mm is desirable. How long (min) will it take to completely roast this stick product?

C. (10 points) The existing flake roasting process uses conveyer belts in a continuous process. The conveyer belt gears limit the roasting time to a maximum of 47 minutes. The stick product must be at least 95% roasted to make acceptable product. Can you use the existing equipment or do you have to buy a new oven?

Corn flake problem

A. For flat plates with reaction controlled rates of reaction, t/tau; = X.
Re-arranging, tau=t/X. Therefore, tau (the time needed for 100% reaction) = 15/0.5 or 30 minutes.

For flat plates under reaction controlled rate conditions, tau=density*(1/2 thickness)/[stochiometric coeff*reaction constant*bulk oxygen concentration]

$$tau := \frac{density \cdot L}{b \cdot k \cdot C}$$

Since L = 2 mm and tau= 30 min, the reaction constant is

$$k := \frac{density \cdot 2}{b \cdot tau \cdot C}$$

B. To make sticks, the cylinder model applies

$$tau := \frac{density \cdot R}{b \cdot k \cdot C} \qquad \frac{t}{tau} := 1 - (1 - X)^{0.5}$$

Since the density, stoichiometric coefficient, and bulk concentration are the same, and we know the radius of the sticks and the reaction constant

$$tau := \frac{density \cdot R}{b \cdot C} \cdot \frac{b \cdot 30 \cdot C}{density \cdot 2}$$

$$tau := \frac{R \cdot 30}{2}$$

So the total roasting time for the sticks is 4*30/2 = 60 minutes

C. To determine whether the existing equipment can be used, calculate the conversion at 47 min.

$$X := 1 - \left(1 - \frac{t}{tau}\right)^2$$

So using 47 min for t and 60 min for tau, the conversion is 95.3%, so you can use the existing oven.

Problem 3 (40 points)

A time release cold medicine is delivered by desorbing the medicine from inert carrier cylindrical pills by ingestion. Values for the various resistances to release (film layer, carrier matrix, dissolution reaction) have been measured and are given below. You may assume the stomach environment to be pure water.

Data:

k_{film}= 0.73 cm/sec	R = 0.5 cm
D_{matrix} = 1.4×10^{-3} cm^2/sec	drug density in carrier = 0.25 mol/cm^3
$k_{reaction}$= 0.013 cm/sec	drug solubility = 0.05 mol/L of water

A. (20 points) Determine which resistance(s) are the most important in this situation. Show all calculations and clearly explain the justification for your solution.

B. (20 points) Based on these resistances, calculate the time (hr) needed to deliver 80% of the medicine. Show all calculations.

Problem 3 Time Release medicine

$k\_film := 0.73\frac{cm}{s}$

$C\_water := 1\frac{gm}{cm^3}\cdot\frac{1mol}{18gm} = 0.056\frac{mol}{cm^3}$

$D\_matrix := 1.4\cdot 10^{-3}\frac{cm^2}{s}$

$R := 0.5cm$

$density := 0.25\frac{mol}{cm^3}$

$k\_reaction := 0.013\frac{cm}{s}$

$solubility := 0.05\frac{mol}{L}$

need to convert the units of solubility to moles medicine/mole water $\frac{1000}{18} = 55.556$

1 L of water contains 1000 gm=55.556 gmol

$molar\_solubility := \frac{0.05}{55.556} = 9\times 10^{-4}$

Part A, To determine which resistances are significant, calculate the total time needed assuming each resistance is the controlling factor

film resistance

$$tau\_film := \frac{density\cdot R}{2\cdot k\_film\cdot C\_water\cdot molar\_solubility}$$

$tau\_film = 0.476hr$

$tau\_film = 1.712\times 10^3 s$

$tau\_film = 28.539min$

inert carrier resistance

$$tau\_matrix := \frac{density\cdot R^2}{4\cdot D\_matrix\cdot C\_water\cdot molar\_solubility}$$

$tau\_matrix = 62.004hr$

$tau\_matrix = 2.232\times 10^5\cdot s$

$tau\_matrix = 3.72\times 10^3\cdot min$

Reaction limited

$$tau\_reaction := \frac{density\cdot R}{k\_reaction\cdot C\_water\cdot molar\_solubility}$$

$tau\_reaction = 53.419hr$

$tau\_reaction = 1.923\times 10^5\cdot s$

$tau\_reaction = 3.205\times 10^3\cdot min$

Clearly, the film resistance is negligible compared to diffusion through the matrix and the reaction resistances

Part B. To calculate the overall time needed to deliver 80% of the drug, i.e. 80% conversion, need to add the times required for each resistance at 80%.

$$t\_matrix(X) := tau\_matrix\cdot[X + (1 - X)\cdot\ln(1 - X)]$$

$$t\_reaction(X) := tau\_reaction\cdot\left[1 - (1 - X)^{\frac{1}{2}}\right]$$

$$t\_overall(X) := t\_matrix(X) + t\_reaction(X)$$

t_overall (X)=29.64+29.53=59.17 hr