Chemical Engineering 140 **December 11, 2017**

Final Examination

(150) 1. Propylene Oxide Production with Side Reaction

Propylene oxide is a highly valuable intermediate in the plastics industry. The catalytic oxidation of propylene to produce propylene oxide involves the following reactions in parallel:

$$2C_3H_6 + O_2 \rightarrow 2C_3H_6O$$
$$C_3H_6 + 9/2O_2 \rightarrow 3CO_2 + 3H_2O$$

The feed to the reactor contains 3 moles of propylene per mole of oxygen. The single-pass conversion of propylene is 10%, and for every 100 moles of propylene consumed in the reactor, 80 moles of propylene oxide emerge in the reactor's products. A multiple-unit process is used to separate the products: propylene and oxygen ~~are recycled back into~~ the reactor, propylene oxide is sold as product, and carbon dioxide and water are discarded. recycled back into

a. (25) Draw a schematic of the process labeling all knowns and unknowns.

b. (85) Calculate the molar composition in the fresh feed.

c. (10) Calculate the selectivity of the process to the desired product as a ratio of lbmol of propylene oxide/ lbmol of carbon dioxide produced.

d. (10) Explain in your own words how to maximize the selectivity calculated in part (c)

e. (20) Calculate the amount of propylene oxide produced in kg/day if 10 kmol/h of fresh feed are used. Molar mass of propylene oxide is 58 kg/kmol.

(75) 2. Physical Meaning of the PFR Energy Balance

In class, we derived the following differential expression for the steady temperature profile in a cylindrical plug flow reactor exposed to a constant external temperature, T_∞:

$$\frac{dT}{dV}=\frac{U(2/R)(T_\infty - T)+r_A\Delta\tilde{H}_{rxn}/(-\nu_A)}{\left[\left(\sum_i \dot{n}_{i,in}\tilde{C}_{Pi}\right)+\dot{n}_{A,in}X_A\Delta\tilde{C}_P/(-\nu_A)\right]}$$

where symbols have their usual definitions.

(15) a. Classify this differential equation

(15) b. What term in this expression gives the strongest temperature dependence?

(15) c. What determines whether the reactor temperature initially increases or decreases along the reactor?

(30) d. Explain the physical meaning of each term in the numerator and denominator of this expression. 4 terms total (2 in numerator, 2 in denominator)

(100) 3. Chemotherapeutic Drug Capture

To be effective in treating tumors, chemotherapeutic drugs must be injected directly into the blood stream at the site of the tumor. Much of the drug, however, circulates through the blood stream. To minimize the harmful circulation, a reactive filter is placed downstream of the kidney to adsorb the excess drug. After a long time, the drug-containing filter is removed from the body.

The drug, species A, is initially injected into the kidney giving an initial concentration C_{A0} in the kidney. As illustrated in Figure 2, model the kidney as a CSTR of volume V and initial concentration C_{A0}. Only clean blood devoid of A flows into the CSTR. Blood contaminated with A flows out at concentration $C_{A1}(t)$. Drug A is dilute so the volumetric flow rate of blood, Q, is constant everywhere.

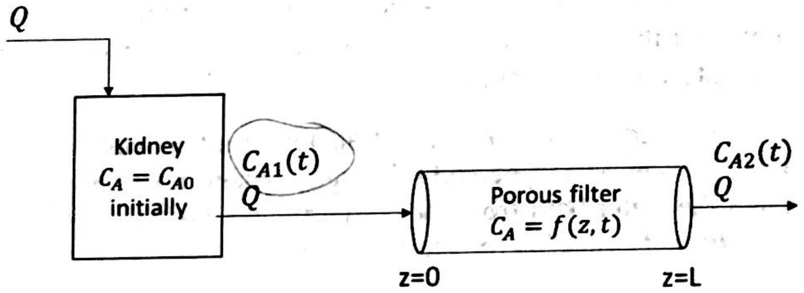

Figure 1. Schematic of drug capture system

a. (35) Calculate the concentration of A leaving the kidney as a function of time C_{A1}.

b. (45) The reactive filter is modeled as a PFR. The rate of adsorption of the drug per unit filter volume is proportional to the concentration of the drug at position z along the axis with a proportionality constant k. Assume that the inlet concentration to the PFR, $C_{A1}(t)$, changes slowly with time such that the filter is at steady state. Thus, the filter operates at steady state but the inlet concentration changes with time (the so-called pseudo steady state approximation). Calculate the concentration profile of A in the reactive filter as a function of time and position, $C_A(t,z)$.

c. (20) Using your result for $C_A(t,z)$, find an expression for the drug concentration eluted into the blood stream, $C_{A2}(t)$. Using this result, multiply by the blood circulation flow rate, Q, and integrate over time to establish the total amount of drug that finally circulates into the blood stream.

(145) 4. Ice Thawing

As an approximate model for predicting how long it takes to slow-thaw a turkey consider the melting of a large chuck of ice in a water bath placed outside (in November). A large sphere of ice with constant density ρ_I , and initially of radius R_o and freezing temperature T_o, is immersed in a large water bath (well stirred) of initial mass M_{Wo} and ambient temperature T_a. The ice melts at a rate of (mass/time) $\dot{m}_{melt} = 4\pi R^2 h_w (T - T_o) / \Delta\hat{H}_{fus}$ where h_w is the heat transfer coefficient between the water bath at temperature T and the melting ice at T_o; $\Delta\hat{H}_{fus}$ is the enthalpy of fusion of ice per unit mass. As the ice melts, the ice sphere shrinks. Concurrently, the melting ice cools the water bath and the surrounding environment heats the water bath. We wish to establish the time taken for the ice to melt completely away, t_f, which estimates the thawing time of the turkey.

(20) a. Write a transient mass balance on the ice sphere to calculate the shrinking ice-sphere radius as function of time, $R(t)$. You are to use the expression for the rate of ice melting given in the problem statement. List the initial condition. Note that your expression cannot be integrated because the bath temperature is not constant.

(40) b. Let the heat transfer coefficient and heat transfer area between the environment and the water bath be labeled as h_a and A, respectively. Write transient mass and energy balances on the water bath. Heat enters the water bath from the environment and the melting ice cools the water bath. As ice melts the mass of water in the bath increases.

(20) c. Assume that the ice sphere shrinks very slowly so that at any given sphere radius the temperature of the bath effectively reaches a steady state (this is called the pseudo steady state approximation). Accordingly, in your transient energy balance of Part b set dT / dt to zero and relate the bath temperature $T(t)$ to the ice-sphere radius, $R(t)$. Assume constant heat capacity of ice bath c_v

In case you do not succeed in obtaining a valid transient energy analysis, reason the following to calculate the pseudo steady bath temperature: At any given time in pseudo steady state, heat input from the environment into the water bath exactly balances that lost to the ice sphere.

(15) d. Does the bath temperature increase or decrease with time. Why?

(20) e. Substitute the result from part c for the pseudo steady bath temperature into the ice mass balance of part a. Obtain a differential equation describing how the ice-sphere radius depends on time.

(15) f. Integrate your differential equation to find t_f

(15) g. The presence of salt lowers the freezing point of water. Will adding salt to the water bath increase the rate of thawing? Explain.