CHFEN 3553 Chemical Reaction Engineering

Final Examination

May 4, 2005; 1 PM – 3 PM

Name:

Student ID:

Answer all questions – Total is 100 points

1. A reversible reaction $A \rightleftarrows B$ is taking place in a PFR. The equilibrium constant (in terms of concentrations) is 4. 50% of the equilibrium conversion is obtained. A CSTR of equal size is placed downstream of the PFR (PFR-CSTR) to increase conversion. What is the total conversion in the reactor sequence with this arrangement?

20 points

$A \Leftrightarrow B$

Solution to the first-order reversible constant volume PFR

$$k\tau = X_e \ln\left(\frac{X_e}{X_e - X}\right)$$

$$K_e = 4 = \frac{C_B}{C_A} = \frac{C_{A0}X_e}{C_{A0}\left(1-X_e\right)} = \frac{X_e}{\left(1-X_e\right)}$$

$$\frac{1}{X_e} = 1 + \frac{1}{K_e}$$

$$X_e = 0.8$$

$$X_1(given) = 0.5 \cdot 0.8 = 0.4$$

In the first situation,

$$k\tau = X_e \ln\left(\frac{X_e}{X_e - X}\right) = 0.8\ln\left(\frac{0.8}{0.8-0.4}\right) = 0.5545$$

CSTR of equal size placed placed downstream

$$\frac{V}{F_{A0}} = \frac{X_2 - X_1}{-r_2}$$

$$-r_2 = k(C_A - \frac{C_B}{K_e}) = kC_{A0}\left((1-X_2) - \frac{X_2}{K_e}\right)$$

$$k\tau = \frac{X_2 - X_1}{\left((1-X_2) - \frac{X_2}{K_e}\right)} = 0.5545$$

$X_1 = 0.4;$ Solve for X_2; $X_2 = 0.5637$

2. A liquid antibiotic containing 500 mg of active ingredient is given to a patient with a body fluid of 40 liters. In the stomach, the antibiotic can either be absorbed into the bloodstream through the stomach walls or can be eliminated through the gastrointestinal tract. Both these processes are first order with rate constants of 0.25 h^{-1} and 0.5 h^{-1} respectively. The only mechanism for the antibiotic to leave the bloodstream is by elimination through urine. This reaction can also be assumed to be first order with a rate constant of 0.4 h^{-1}. The doctor wants to find out the exact time at which the concentration of this antibiotic in the blood peaks in the patient. Determine this time and the concentration of the antibiotic in the blood stream at this time.

20 points

$C_A -$ Concentration of drug in stomach

$C_B -$ Concentration of drug in blood

$$\frac{dC_A}{dt} = -k_1 C_A - k_2 C_A$$

$$\frac{dC_B}{dt} = k_1 C_A - k_3 C_B$$

Series reaction

$$C_B = \frac{k_1 C_{A0}}{k_3 - k}\left[e^{-kt} - e^{-k_3 t}\right]$$

$$k = k_1 + k_2$$

$$C_{A0} = 12.5 \text{ mg/l}$$

Maximum concentration is when $\frac{dC_B}{dt} = 0$

$$t = \frac{1}{k - k_3}\ln\frac{k}{k_3} = 1.796 \text{ hours}$$

Substitute in the concentration equation

$$C_B = 2.03 \text{ mg/liter}$$

3. The liquid-phase irreversible reaction $A \rightarrow B$ is carried out in a CSTR. To learn the rate law, the residence time, τ is varied and the effluent concentrations of species A are measured. Pure A enters the reactor at a concentration of 7.5 mol/liter in all the runs given below.

Run	1	2	3	4
τ (min)	1	15	30	100
C_A (mol/lit)	3.2	0.72	0.46	0.21

a. Write the mole balance for the CSTR where an n[th] order equation is taking place (in terms of concentrations and residence time).
b. Show how you will plot the above data to obtain a straight line, and thus determine the reaction order (n) and reaction rate constant k.
c. Plot the data on the paper provided and find n and k by the method you describe in step b.

20 points

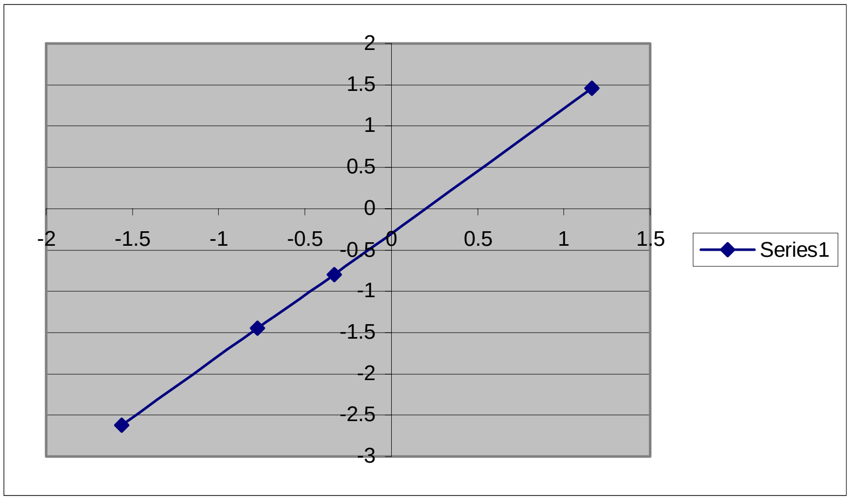
CSTR Eqaution

$$\frac{C_{A0} - C_A}{\tau} = kC_A^n$$

$$\ln\left(\frac{C_{A0} - C_A}{\tau}\right) = \ln(k) + n \ln C_A$$

Plot

$$\ln\left(\frac{C_{A0} - C_A}{\tau}\right) versus \ln C_A$$



n=1.5
k=0.75

4. The elementary reversible liquid-phase reaction $A \rightleftarrows B$ is carried out in a CSTR. The reactor is jacketed and is surrounded by a jacket. Pure A enters the reactor at a temperature of 27^0C. The following parameters are given.

Rate constant k at 100^0C = 1.25 min^{-1}, $E = 40,000$ cal/mole

Equilibrium constant K_e at 120^0C = 75

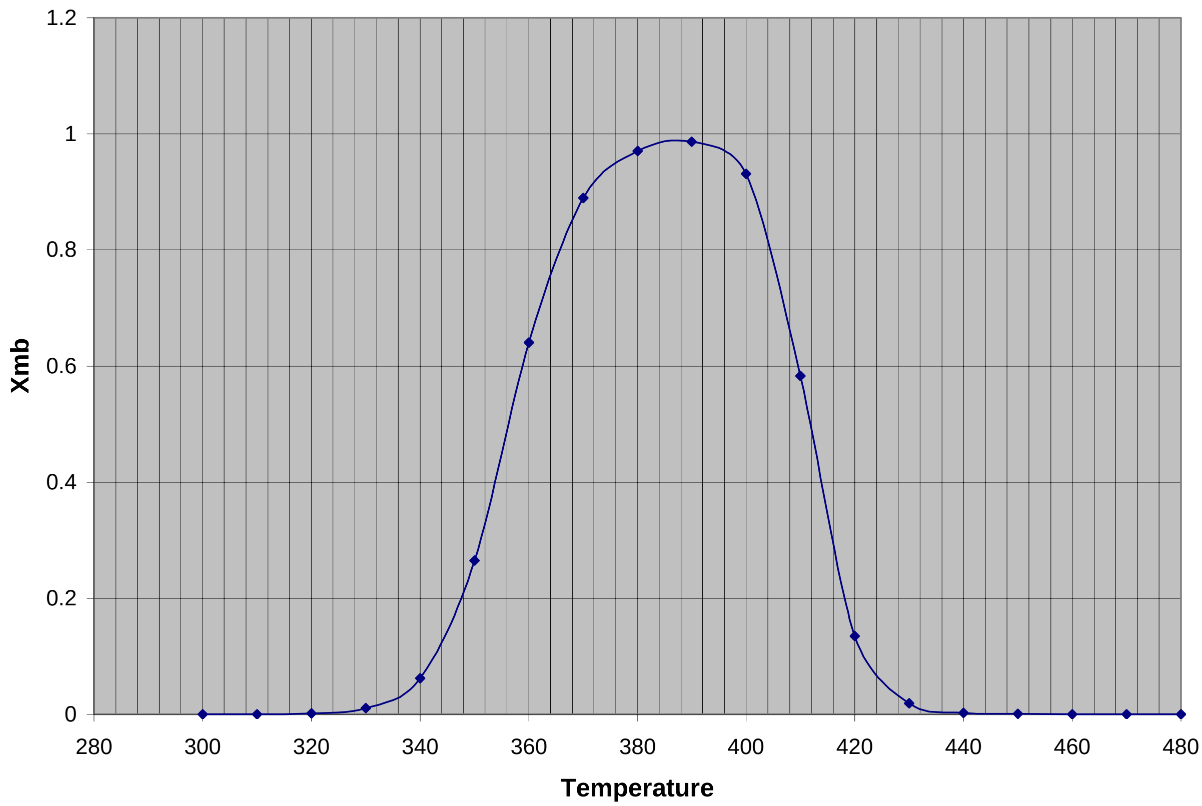
$UA = 4000$ cal/min K; $T_a = 37^0 C; C_{pA} = C_{pB} = 45$ cal/mol K; $\Delta H_{Rx} = -75$ kcal/mol A

$V = 100$ liters, $v_0 = 10$ lit/min, $F_{A0} = 10$ mol/min

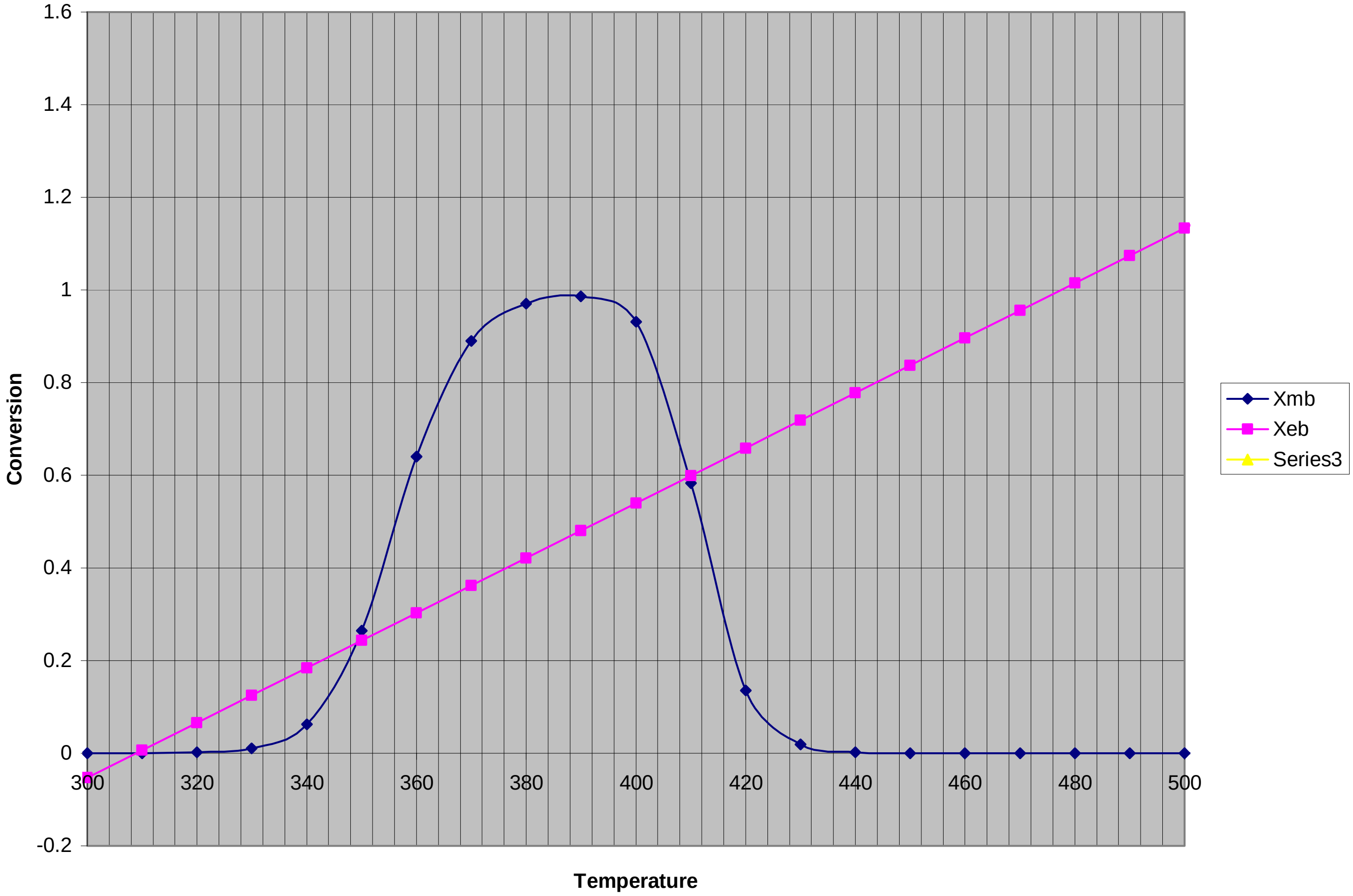
Using the mole balance equation only, a relationship between conversion in the reactor and the reactor temperature can be obtained. This relationship is shown in the following figure as a plot of X_{MB} versus reactor temperature.

a. Show the equation that was used to create this plot.
b. Develop an energy balance equation for the CSTR. Show how many steady states are possible and determine the conversions and temperatures at the *stable* steady states.
c. Identify at least two strategies for obtaining higher conversions in this unit.

20 points



$$X_{EB} = \frac{UA(T - T_a)/F_{A0} + \tilde{C}_{pA}(T - T_0)}{-\Delta H_{Rx}}$$ is the energy balance equation. Superimpose on the curve given.



Three steady states – X=0, T=310K; X=0.22, T=350K; X=0.6,T=412 K

Two strategies – Increase U or reduce Ta

5. A first-order, gas-phase reaction $A \rightarrow \frac{B}{2}$ is performed in a PBR at 450 K and 4 atm. Feed rate is 4 mol/s containing 10% A and the rest inerts. The PBR is packed with 10 mm diameter spherical porous particles. The intrinsic reaction rate is given as: $r_A^{'} = 2\,C_A$ mol/kg(cat)-s. Bulk density of the catalyst is 2.5 kg/liter. The diffusivity is 0.075 cm^2/s. The pressure drop parameter alpha (α) is found to be $0.001\,kg^{-1}$.
   a. What is the value of the internal effectiveness factor?
   b. How much catalyst (kg) is required to obtain 15% conversion in the reactor?
   c. Find the pressure at the exit of the reactor.

20 points

$$\phi = R\sqrt{\frac{k\rho}{D}} = 0.5\sqrt{\frac{2 \cdot 2.5}{0.075}} = 4.0824$$

$$\eta = \frac{3}{\phi^2}\left(\frac{\phi}{\tanh\phi} - 1\right) = 0.5553$$

$$F_{A0}\frac{dX}{dW} = -r_A^{'} = kC_A = \eta k C_{A0}\frac{(1-X)}{(1+\varepsilon X)}\frac{P}{P_0}$$

$$= \eta k C_{A0}\frac{(1-X)}{(1+\varepsilon X)}(1-\alpha W)^{1/2}$$

$$\frac{dX}{dW} = \frac{\eta k C_{A0}}{F_{A0}}\frac{(1-X)}{(1+\varepsilon X)}(1-\alpha W)^{1/2}$$

$$\int_0^X \frac{1+\varepsilon X}{1-X}dX = \frac{\eta k}{v_0}\int_0^W (1-\alpha W)^{\frac{1}{2}} dW$$

$$(1+\varepsilon)\ln\frac{1}{(1-X)} - \varepsilon X = \frac{\eta k}{v_0}\frac{2}{3\alpha}\left[1-(1-\alpha W)^{3/2}\right]$$

$$v_0 = 36.9\frac{lit}{s};\ X = 0.15;\ \varepsilon = -0.05;\ \alpha = 0.001;\ \eta = 0.5553;$$

$$k = 2$$

$$W = 5.387\ kg$$

$$\frac{P}{P_0} = (1-\alpha W)^{1/2} = 0.9973$$

$$P = 3.989\ atm$$