Instructions

1. Write your name at the top of each answer sheet and on the front page of the exam questions.
2. Start each problem at the top of a new page.
3. The exam consists of three equally weighted problems.
4. Useful integrals and equations are listed beginning on page 3.
5. Return the exam questions or you will receive a grade of zero.

R = 82.06 cm^3-atm/gmole-K; R = 1.987 cal/gmole-K

The van't Hoff relation is $\frac{\partial \ln K}{\partial T} = \frac{\Delta H^\circ}{RT^2}$

Problem 1 (34 points) The gas-phase reaction

$$\mathrm{A} \rightarrow 2\mathrm{B} \qquad r = kc_A \qquad k = 4.08 \times 10^9 \exp\left(\frac{-27,000 \text{ cal/gmol}}{RT}\right) \text{ sec}^{-1}$$

is carried out in a PFR operating isothermally at 650 K and at a constant pressure of 3 atm. The feed consists of a mixture of A and an inert that is twice the concentration (and molar flowrate) of A. There is a disruption in the upstream process and the inlet flowrate of A is now reduced by a factor of 2 (*i.e.,* $N_{Af,new} = 0.5N_{Af}$). You must keep the conversion of A in the reactor at 90%. You cannot change the pressure or the reactor volume so you decide to change the temperature. What temperature do you recommend to maintain a constant conversion of A?

Problem 2 (33 points) Consider the reversible liquid-phase reaction

$$\mathrm{A} \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} \mathrm{B} + \mathrm{C} \qquad r = k_1 c_A - k_{-1} c_B c_C$$

that will be conducted in a steady-state CSTR. The inlet concentrations are $c_{Af} = 6.5$ gmol/liter, $c_{Bf} = c_{Cf} = 0$. At 328 K, $k_1 = 3.8 \times 10^{-3}$ sec^{-1} and $k_{-1} = 0.3 \times 10^{-4}$ liter/gmol-sec. Because this is liquid-phase you may assume constant density.

Part (a) What residence time is required to get within 20% of the equilibrium concentration of A ($c_{A,eq}$), *i.e.,*

$$\frac{c_A - c_{A,eq}}{c_{A,eq}} = 0.2$$

Part (b) What residence time is required to realize the equilibrium concentration of A?

Problem 3 (33 points) The water-gas shift reaction is used commercially to generate hydrogen from carbon monoxide in a catalytic reaction.

$$CO + H_2O \rightleftharpoons CO_2 + H_2$$

The reaction is operated under conditions that produce an equilibrium mixture. You can select one of two catalysts for the process. Catalyst 1 is based on Fe-Cr, is thermally unstable and cannot be operated above 500 K. Catalyst 2 is based on Cu-ZnO and needs to be operated at 700 K to prevent other gas phase impurities from contaminating the surface. Using the data below at 600 K, which catalyst would you choose to maximize the amount of H_2 produced? Explain your answer and provide a justification for your choice.

	ΔG_f^{600} (kcal/mol)	ΔH_f^{600} (kcal/mol)
CO	-39.36	-26.33
H_2O	-51.16	-58.50
CO_2	-94.45	-94.12
H_2	0	0

Batch Reactor

$$\frac{d(V_R c_j)}{dt} = \sum_i^{n_{rxns}} \nu_{ij} r_i V_R$$

$$\frac{dT}{dt} = \frac{UA(T_a - T) - \sum_i^{n_{rxns}} r_i \Delta H_{Ri} V_R}{V_R \sum_j^{n_{components}} c_j \overline{C}_{pj}}$$

Plug Flow Reactor

$$\frac{d(Qc_j)}{dV} = \sum_i^{n_{rxns}} \nu_{ij} r_i$$

$$\frac{dT}{dV} = \frac{\frac{2}{R} U(T_a - T) - \sum_i^{n_{rxns}} r_i \Delta H_{Ri}}{Q \sum_j^{n_{components}} c_j \overline{C}_{pj}}$$

Stirred Tank Reactor

$$\frac{d(V_R c_j)}{dt} = Q_f c_{jf} - Q c_j + \sum_i^{n_{rxns}} \nu_{ij} r_i V_R$$

$$\frac{dT}{dt} = \frac{UA(T_a - T) - \sum_i^{n_{rxns}} r_i \Delta H_{Ri} V_R + Q_f \sum_j^{n_{components}} c_{jf}(\overline{H}_{jf} - \overline{H}_j)}{V_R \sum_j^{n_{components}} c_j \overline{C}_{pj}}$$

Continuous Stirred Tank Reactor at Steady-state (constant phase)

$$0 = Q_f c_{jf} - Q c_j + \sum_i^{n_{rxns}} \nu_{ij} r_i V_R$$

$$0 = UA(T_a - T) - \sum_i^{n_{rxns}} r_i \Delta H_{Ri} V_R + \sum_j^{n_{components}} Q_f c_{jf} \int_T^{T_f} \overline{C}_{pj} dT$$

$$\int \frac{1}{a+bx}dx = \frac{1}{b}\ln(a+bx)$$

$$\int (a+bx)^n\,dx = \frac{(a+bx)^{n+1}}{(n+1)b} \qquad ; n \neq -1$$

$$\int \frac{dx}{(a+bx)(a'+b'x)} = \frac{1}{ab'-a'b}\ln\left(\frac{a'+b'x}{a+bx}\right)$$

$$\int \frac{a+bx}{a'+b'x}dx = \frac{bx}{b'} + \frac{ab'-a'b}{b'^2}\ln\left(a'+b'x\right)$$

$$\int \frac{(a+bx)^m}{(a'+b'x)^n}dx = \frac{-1}{(n-1)b'}\left[\frac{(a+bx)^m}{(a'+b'x)^{n-1}} - mb\int \frac{(a+bx)^{m-1}}{(a'+b'x)^{n-1}}dx\right]$$

$$\int x^m\,(a+bx)^n\,dx = \frac{x^{m+1}\,(a+bx)^n}{m+n+1} + \frac{an}{m+n+1}\int x^m\,(a+bx)^{n-1}\,dx$$

Simpson's three-eighth's rule for numerical integration:

$$\int_{X_0}^{X_3} f(X)dX = \frac{3h}{8}\left[f(X_0)+3f(X_1)+3f(X_2)+f(X_3)\right]$$

where:

$$h = \frac{X_3 - X_0}{3} \qquad X_1 = X_0 + h \qquad X_2 = X_0 + 2h$$

Integration of $N+1$ points, where N is even:

$$\int_{X_0}^{X_N} f(X)dX = \frac{h}{3}\left[f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + \ldots + 4f_{(N-1)} + f_N\right]$$

where:

$$h = \frac{X_N - X_0}{N}$$