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

It takes 2.52 hr for 75% of A to react in a batch reactor at 338 K and it takes 0.19 hr for 75% of A to react at 363 K when the reactor is charged with 2.5 mol/l of A ($c_{Ao} = 2.5$ mol/l) and 4 mol/l of B. The liquid-phase reaction is

$$\mathrm{A} + \mathrm{B} \longrightarrow \mathrm{C} \qquad r = kc_Ac_B$$

What reaction temperature is required to realize a conversion of 90% of A in 0.2 hr if the feed is 3.5 mol/l of A and 4 mol/l of B?

Problem 2

Consider the liquid-phase reaction

$$\mathrm{A} \longrightarrow \mathrm{B} \qquad r = kc_A^2$$

A 5,000 liter plug flow reactor is fed with A at $c_{Af} = 2.5$ gmol/l at a flowrate of $Q = 1,000$ liter/min. Under these conditions the conversion of A is $x_A = 95\%$.

You are to conduct the same reaction using the same inlet feed and flowrate in a series arrangement of four different CSTRs. The CSTRs can be arranged anyway you wish and your objective is to maximize the conversion of A. The four reactors have volumes of 1,000, 2,000, 3,000 and 4,000 liters each and the combined volume of the cascade will be 10,000 liters. Determine which order to sequence the reactors to maximize the conversion of A, **AND** calculate this conversion. Also explain why this sequence should be the one that optimizes the conversion of A.

Table 1: Thermodynamic Data for Ethane Pyrolysis

Component	Temperature (K)	ΔG (kcal/mole)
C_2H_6	900	21.00
	1000	26.13
C_2H_4	900	26.35
	1000	28.25
H_2	900	0.0
	1000	0.0
H_2O	900	-47.36
	1000	-46.04

Problem 3

The thermal cracking of ethane

$$C_2H_6 \rightleftharpoons C_2H_4 + H_2$$

is typically performed in a steam diluent. Use the data in Table 1 to answer the following questions.

1. Prove that the reaction is either exothermic or endothermic and tell me which one it is.
2. What is the equilibrium mixture (in partial pressure) at 1000 K, 1 atm total pressure for a mixture that is initially 1 mole of ethane and 5 moles of steam.

Batch Reactor

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

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

Plug Flow Reactor

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

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

Stirred Tank Reactor

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

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

Continuous Stirred Tank Reactor (constant phase)

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

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

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

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

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

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

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

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

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:

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