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 4.
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

Problem 1 (34 points) Determine the operating temperature of a steady-state CSTR for the following set of liquid-phase reactions. The solution requires simultaneous solution of a set of equations and if you do not have a programmable calculator capable of solving the set of equations, you should show you have properly defined the problem by performing TWO iterations of a trial and error solution. In this trial and error solution, using a guess of $T = 370$ K, determine if this was the right guess and make one more iteration. If you have a programmable calculator, give us the answer.

		k_o (min^{-1})	E_a (cal/gmol)	ΔH_R (cal/gmol)
$A \xrightarrow{k_1} B$	$r_1 = k_1 c_A$	8.25×10^{12}	19,500	-23,000
$B \xrightarrow{k_2} C$	$r_2 = k_2 c_B$	2.27×10^{10}	17,500	-27,000
$B \xrightarrow{k_3} D + E$	$r_3 = k_3 c_B$	1.28×10^{9}	15,800	-19,000

The process parameters are listed below. The feed is pure A.

Parameter	Value	Units
V_R	1,000	liter
$\bar{C}_{pA}$	45	cal/gmol-K
Q_f	100	liter/min
T_f	338	K
T_a	323	K
UA	377,300	cal/min-K
c_{Af}	5.0	gmol/liter

Problem 2 (33 points) The reaction

$$H_2 + Br_2 \rightleftharpoons 2HBr$$

serves as one of the classics to illustrate how statements of mass action, such as listed above, actually proceed by a series of elementary reactions. Use the mechanism of elementary reactions presented below and the concepts developed in the text and in class to show that the rate of HBr formation (R_{HBr}) is given by

$$R_{\mathrm{HBr}} = \frac{k c_{H_2} c_{Br_2}^{0.5}}{1 + k' \frac{c_{HBr}}{c_{Br_2}}}$$

where k and k' are effective rate constants **AND** relate these effective rate constants to the rate constants for the individual elementary reactions. Note the first reaction, which is reversible, cannot be treated as being at equilibrium. Also, Br and H atoms are reaction intermediates. List any assumptions you make,

$$Br_2 \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} 2Br$$

$$Br + H_2 \xrightarrow{k_2} H + HBr$$

$$H + Br_2 \xrightarrow{k_3} Br + HBr$$

$$H + HBr \xrightarrow{k_4} H_2 + Br$$

Problem 3 (33 points) An adiabatic batch reactor is used for the liquid phase reaction.

$$\mathrm{A} \rightarrow \mathrm{B} \qquad r = kc_A \qquad k = A_1 \exp(-E_1/RT)$$

The kinetic constants, thermodynamic data and initial conditions are listed below. You may assume constant density and volume, and that the heat capacity and heat of reaction are independent of temperature. How long does it take for the conversion of A to equal $x_A = 0.9$?

Item	Units	Value
A_1	hr^{-1}	75.96×10^{15}
E_1	cal/gmol	30,400
ΔH_R	cal/gmol	-2,700
$\hat{C}_p$	cal/g-K	0.25
T_o	K	358
ρ	$\mathrm{g/cm^3}$	0.9
c_{Ao}	$\mathrm{gmol/cm^3}$	5×10^{-3}

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

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

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

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

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

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

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

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

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

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

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

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

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:

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