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

Problem 1 (34 points)
The following gas-phase reaction will be conducted in a PFR

$$2\text{ A} \rightarrow \text{B} \qquad r = kc_A^2$$

where,

$$k = 8 \times 10^{10} \exp(\frac{-16,500 \text{ cal/gmol}}{RT}) \text{ cm}^3\text{/gmol-sec}$$

The reactor operates at a constant pressure of 2 atm. The feed consists of pure A at at a volumetric flow rate of 50,000 cm^3/sec and enters at 650 K. The thermodynamic properties, which can be assumed constant with temperature, are given below.

Component	$\overline{C}_p$ (cal/gmol-K)	$\overline{H}_f$ (cal/gmol)
A	40	20,460
B	65	16,710

Part A: The temperature in the reactor cannot exceed 875 K or the product B becomes thermally unstable and explodes. Determine the conversion of A that is possible if the reactor operates adiabatically and a maximum temperature is set to 850 K.

Part B: List two possible ways to increase the conversion of A for the same maximum temperature constraint.

Problem 2 (33 points)
One possible mechanism for the gas-phase chlorination of chloroform

$$2\ CHCl_3 + Cl_2 \rightarrow 2\ CCl_4 + 2\ HCl$$

involves the following set of elementary reactions

$$Cl_2 \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} 2\ Cl$$

$$Cl + CHCl_3 \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} HCl + CCl_3$$

$$CCl_3 + Cl_2 \underset{k_{-3}}{\overset{k_3}{\rightleftharpoons}} CCl_4 + Cl$$

$$CCl_3 + Cl \overset{k_4}{\rightarrow} CCl_4$$

$$2\ CCl_3 \overset{k_5}{\rightarrow} C_2Cl_6$$

Part A: Determine the rate of production of CCl_4 in terms of stable molecules. The Cl and CCl_3 radicals are reaction intermediates. Under the conditions of the experiments Reaction 1 is so fast it can be assumed to be at equilibrium.

Part B: This reaction has been studied in a batch reactor charged with 94.4 Torr of Cl_2 and $CHCl_3$ (the total reactor pressure was 116.7 Torr initially). List the necessary design equations needed to determine the partial pressure of Cl_2 versus time. You may assume the reactor is isothermal.

Problem 3 (33 points)
The liquid-phase series reactions

$$\mathrm{A} \xrightarrow{k_1} \mathbf{B} \xrightarrow{k_2} \mathbf{C} \qquad r_1 = k_1 c_A \qquad r_2 = k_2 c_B$$

$$k_1 = 3.16 \times 10^{14} \exp(-12,500/T)\ \mathrm{min}^{-1};\ \mathrm{T\ in\ K}$$

$$k_2 = 2.52 \times 10^{9} \exp(-8,500/T)\ \mathrm{min}^{-1};\ \mathrm{T\ in\ K}$$

are to be carried out in a steady-state CSTR. The feed enters at 45 °C and consists of pure A at a concentration of $c_{Af} = 5$ mol/liter. Determine the temperature of the cooling fluid, which will be constant, that is required for the reactor to operate at 75 °C.

Parameter	Value	Units
$\rho \times Q_f$	93,000	g/min
ΔH_{R1}	-6,200	cal/gmol
ΔH_{R2}	8,000	cal/gmol
V_R	1,000	liter
Q_f	100	liter/min
$\hat{C}_{Pf}$	0.22	cal/g-K
U	0.65	cal/min-cm^2-K
A	15,400	cm^2

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)

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

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

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

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

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

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

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

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

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:

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