

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.

$$R = 82.06 \text{ cm}^3\text{-atm/gmole-K}; R = 1.987 \text{ cal/gmole-K}$$

**Problem 1 (34 points)**

The following gas-phase reaction will be conducted in a PFR



where,

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

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

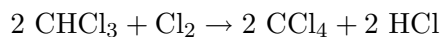
Component	$\bar{C}_p$ (cal/gmol-K)	$\bar{H}_f$ (cal/gmol)
A	40	20,460
B	65	16,710

**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.

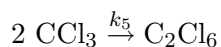
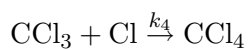
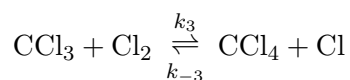
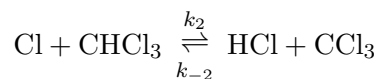
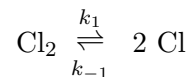
**Part B:** List two possible ways to increase the conversion of A for the same maximum temperature constraint.

**Problem 2 (33 points)**

One possible mechanism for the gas-phase chlorination of chloroform



involves the following set of elementary reactions

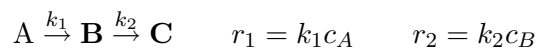


**Part A:** Determine the rate of production of  $\text{CCl}_4$  in terms of stable molecules. The  $\text{Cl}$  and  $\text{CCl}_3$  radicals are reaction intermediates. Under the conditions of the experiments Reaction 1 is so fast it can be assumed to be at equilibrium.

**Part B:** This reaction has been studied in a batch reactor charged with 94.4 Torr of  $\text{Cl}_2$  and  $\text{CHCl}_3$  (the total reactor pressure was 116.7 Torr initially). List the necessary design equations needed to determine the partial pressure of  $\text{Cl}_2$  versus time. You may assume the reactor is isothermal.

**Problem 3 (33 points)**

The liquid-phase series reactions



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

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

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
$\Delta H_{R1}$	-6,200	cal/gmol
$\Delta H_{R2}$	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 <sup>2</sup> -K
$A$	15,400	cm <sup>2</sup>

**Batch Reactor**

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

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

**Plug Flow Reactor**

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

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

**Stirred Tank Reactor**

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

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

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

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

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

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

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

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

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

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

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

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

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

where:

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

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

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

where:

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