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) Consider the chlorination of ethane

$$Cl_2 + C_2H_6 \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} 1,1-C_2H_2Cl_2 + 2H_2$$

The thermodynamic properties are

Component	ΔH_f^{600K} (kcal/mol)	ΔG_f^{600K}
chlorine	0.0	0.0
ethane	-23.29	5.96
1,1-dichloroethylene	-0.33	11.61
hydrogen	0.0	0.0

in which ΔH_f^{600K} and ΔG_f^{600K} are the heats of formation and the Gibbs free energy of formation of the compounds at 600 K from the elements, respectively. You need to find the temperature at which the mole fraction of chlorine is 0.001 at equilibrium for the following two conditions.

(a) If a constant pressure (1 atm) batch reactor is charged with a mixture of chlorine:ethane:dichloroethylene:hydrogen that is 0.2:0.8:0:0.

(b) If a constant pressure (1 atm) batch reactor is charged with a mixture of chlorine:ethane:dichloroethylene:hydrogen that is 0.2:0.4:0:0.4.

Problem 2 (33 points) The reaction of chlorine with propylene to produce dichloropropane will be conducted in an isothermal PFR operating at 2 atm of total pressure.

$$\mathrm{Cl_2} + \mathrm{C_3H_6} \longrightarrow \mathrm{C_3H_6Cl_2}$$

where:

$$r = kP_{C_3H_6}P_{Cl_2} \qquad k = 11.7\exp(-3,452/T)$$

P in atm, T in Rankine, and the units of k are lbmole/(hr-ft^3-atm^2). The feed consists of a 4:1 molar ratio of propylene to chlorine at a total molar flow of 0.85 lbmole/hr. Find the temperature that will lead to 90% conversion of chlorine in a 25 ft-long reactor that is 4 inches ID.

Problem 3 (33 points) The following liquid-phase reactions take place in a steady-state CSTR.

$$\mathrm{A} \xrightarrow{k_1} \mathrm{B} \xrightarrow{k_2} \mathrm{C} \xrightarrow{k_3} \mathrm{D}$$

$$\xrightarrow{k_4} \mathrm{E} \xrightarrow{k_5} \mathrm{F}$$

where:

Reaction	Rate Constant
$r_1 = k_1 c_A$	$k_1 = 3.0$ hr^{-1}
$r_2 = k_2 c_B$	$k_2 = 2.5$ hr^{-1}
$r_3 = k_3 c_C$	$k_3 = 2.0$ hr^{-1}
$r_4 = k_4 c_B$	$k_4 = 4.5$ hr^{-1}
$r_5 = k_5 c_E$	$k_5 = 1.5$ hr^{-1}

(c) Determine the concentration of E (c_E) exiting this reactor if the feed contains only A at a concentration $c_{Af} = 7$ moles/liter and the residence time is $\theta = 2.16$ hr.

(d) Discuss what process conditions you would consider and how you would go about selecting a set of conditions that would maximize the production of E and minimize the production of C, D and F.

Design Equations

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

$$\frac{d(Q c_j)}{dV} = \sum_{i}^{n_{rxns}} \nu_{ij} r_i$$

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

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)

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

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

Useful Integrals

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

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

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

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

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

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

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

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

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:

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