

Instructions

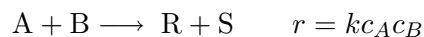
1. Write your name at the top of each answer sheet and on the front page of the exam questions.
2. Start each problem at the top of a new page.
3. The exam consists of three equally weighted problems.
4. Useful integrals and equations are listed beginning on page 4.
5. Return the exam questions or you will receive a grade of zero.

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

The van't Hoff relation is $\frac{\partial \ln K}{\partial T} = \frac{\Delta H^\circ}{RT^2}$

Problem 1

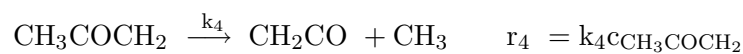
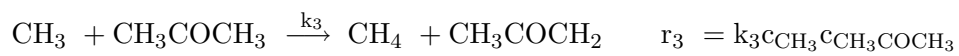
The irreversible aqueous-phase reaction



is carried out isothermally as follows. Equal volumetric flowrates of two liquid streams are introduced into a 30 lit CSTR. One stream contains 0.020 mol A/lit, and the other contains 1.40 mol B/lit. The CSTR effluent then passes through a plug flow reactor. We measure the concentration of the R species in the effluent of the CSTR and it is 0.002 mol R/lit. What must the volume of the plug flow reactor be in order to achieve 36% conversion of the A in the system (the CSTR in series with the PFR).

Problem 2

The thermal decomposition of acetone involves the following gas phase reactions.

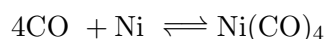


These reactions will be carried out in a constant pressure, isothermal PFR. The reactor operates at 1 atm and the feed is an acetone:nitrogen mixture with a molar ratio of 1:4.

Develop the necessary design equations needed to follow the molar flow of acetone and determine the effluent composition from the reactor. It will be necessary for you to define all terms and specify how you would calculate any variables in the balances for you to receive full credit.

Problem 3

Nickel tetracarbonyl is known to form in stainless steel tubing according to the following reaction between gaseous CO and Ni in the steel alloy.



Nickel tetracarbonyl is a gas and is extremely toxic so it must be destroyed before the gas can be vented from the tubing. The following thermodynamic data are available for the reaction written above.

Temperature (K)	ΔG (cal/gmole)
318	-4,621
338	-2,519
358	-477
378	1,568
398	3,623
418	5,630
438	7,736

- (a) Use the thermodynamic data to determine if the reaction, as listed above, is endothermic or exothermic. Be sure to show your work and explain your reasoning.
- (b) Determine the temperature at which the equilibrium mole fraction of nickel tetracarbonyl is 1 ppm (1×10^{-6}) for a total pressure of 1 atm in an isothermal closed system that is initially charged with pure CO. You may assume the activity of Ni is unity.

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

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

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)

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

Useful Integrals

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

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

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

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

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

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

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:

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