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

The following gas-phase reaction operates at equilibrium in a constant pressure reactor.

$$N_2 + 3H_2 \rightleftharpoons 2NH_3$$

The feed only contains a 3:1 molar mixture of H_2:N_2. The equilibrium constant at 298 K is $K = 5.27 \times 10^5$ and the heat of reaction, which may be assumed constant, is $\Delta H = -23,000$ cal/mol. Determine the temperature to operate the reactor at a pressure of 300 atm that will lead to the mole fraction of NH_3 being 70 %, (*i.e.*, $y_{NH_3} = 0.70$).

Problem 2

Consider the liquid-phase reaction

$$\mathrm{A} + \mathrm{B} \longrightarrow \mathrm{C} \qquad r = k c_A c_B \qquad k = 6.35 \times 10^{15} \exp(-26,000/RT)$$

where the units on k are liter/gmol-hr, T is in degrees Kelvin and $R = 1.987$ cal/gmol-K. This reaction will be conducted in a 1000-liter batch reactor. The reactor is operated isothermally at 358 K and you may assume constant density.

(a) What time is required to acheive 95% conversion of A ($x_A = 0.95$) if the reactor is charged with A at a concentration of $c_{Ao} = 5$ gmol/l and B at a concentration of $c_{Bo} = 10$ gmol/l?

(b) What time is required to achieve 95% conversion of A ($x_A = 0.95$) if the reactor is charged with A at a concentration of $c_{Ao} = 5$ gmol/l and B at a concentration of $c_{Bo} = 5$ gmol/l?

(c) Explain why the times calculated above are so different.

Problem 3

Consider the series, first-order, liquid-phase reactions.

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

$$\begin{array}{ll} r_1 = k_1 c_A & k_1 = 0.95 \text{ min}^{-1} \\ r_2 = k_2 c_B & k_2 = 0.10 \text{ min}^{-1} \\ r_3 = k_3 c_C & k_3 = 0.30 \text{ min}^{-1} \end{array}$$

(a) Determine the residence time in the CSTR that maximizes the production of B if the same feed contains pure A at a concentration of $c_{Af} = 5$ gmol/l.

(b) What is the maximum concentration of B that forms at this residence time?

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)

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

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

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

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

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

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

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

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

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:

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