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 five problems; they are equally weighted.
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 $cm^3$-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 leads to a mole fraction of $NH_3$ of 0.7 ($y_{NH_3} = 0.70$).

**Problem 2**
Determine the mass of catalyst required to achieve a conversion for A of $x_A = 0.8$ in an isothermal fixed bed reactor for the second order reaction. Both A and B are gases.

$$A \xrightarrow{k} B \qquad r = kc_A^2 \qquad k = 1.3 \times 10^5 \text{ cm}^3\text{/gmol-sec}$$

The catalyst is spherical, with a radius of $R = 0.45$ cm. The feed consists of pure at a concentration of $c_{Af} = 1.11 \times 10^{-5}$ gmol/$cm^3$ and a molar flow of $N_{Af} = 0.8$ gmol/sec. The effective diffusivity of A is $D_A = 0.008$ $cm^2$/sec. The bed porosity is $\epsilon_B = 0.41$. The bed density is $\rho_B = 0.40$ g/$cm^3$ You may assume the bulk fluid and the pellet surface concentrations are equal.

**Problem 3**

The reaction

$$\mathrm{A} + \mathrm{B} \rightleftharpoons \mathrm{C} + \mathrm{D}$$

is carried out in a series of adiabatic tubular reactors with interstage cooling as shown in Figure 1. The gaseous feed is equimolar in A and B and enters each reactor at 27 °C. The heat is removed between the reactors at a rate of $\dot{Q} = -87.5$ kcal/min. The following data apply

| | |
|---|---|
| $\Delta H_R$ | -30 kcal/mol |
| $C_P$ | 25 cal/mol-K |
| $K$ at 50 °C | $5.0 \times 10^5$ |
| $N_{Af}, N_{Bf}$ | 10 mol/min |
| $\dot{Q}$ | -87.5 kcal/min |

State any assumptions you make while solving

**(a)** What is the outlet temperature of the first reactor?

**(b)** What is the conversion of A at the outlet of the first reactor?

**(c)** Is the first reactor close to equilibrium at the exit?

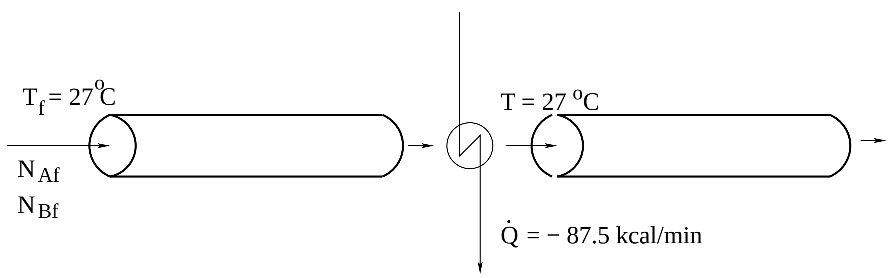


Figure 1: Tubular Reactors with Interstage Cooling.

**Problem 4**

Determine the isothermal(625 K) plug flow reactor volume required for 80 % of A to react for the following second-order gas phase reaction.

$$\mathrm{A} \rightarrow \mathrm{B} + \mathrm{C} \qquad r = kc_A^2 \qquad k = 800\ \mathrm{cm^3/gmol\text{-}sec}$$

The feed is pure A at a total pressure of 2 atm and a feed rate of $N_{Af} = 2.5$ gmol/sec. You may assume a constant pressure.

**Problem 5**

A pulse input experiment was performed on a flow reactor. The effluent pulse data ($c_{\text{pulse}}$) are tabulated below. Determine the effluent concentration for A from this reactor if $c_{Af} = 0.07$ gmol/liter for the liquid-phase reaction.

$$\text{A} \rightarrow \text{B} \qquad r = kc_A^2 \qquad k = 16.56 \text{ liter/gmol-min}$$

| $t$ (min) | $c_{\text{pulse}}$ ($\mu$mole/liter) | $t$ (min) | $c_{\text{pulse}}$ ($\mu$mole/liter) | $t$ (min) | $c_{\text{pulse}}$ ($\mu$mole/liter) |
|---|---|---|---|---|---|
| 0 | 0.00 | 7 | 7.40 | 14 | 0.10 |
| 1 | 0.20 | 8 | 3.00 | 15 | 0.02 |
| 2 | 0.50 | 9 | 1.50 | 16 | 0.00 |
| 3 | 0.75 | 10 | 1.10 | | |
| 4 | 2.10 | 11 | 0.80 | | |
| 5 | 6.50 | 12 | 0.50 | | |
| 6 | 8.90 | 13 | 0.20 | | |

**In general:**

$$\bar{\theta} = \int_0^\infty \theta p(\theta) d\theta \qquad \sigma^2 = \int_0^\infty (\theta - \bar{\theta})^2 p(\theta) d\theta$$

**For segregated flow**

$$c_s(\theta) = \int_0^\infty p(\theta) c(\theta) d\theta$$

**For CSTRs-in-series**

$$p(\theta) = \left(\frac{n}{\bar{\theta}}\right)^n \frac{\theta^{n-1}}{(n-1)!} \exp^{n\theta/\bar{\theta}} \qquad n = \frac{\bar{\theta}^2}{\sigma^2}$$

**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**

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

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

**Continuous Stirred Tank Reactor** (steady-state and constant phase)

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

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

For heterogeneous reactions one must determine the rate per unit volume of pellet.

$$R_{jp} = \frac{1}{V_p} \int_{V_p} R_j dV = -\frac{S_p}{V_p} D_j \left. \frac{dc_j}{dr} \right|_{r=R_p}$$

The dimensionless steady-state concentration within a symmetrical pellet is found with

$$\overline{\nabla}^2 \overline{c} + \left[ \frac{a^2 |R_{js}|}{c_{js} D_j} \right] \overline{R} = 0 \qquad \overline{R} = \frac{R_j}{R_{js}}$$

For a first-order reaction (A $\rightarrow$ B) with a spherical pellet surface concentration of $c_{\mathrm{A}s}$

$$c_{\mathrm{A}} = c_{\mathrm{A}s} \frac{R}{r} \times \frac{\sinh\left(\Phi(\frac{3r}{R})\right)}{\sinh(3\Phi)}$$

$$R_{\mathrm{A}p} = \frac{1}{\Phi} \left[ \frac{1}{\tanh 3\Phi} - \frac{1}{3\Phi} \right] \times (-k_1 c_{\mathrm{A}s})$$

$$\Phi = \frac{R}{3} \times \sqrt{\frac{k_1}{D_e}}$$

For some heterogeneous cases it is appropriate to use

$$\eta = \frac{R_j}{R_{js}}$$

$$\eta \approx \frac{1}{\Phi} \left[ \frac{1}{\tanh 3\Phi} - \frac{1}{3\Phi} \right]$$

$$\Phi = \frac{V_p}{S_p} \left[ \frac{n+1}{2} \times \frac{k_n c_s^{n-1}}{D_e} \right]^{0.5}$$

where

$$\tanh x = \frac{\mathrm{e}^x - \mathrm{e}^{-x}}{\mathrm{e}^x + \mathrm{e}^{-x}}$$

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

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

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

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

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

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

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:

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