

Instructions

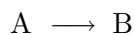
1. Write your name at the top of each answer sheet and on the front page of the exam questions.
2. Start each problem at the top of a new page.
3. The exam consists of three problems; they are not equally weighted.
4. Useful integrals and equations are listed beginning on page 3.
5. Return the exam questions or you will receive a grade of zero.

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

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

Problem 1

[40 POINTS.] The Hougen-Watson expression for the heterogeneous reaction



reduces to

$$r = kc_A^{1.5}$$

This reaction was studied in a 0.65 cm radius spherical pellet ($R = 0.65 \text{ cm}$) at 575K. When the partial pressure of A is 1 atm, the rate of production of A was found to be $R_A = -4.78 \times 10^{-6} \text{ mol/cm}^3\text{-sec}$. The diffusivity of A in the pellet is $D_A = 0.0075 \text{ cm}^2/\text{sec}$. What is R_A if the partial pressure of A is doubled to 2 atm?

Problem 2

[40 POINTS.] Determine the mass of catalyst required to realize a conversion of A_2 of 90% for the heterogeneous reaction



if the reaction is carried out in an isothermal fixed-bed reactor.

The reactor operates at 1 atm total pressure and 600 K. The feed is a 50:50 molar mixture of A_2 :B and the inlet molar flowrate of A_2 is $N_{A_2f} = 12 \text{ mol/sec}$. The catalyst is a spherical pellet with a radius of $R = 0.5 \text{ cm}$. The bed density is $\rho_B = 0.76 \text{ g/cm}^3$ and the bed porosity is $\epsilon_B = 0.31$. The diffusivity of A in the catalyst is $D_A = 0.008 \text{ cm}^2/\text{sec}$. You may neglect external transport limitations. The reactants and products are gases.

Problem 3**[20 POINTS.]**

- (a) Why does it take increasingly higher pressures to saturate a surface with a chemisorbed species as the temperature is increased?
- (b) Show how the steady state material balance in a pellet

$$D_e \nabla^2 c_j + R_j = 0$$

where, for example the Laplacian $\nabla^2 c_j$ in spherical coordinates is

$$\nabla^2 c_j = \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dc_j}{dr} \right)$$

reduces to the dimensionless form

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

- (c) Why was the characteristic length in a catalyst pellet defined to be

$$a = \frac{V_p}{S_p}$$

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:

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

General Information on Mass Transfer with Reaction

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

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

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

$$c_A = c_{As} \frac{R}{r} \times \frac{\sinh\left(\Phi\left(\frac{3r}{R}\right)\right)}{\sinh(3\Phi)}$$

$$R_{Ap} = \frac{1}{\Phi} \left[\frac{1}{\tanh 3\Phi} - \frac{1}{3\Phi} \right] \times (-k_1 c_{As})$$

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

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

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