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 cm^3-atm/gmole-K; R = 1.987 cal/gmole-K

Problem 1

The heterogeneously catalyzed reaction

$$2A \longrightarrow B$$

will be conducted in a cylindrical catalyst pellet. The rate of reaction is given by

$$r = \frac{kc_A^2}{(1 + Kc_A)^2}$$

Parameter	Value	Units
K	35,000	cm^3/mol
k	4.55×10^6	cm^3/mol-sec
D_A	0.095	cm^2/sec
pellet radius	0.15	cm
pellet length	0.30	cm

The external mass transfer rate is fast enough that the bulk fluid and the pellet exterior concentration are the same. If the external surface concentration is $c_A = 6.25 \times 10^{-5}$ gmol/cm^3, can you assume the concentration of A within the pellet is the approximately the same as the concentration at the pellet exterior surface? Why or why not? Justify your answer with suitable calculations.

Problem 2

Consider the catalytic reaction $A + B \longrightarrow P$ to preceed by two pathways. In the first, Mechanism 1 adsorbed A reacts with adsorbed B in the rate limiting step and the adsorbed B in the rate limiting step and the adsorption of A, B and P are fast enough they can be considered at equilibrium.

Mechanism 1

$$A_{(g)} + S \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} A_{(ads)}$$

$$B_{(g)} + S \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} B_{(ads)}$$

$$A_{(ads)} + B_{(ads)} \overset{k_3}{\longrightarrow} P_{(ads)} + S$$

$$P_{(g)} + S \underset{k_{-4}}{\overset{k_4}{\rightleftharpoons}} P_{(ads)}$$

In the second mechanism, Mechanism 2, adsorbed A reacts with gas phase B in the rate limiting step and the adsorption of A, B and P are fast enough they can be considered at equilibrium.

Mechanism 2

$$A_{(g)} + S \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} A_{(ads)}$$

$$B_{(g)} + S \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} B_{(ads)}$$

$$A_{(ads)} + B_{(g)} \overset{k_5}{\longrightarrow} P_{(ads)}$$

$$P_{(g)} + S \underset{k_{-4}}{\overset{k_4}{\rightleftharpoons}} P_{(ads)}$$

(a) Develop the Hougen-Watson (Langmuir-Hinshelwood) rate expressions for the rate of reaction of A (R_A) for each mechanism.

(b) Describe experiments you would perform to establish which mechanism is correct. Be sure to detail how the experimental data would be analyzed/interpreted.

Problem 3

The second-order heterogeneous reaction

$$\text{A} \xrightarrow{k} \text{B} \qquad r = kc_A^2 \qquad k = 1.3 \times 10^5 \text{cm}^3\text{-gmole}^{-1}\text{sec}^{-1}$$

is conducted in an isothermal fixed bed reactor over a spherical catalyst (pellet radius $R = 0.45$cm). The reactor feed contains pure A (a gas) at a concentration of $c_{Af} = 1.11 \times 10^{-5}$ gmole/cm^3 and a molar flow rate of $N_{Af} = 0.8$ gmole/sec. The pellet density is $\rho_p = 0.68$ g/cm^3, the bed density is $\rho_B = 0.40$ g/cm^3 and the bed porosity is $\epsilon_B = 0.41$. The effective diffusivity of A is $D_A = 0.008$ cm^2/sec. You may assume the bulk fluid and the pellet surface concentrations are equal.

Determine the mass of catalyst required for a conversion of A of $x_A = 0.85$