Chemical Kinetics and Reaction Engineering

MIDTERM EXAMINATION I
Question 1 of 2
Friday, February 19, 2010

The exam is 100 points total and 20% of the course grade.

Please read through the questions carefully before giving your response.

Question Number	Possible Points
1	50

Name:____

SID:____

You are allowed one 8.5” x 11” sheet of paper and a calculator for this exam. A list of (possibly) useful integrals is provided on the last page of this packet.

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Problem 1 (50 points)

Consider the following elementary, gas-phase reaction

$$A + 2B \rightarrow C$$

that occurs in a well-mixed, isothermal batch reactor with constant volume. The reactor is initially charged with an equimolar mixture of A and B, and the reaction rate constant at 273 K is 0.45 $L^2\ mol^{-2}\ min^{-1}$. Consider all species as ideal gases.

(i) (10 points) Derive an expression for the rate of depletion of A ($-r_A$) in terms of the conversion of A (X_A), the rate constant (k), and the inlet concentration of A (C_{A0}).

(ii) (15 points) You are to perform this reaction at 303 K and an initial pressure of 300 kPa. Calculate the time required to achieve 25% conversion for species A in this system.

(iii) (15 points) Consider now an isothermal system with variable volume and variable pressure. The initial volume (V_0) is 1.0 L, and the volume (V) varies with pressure (P) according to V = 0.6P. Develop expressions for the volume (V) and concentrations of A and B (C_A, C_B) as functions of the conversion of the limiting reactant in this system, and relevant feed parameters.

(iv) (10 points) For the case considered in part (iii), now derive an expression for ($-r_A$) solely in terms of the conversion of the limiting reactant, while evaluating numerically all other constants.

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List of Integrals

$$\int \frac{1}{(1-X)} dX = \ln\left(\frac{1}{1-X}\right)$$

$$\int \frac{1}{(1-X)^2} dX = \left(\frac{1}{1-X}\right)$$

$$\int \frac{1}{(1+aX)} dX = \frac{1}{a}\ln(1+aX)$$

$$\int \frac{1}{(1-X)(1-aX)} dX = \frac{\ln(X-1)-\ln(aX-1)}{a-1}$$

$$\int \frac{1}{(1-X)(1-aX)^2} dX = -\frac{(aX-1)\ln(a(X-1))+(1-aX)\ln(aX-1)+a-1}{(a-1)^2(aX-1)}$$

$$\int \frac{(1+bX)}{(1-aX)} dX = -\frac{abX+(a+b)\ln(aX-1)}{a^2}$$

$$\int \frac{(1+bX)^2}{(1-aX)} dX = -\frac{abX(a(bX+4)+2b)+2(a+b)^2\ln(aX-1)}{2a^3}$$

NAME
SID#

Chemical Kinetics and Reaction Engineering

MIDTERM EXAMINATION I
Question 2 of 2
Friday, February 19, 2010

The exam is 100 points total and 20% of the course grade.

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Question Number	Possible Points
2	50

Name:____

SID:____

You are allowed one 8.5" x 11" sheet of paper and a calculator for this exam.

NAME
SID#

Problem 2 (50 points)

Acid-catalyzed hydrolysis reactions are very common in the synthesis of many organic compounds and synthesis of biofuels. The overall reaction for this type of transformation for esters can be written as:

$$RCOOR' + H_2O \xrightarrow{H^+} RCOOH + R'OH$$

A mechanism for this reaction based on a sequence of elementary steps is:

$$RCOOR' + H^+ \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} RCOHOR'^+$$

$$RCOHOR'^+ \xrightarrow{k_2} RCOOH + R'^+$$

$$R'^+ + H_2O \xrightarrow{k_3} R'OH + H^+$$

where $k_1 = 1$ L mol^{-1} s^{-1}), $k_{-1} = 0.1$ s^{-1}, $k_2 = 0.05$ s^{-1} and $k_3 = 0.01$ L mol^{-1} s^{-1}).

(i) (15 points) Derive an expression for the overall reaction rate in terms of the concentration of reactants, products, protons (H^+) as well as the rate constants k_1, k_{-1}, k_2, k_3.

(ii) (5 points) Now consider the case in which reaction (2) is the rate-determining step. Draw a rate arrow diagram for the reaction, including the rates of all the steps involved in the mechanism as well as the overall reaction rate.

(iii) (5 points) Derive a simplified rate expression under these conditions where step 1 is quasi-equilibrated.

(iii) (5 points) If the only rate constant that appears in the overall reaction rate expression is k_1, how would your rate arrow diagram in (ii) change? Re-draw the rate arrow diagram of part (ii) under these new circumstances.

(iv) (10 points) Using your expression for part (i), calculate the time that a batch stirred tank reactor (BSTR) would need in order to hydrolyze 90% of RCOOR' in), if the reaction is carried out with a concentration of H^+ equal to 10^{-3} mol L^{-1}

(v) (10 points) Now consider that this reaction is conducted in a continuous stirred tank reactor (CSTR), with the same conversion and under the same conditions as part (iv). Is the residence time higher or lower than the time calculated in part (iv)? Explain why in 2 sentences or fewer. Answers without an explanation or answers exceedingly long will not receive credit.

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