04-CHEM-A4, CHEMICAL REACTOR ENGINEERING

DECEMBER 2015

3 hours Duration

1. If doubt exists as to the interpretation of any question, please submit with your answer a clear statement of any assumption(s) you make. If possible, please underline or enclose any such statement in a box.

2. This is an OPEN BOOK EXAM. However only the items listed below are permitted into the exam.
   - One textbook of your choice with notations listed on the margins etc but no loose notes are permitted into the exam.
   - your own unit conversion tables and/or mathematical tables such as a CRC Handbook.
   - a non-communicating, programmable electronic calculator using a small operating guide. Please write the name and model of your calculator on the first inside left-hand sheet of the exam workbook.

3. Answering any **four** questions will constitute a complete paper. Unless you indicate otherwise, only the first four answers as they appear in your answer booklet will be marked.

4. Each question is worth 25 points. Marking schemes are provided in brackets after each question.

5. Technical content is the key ingredient in your answers. However, no credit will be given for deriving rate expressions, or standard formulas that are available in the textbook. Clear writing is essential, particularly when explanations are required.

6. It will help the examiner if you could cite the origin of significant formula used – e.g., Fogler, eq. (3-44).

Marking Scheme – Four questions comprise a complete exam.

1. 25 points – a) 8 points, b) 17 points
2. 25 points
3. 25 points
4. 25 points – a) 12 points, b) 13 points
5. 25 points – a) 10 points, b) 12 points, c) 3 points

QUESTION 1

The following reactions are performed isothermally in the gas phase in a plug flow reactor (PFR):

$$A \rightarrow B \qquad r_{A1} = k_1 P_A$$

$$A \rightarrow 2C \qquad r_{A2} = k_2 P_A$$

$$A \rightarrow 3D \qquad r_{A3} = k_3 P_A$$

The reaction rate constants (in moles per second per cubic meter per bar) are given by:

$$k_1 = 5.4 \times 10^2\ e^{(-20{,}000/RT)}$$

$$k_2 = 6.5 \times 10^3\ e^{(-40{,}000/RT)}$$

$$k_3 = 2.1 \times 10^2\ e^{(-20{,}000/RT)}$$

where RT is in Joules per mole.

a) At what temperature should the reactor be operated to achieve a 20% selectivity for D (i.e., one mole of A reacts through reaction equation #3 for every five moles of A reacted)?

b) At this temperature, what reactor volume is required for a 10% yield of D (i.e., one mole of A reacts through reaction equation #3 for every ten moles of A fed to the reactor) if pure A is fed to the reactor at a rate of 2 moles per second? The reactor pressure is 1 bar.

QUESTION 2

A stream of methanol (**A**) in benzene at a concentration of 0.054 moles per liter is added at the rate of 3.78 liters per minute to a continuous stirred tank reactor (CSTR) containing 40 moles of triphenylmethylchloride (**B**) in dry benzene. The initial volume of the reactor is 378 liters. A reaction proceeds as follows:

$$CH_3OH\ (\mathbf{A}) + (C_6H_5)_3CCl\ (\mathbf{B}) \rightarrow (C_6H_5)_3COCH_3\ (\mathbf{C}) + HCl\ (\mathbf{D})$$

The reaction is essentially irreversible, and the reaction rate (in moles per liter per minute) is given by the equation:

$$\mathbf{r = 0.263C_A^2C_B}$$

Determine the concentration (in moles) of the product triphenylmethylether (**C**) as a function of time (in minutes).

QUESTION 3

A continuous stirred tank reactor (CSTR) and a plug flow reactor (PFR) are used to decompose a reactant **A** via a second-order process with rate constant of 2 x 10^{-3} liter per mole per second. The reaction is performed in the liquid phase. The inlet concentration of **A** to the reactor is 5 moles per liter at a flow rate of 0.02 liters per second. The volume of the CSTR is 2 liters and the volume of the PFR is 2 liters.

What order should the CSTR and PFR be placed in order to maximize conversion? Please show calculations. What is the maximum conversion?

QUESTION 4

The nitration of aromatic compounds is a highly exothermic reaction that generally uses catalysts that tend to be corrosive (like HNO_3/H_2SO_4). A less corrosive reaction employs nitrogen pentoxide (N_2O_5) as nitrating agent as shown below:

$$N_2O_5\ \mathbf{(A)} + 2C_6H_6\ \mathbf{(B)} \rightarrow 2C_6H_5NO_2\ \mathbf{(C)} + H_2O\ \mathbf{(D)}$$

The reaction rate is first order in A and second order in B, and the rate constant (in liters^2 per mole^2 per minute) is given by the equation

$$k = 0.090 \exp\{(\Delta E_a/R)(0.0033 - 1/T)\}$$

where ΔE_a is the activation energy, R is the universal gas constant and T is the temperature.

a) If this reaction is conducted in an adiabatic continuous stirred tank reactor (CSTR) at a volumetric flow rate of 1000 liters per minute, initial N_2O_5 concentration of 0.01 moles per liter, and at an initial temperature of 303 K, what is the reactor volume and space-time necessary to achieve 35% conversion of N_2O_5?

b) If this reaction is conducted in a continuous stirred tank reactor (CSTR) at a volumetric flow rate of 100 liters per minute and an initial N_2O_5 concentration of 0.1 moles per liter, what is the reactor volume and space-time necessary to reach 35% conversion of N_2O_5 if it is cooled to a temperature of 323 K. The heat transfer coefficient (UA_H) is 9000 Joules per minute per Kelvin.

DATA:

Heat of Reaction = -370.1 kJ/mol

Activation Energy = 40 kJ/mol

Specific Heat Capacity of N_2O_5 = 84.5 J/mol.K

Specific Heat Capacity of C_6H_6 = 137 J/mol.K

Specific Heat Capacity of $C_6H_5NO_2$ = 170 J/mol.K

Specific Heat Capacity of H_2O = 75 J/mol.K

Initial Molar Flow Rate of N_2O_5 = 10 mol/min

Initial Molar Flow Rate of C_6H_6 = 30 mol/min

QUESTION 5

The second-order reaction **A → R** is studied in a recycle reactor with a very large recycle ratio, and the following data are recorded:

Void Volume of Reactor = 1 liter

Weight of Catalyst Used = 3 grams

Feed Concentration of **A** to the Reactor (C_{A0}) = 2 mol/L

Feed Volumetric Flow Rate to the Reactor (v_0) = 1 L/hr

Concentration of **A** at Reactor Exit (C_{Aexit}) = 0.5 mol/L

a) Find the rate constant for this reaction. Please give units.

b) Assuming no recycle, calculate the amount of catalyst needed in a packed bed reactor for 80% conversion of 1000 L/hr of feed of concentration C_{A0} = 1 mol/L.

c) Repeat part (b) if the reactor is packed with 1 part catalyst to 4 parts inert solid. This addition of inerts helps maintain isothermal conditions and reduce possible hot spots.