# 04-CHEM-A4, CHEMICAL REACTOR ENGINEERING

December 2016

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) 5 points, b) 12 points, c) 8 points
2. 25 points
3. 25 points
4. 25 points – a) 5 points, b) 12 points, c) 8 points
5. 25 points – a) 9 points, b) 5 points, c) 11 points

## QUESTION 1

Consider the liquid phase reaction **A + B → Products**. The reaction rate equation is of the form

$$-r_A = kC_AC_B/(1 + K_AC_A)^2$$

Reactant B is present in substantial excess, so that $C_B$ does not change appreciably as reactant A is consumed.

**a)** The value of reaction rate ($-r_A$) goes through a maximum as $C_A$ is increased. At what value of $C_A$ does this maximum occur?

**b)** The concentration of A in the feed to a continuous reactor is $C_{A0} = 1.5/K_A$. The concentration of A in the outlet is $0.5/K_A$. Plot a graph of $(1/-r_A)$ versus $C_A$ that covers this range of concentration. One ideal continuous reactor will be used to carry out this reaction. Should it be a continuous stirred tank reactor (CSTR) or a plug flow reactor (PFR)? Explain your answer.

**c)** Would your answer to Part (b) be different if the inlet concentration was $C_{A0} = 1.5/K_A$ and the outlet concentration of A is $1/K_A$? Explain your answer.

## QUESTION 2

An adiabatic mixed-flow reactor processes 56.64 liters per minute of a liquid feed containing reactant R and inerts I flowing at a rate of 0.67 mol/min and 0.33 mol/min, respectively. In the reactor, reactant R gives products S and T by the elementary reaction **A → S + T**. Feed enters the reactor at 300 K, and the data on the system are as follows:

**Heat Capacities**: For R → 7 cal/mol °C; For S → 4 cal/mol °C; For T → 4 cal/mol °C; For I → 8 cal/mol °C

**Rate Constant**: $k = 0.12\ hr^{-1}$ at 298 K

**Activation Energy**: $E_a = 25$ kcal/mol

**Heat of Reaction**: $\Delta H_r = -333$ cal/mol of R

Calculate the volume of the reactor required to achieve 90% fractional conversion of R.

## QUESTION 3

The irreversible reaction **A → B** takes place in a solvent, and the kinetics of the reaction have been studies at concentrations of A from 2.0 mol/liter to 0.25 mol/liter. Over this range, the kinetic data are well correlated by the rate equation

$$-r_A = kC_A^{0.5}$$

In an ideal isothermal batch reactor operating at 25 °C, the concentration of A drops from an initial $C_{A0}$ of 2.0 mol/liter to 1.0 mol/liter in 15 minutes. When this reactor operates at 50 °C, it takes 20 seconds for the concentration of A to drop from an initial $C_{A0}$ of 2.0 mol/liter to 1.0 mol/liter.

What will the concentration of A be in an ideal batch reactor operating isothermally at 40 °C after 10 minutes if the initial concentration $C_{A0}$ is 2.0 mol/liter?

## QUESTION 4

The irreversible gas-phase reaction **A → B** is carried out in a fixed-bed catalytic reactor that operates as an ideal plug flow reactor (PFR). The reaction is second order in A ($-r_A = kC_A^2$) and the value of the rate constant (k) is $2.5 \times 10^{-3}$ $m^6$ per mole per kg of catalyst per second. The concentration of A in the feed to the reactor is 12 $mol/m^3$, and the volumetric flow rate is 0.5 $m^3/s$. The total pressure is 1 atm and pressure drop through the reactor can be neglected.

**a)** If the reaction is controlled by intrinsic kinetics, what weight of catalyst is required to achieve 90% conversion of A?

**b)** The catalyst particles are in the shape of rings. The outer diameter is 2 cm, the inner diameter is 1 cm, and the length is 2 cm. The particle density of the catalyst is 3000 $kg/m^3$ and the effective diffusivity of A in the catalyst particle is $10^{-7}$ $m^2/s$. Estimate the values of the effectiveness factor at the very beginning of the bed and at the very end of the bed. You may assume that external transport resistances are negligible, and that catalyst particles are isothermal.

**c)** If the external transport resistances are negligible, what weight of catalyst is required to achieve 90% conversion of A when the internal transport resistances are taken into account?

## QUESTION 5

A fluid is flowing at a rate of 0.1 liter/min through a reactor vessel at steady state. The response to a pulse input of tracer at t = 0 is given the table below.

| Time (min) | Outlet Concentration of Tracer (mmol/liter) |
|---|---|
| 0 | 0 |
| 1 | 0 |
| 2 | 0 |
| 3 | 1 |
| 4 | 2 |
| 5 | 8 |
| 6 | 18 |
| 7 | 25 |
| 8 | 22 |
| 9 | 19 |
| 10 | 16 |
| 11 | 13 |
| 12 | 10 |
| 13 | 7 |
| 14 | 5 |
| 15 | 3 |
| 16 | 2 |
| 17 | 1 |
| 18 | 0 |
| 19 | 0 |

a) How much tracer (in mmoles) was injected into the reactor vessel?

b) What is the volume of the reactor vessel?

c) What is the variance of the external-age distribution?