04-CHEM-A4, CHEMICAL REACTOR ENGINEERING

MAY 2014

- 1) If you have any doubt as to the interpretation of a 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) Open Book Exam: You may bring to this examination
 - the official designated textbook by Fogler any edition (annotated in margins, etc. as desired).
 - your own unit conversion tables and/or mathematical tables, (such as a CRC Handbook).
 - a non-communicating, programmable electronic calculator including a small operating guide. Please write the name and model of your calculator on the first inside left-hand sheet of the exam work book.
- 3) Graph paper will be provided.
- 4) Any **four** questions constitute a complete paper and, unless you indicate otherwise, only the first four answers as they appear in your answer booklet will be marked.
- 5) Each question is worth 20 marks. Marking schemes are provided in brackets after each question.
- 6) Technical content is the key ingredient in your answers. However, no credit will be given for deriving reaction rate expressions, or standard formulas that are available in the textbook. Clear writing is essential, particularly when explanations are required.
- 7) It will be help to the examiner if you would cite the origin of significant formulas used e.g., Fogler, eq. (3-44).

Marking Scheme Four questions comprise a complete examination.

- 1. 20 marks a) 10 marks, b) 10 marks.
- 2. 20 marks a) 10 marks, b) 10 marks.
- 3. 20 marks a) 7 marks, b) 7 marks, c) 6 marks
- 4. 20 marks a) 10 marks, b) 10 marks
- 5. 20 marks a) 20 marks

Question 1:

An aqueous solution of ethyl acetate is to be saponified in a CSTR which can be assumed to be perfectly mixed. The reaction is:

$$CH_3 COO C_2H_5 + NaOH = CH_3 COO Na + C_2H_5 OH$$

And under the specified conditions the reaction is second order and essentially irreversible. The reactants are fed to the reactor in two streams as follows:

Ethyl acetate: 0.1 gmole/litre, flowrate 70 litre/min NaOH: 0.2 gmole/litre, flowrate 50 litre/min

Rate constant: k=23.5 litre/gmole min at 0°C k=92.4 litre/gmole min at 20 °C

- a) The reactor volume is 200 litre and it is operated at 30 °C. Estimate the composition of the outlet stream:
- b) The reactor is to be replaced by two CSTRs in series (equal volume tanks). What tank volume will give the same conversion under the above flow conditions?

Question 2:

A certain liquid phase isomerization reaction is first order in each direction and exothermic in the forward direction.

$$A \underset{k_2}{\overset{k_1}{\rightleftharpoons}} B$$

$$k_1 = 10^5 e^{(-\frac{6500}{RT})} \text{min}^{-1} \text{ (R = 1.98 cals/g mole K)}$$

The heat of reaction $(-\Delta H)$ is 4500 calories and is essentially independent of temperature.

At 298 °K the standard free energy of change is given by ΔG^{o}_{298} =-710 cals.

A feed solution is available containing A and B in the molar ratio 2:1 and in the product stream a molar ration of 1:2 is required.

- a) Derive an expression which gives the temperature at which the reaction rate is a maximum as a function of the degree of conversion. Hence calculate the optimal operating temperature for a CSTR.
- b) If the reaction is to be carried out in an isothermal tubular reactor (plug flow) between what limits must the optimum operating temperature lie?
- c) If the reaction is to be carried out in a temperature programmed batch reactor, what should the initial and final temperature be for the optimal system?

Question 3:

The vapour phase decomposition of acetaldehyde is carried out isothermally in a constant volume batch reactor at $450\,^{\circ}\text{C}$.

$$CH_3CHO = CH_4 + CO$$

The system contains initially a 50-50 mixture of acetaldehyde vapour and nitrogen.

a) Show that the following observations of total pressure are consistent with a first order irreversible reaction and calculate the rate constant.

Time (min)	0	2.2	5.1	9.2	16.1
P (atm)	1	1.1	1.2	1.3	1.4

b) A mixture of 40% acetaldehyde and 60% N_2 at a pressure of 5 atm is passed through an isothermal plug flow reactor of volume 15 litres which is maintained at 450 °C. Calculate the flowrate at which 50% of the acetaldehyde will be decomposed.

Question 4:

A second order liquid phase reaction can be represented by:

$$2A \rightarrow R$$

The reaction rate expression for the reaction is given by:

$$-r_A = k_2 C_A^2$$

The plant has two spare tanks available of volumes V1 and V2 where V=2V2. These tanks are to be operated in series at steady state and can be assumed to be well mixed. The reactant stream entering the first reactor contains no product.

- a) Determine quantitatively in which order these two tanks should be connected in order to give the highest conversion to product R.
- b) Determine quantitatively if there is any merit in putting the two tanks in parallel.

Question 5:

The homogeneous decomposition of phosphine:

$$4PH_3 \rightarrow P_4 + 6H_2$$

Proceeds at 1200 °F with first order rate:

$$-r_{PH3} = (10/hr) C_{PH3}$$

a) What size of plug flow reactor operating at 1200 °F and 4.6 atm can produce 80% conversion of a feed consisting of 4 lb-mol. of pure phosphine per hour?