16-CHEM-A4, CHEMICAL REACTOR ENGINEERING

MAY 2019

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.
   - any non-communicating calculator is allowed.
     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
2. 25 points – a) 20 points, b) 5 points
3. 25 points – a) 22 points, b) 3 points
4. 25 points
5. 25 points – a) 13 points, b) 5 points, c) 7 points

QUESTION 1

An irreversible reaction, **A → B**, obeys the following rate equation:

$$-r_A = \frac{kC_A}{[1 + KC_B]}$$

where C_A → concentration of A at any instant of time

C_B → concentration of B at any instant of time

k → reaction rate constant

K → a constant

At 50 °C, the value of k is 4.08 min^{-1} and the value of K is 10 liters per mole. Liquid feed containing A at a concentration of 1 mole per liter and no B is fed to a plug flow reactor with a volume of 200 liters at volumetric flow rate of 1200 liters per hour. If the reactor behaves as an ideal flow reactor and operates isothermally at 50 °C, what is the fractional conversion of A?

QUESTION 2

The dehydration of mixtures of methanol (CH_3OH) and butanol ($(CH_3)_2CHCH_2OH$) to form ethers and olefins over a sulfonic acid catalyst. At high pressures, dimethylether or DME (CH_3OCH_3) is the predominant product. The reaction of methanol to form DME is a reversible dehydration reaction as shown below:

$$2CH_3OH \leftrightarrow CH_3OCH_3 + H_2O$$

where $k_1 \rightarrow$ forward reaction rate constant for formation of DME from methanol

The postulated reaction rate equation for the formation of DME is given by:

$$r_{DME} = \frac{k_1\, K_M^2\, p_M^2}{[1 + K_M\, p_M + K_B\, p_B]^2}$$

where $p_M \rightarrow$ partial pressure of methanol

$p_B \rightarrow$ partial pressure of butanol

$K_M \rightarrow$ adsorption equilibrium constant for methanol

$K_B \rightarrow$ adsorption equilibrium constant for butanol

For a feed consisting only of methanol and nitrogen, the following kinetic data was obtained using a plug flow reactor operating at 375 K and a total pressure of 1340 kPa:

r_{DME} (moles per kg of catalyst per hour)	p_M (kPa)
0.155	30
0.156	40
0.200	80
0.217	120
0.219	160
0.220	240

(a) Does the postulated reaction rate equation fit the above experimental data?

(b) Determine the best fit values of k_1 and K_M.

QUESTION 3

Water at a flow rate of 1000 gallons/hr is passed continuously through a small, continuous polymerization reactor. At the time of purchase, the volume of the reactor was 500 gallons. The performance of the reactor appears to have deteriorated over time and there is some concern that solid polymer has built up in the reactor, thereby reducing the volume in which the polymerization reaction takes place. Therefore, a tracer test was run. A sharp pulse of tracer was injected right at the point where the water stream entered the reactor at steady-state. The total amount of injected tracer was 100,000 units. The concentration of tracer was measured at the point where water stream left the reactor and the following data was obtained:

Time After Injection (min)	**Tracer Concentration in Effluent** (units/gal)
0	0
1	205
2	225
3	222
4	215
5	205
10	165
15	138
20	111
25	92
30	76
40	53

50	35
60	24
70	16
80	10
90	4
100	0

(a) Calculate the volume of the reactor available for polymerization reaction.

(b) Estimate the amount of polymer that has built up in the reactor over time.

QUESTION 4

An irreversible first-order reaction, **A → Products**, was carried out in a differential reactor using various catalysts. The catalyst particles are spherical and essentially isothermal. The effective diffusivity ($D_{A,eff}$) is constant throughout each particle. The effect of particle size was investigated for one type of catalyst and the following results were obtained:

Particle Radius (mm)	**Measured Reaction Rate** (moles of A per liter of catalyst per second)
2	2.5
0.5	8.9
0.15	20.1

What is the effectiveness factor for each particle size? You may assume the reaction rate constant and effective diffusivity do not depend on particle size and external transport resistances are insignificant.

QUESTION 5

An irreversible first-order reaction, **A → R**, was carried out in an isothermal, ideal plug flow reactor with 3.9 mm diameter spherical catalytic particles. The heat of reaction (ΔH_r) is essentially zero and the inlet concentration of A is 1.1×10^{-4} mol/cm^3 for all experiments. The following data was obtained for reaction carried out at 400 °C:

Experiment #	**Space Time** (g-s/cm^3)	**Conversion of A** (%)	**Superficial Mass Velocity** (g-s/cm^2)
1	0.18	50	0.19
2	0.36	75	0.19
3	0.72	94	0.19
4	1.08	98	0.19

(a) For the four experiments at 400°C, does the first-order rate equation fit the data? What is the value of apparent reaction rate constant?

Two additional experiments were carried out at 400°C and the following data was obtained:

Experiment #	**Space Time** (g-s/cm^3)	**Conversion of A** (%)	**Superficial Mass Velocity** (g-s/cm^2)
5	0.18	75	0.57
6	0.36	94	0.57

(b) Based on six experiments carried out at 400°C, does the process of external mass transfer have any influence on the performance of the catalysts? Explain your answer and be as quantitative as possible.

One additional experiment was carried out at 425°C and the following data was obtained:

Experiment #	**Space Time** (g-s/cm^3)	**Conversion of A** (%)	**Superficial Mass Velocity** (g-s/cm^2)
7	0.18	54	0.19

(c) Is the result for experimental data at 425 °C consistent with your answer obtained in part (b)? Explain your answer and be as quantitative as possible.