16-CHEM-A4, CHEMICAL REACTOR ENGINEERING

DECEMBER 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.
   - a non-communicating, programmable electronic calculator using a small operating guide. Any non-communicating calculator is permitted. 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) 15 points, b) 10 points
2. 25 points – a) 8 points, b) 5 points, c) 12 points
3. 25 points
4. 25 points – a) 12 points, b) 3 points, c) 3 points, d) 7 points
5. 25 points – a) 3 points, b) 7 points, c) 9 points, d) 6 points

QUESTION #1

The decomposition of gaseous reactant A in a constant-volume batch reactor at 100 °C yielded the following data:

Time t, in sec	Pressure p_A, in atm
0	1.00
20	0.80
40	0.68
60	0.56
80	0.45
100	0.37
140	0.25
200	0.14
260	0.08
330	0.04
440	0.02

The stoichiometry of the reaction is **2A → R + S**.

(a) What size of plug flow reactor (in liters) operating at 100 °C and 1 atm can treat 120 moles of A per liter in a feed containing 20% inerts to obtain 95% conversion of A?

(b) What size of mixed flow reactor (in liters) operating at 100 °C and 1 atm can treat 120 moles of A per liter in a feed containing 20% inerts to obtain 95% conversion of A?

QUESTION #2

You are asked to explore various reactor setups for the transformation of A into R. The transformation takes place by means of the following elementary reaction **A + R → R + R**. The rate constant (k) for the reaction is 1 liter per mole per minute and the concentration of active materials is $C_{A0} + C_{R0} = C_A + C_R = C_0 = 1$ mol/liter throughout. For a product in which $C_R = 0.9$ mol/liter, calculate the reactor holding time for the following reactor setups:

(a) Plug flow reactor

(b) Mixed flow reactor

(c) Minimum-size combination reactors setup without recycle

QUESTION #3

A small reactor fitted with a sensitive pressure-measuring device is flushed out and then filled with pure reactant A at 1 atm pressure. The operation is carried out at 25 °C, a temperature low enough that the reaction does not proceed to any appreciable extent. The temperature is then raised as rapidly as possible to 100 °C by plunging the reactor into boiling water. The stoichiometry of the reaction is **2A → R**. After leaving the reactor in the bath over the weekend, the contents are analyzed for reactant A and none could be found. Find a rate equation in units of moles, liters and minutes which will satisfactorily fit the following data:

Time t (min)	**Pressure** π (atm)
1	1.14
2	1.04
3	0.982
4	0.940
5	0.905
6	0.870
7	0.850
8	0.832
9	0.815
10	0.800
15	0.754
20	0.728

QUESTION #4

Transesterification of vegetable oils with alcohols such as methanol is a key step in producing bio-diesel fuel. The reaction of triglyceride triacetin with methanol (CH_3OH) is a model reaction used to evaluate the performance of various solid transesterification catalysts. The reactions taking place are:

Triacetin (TA) + CH_3OH (MeOH) → Diacetin (DA) + Methyl Acetate (MeAc)

Diacetin (DA) + CH_3OH (MeOH) → Monoacetin (MA) + Methyl Acetate (MeAc)

Monoacetin (MA) + CH_3OH (MeOH) → Glycerol (G) + Methyl Acetate (MeAc)

The above liquid-phase reactions were studied using an ETS-10 catalyst at 60 °C in an ideal batch reactor and the following concentration data as a function of time was obtained:

Time (min)	C_{TA} (mol/liter)	C_{DA} (mol/liter)	C_{MA} (mol/liter)	C_G (mol/liter)	C_{MeAc} (mol/liter)	C_{MeOH} (mol/liter)
0	2.33	0.00	0.00	0.00	0.00	13.44
5	1.56	0.51	0.06	0.00	1.29	
10	1.29	0.77	0.20	0.00	1.89	
15	1.10	0.90	0.37	0.04	2.29	
20	0.99	0.99	0.50	0.10	2.56	
30	0.80	0.94	0.71	0.17	2.96	

40	0.67	0.86	0.83	0.24	3.26	
50	0.54	0.74	0.89	0.33	3.57	
60	0.43	0.66	0.90	0.43	3.89	

(a) Based on the high initial ratio of methanol to triacetin, it might be hypothesized that the reaction is pseudo-first-order with respect to triacetin. Test the hypothesis based on the data obtained and comment on how well the model fits the data.

(b) What is the ratio on methanol concentration after 60 minutes of reaction to the initial methanol concentration? How reasonable is the pseudo-first-order assumption?

(c) What is the selectivity to glycerol based on triacetin after 60 minutes of reaction? What is the yield of glycerol based on triacetin after 60 minutes of reaction?

(d) The rate equation for disappearance of triacetin may be given by the equation

$$-r_{TA} = k\, C_{TA}\, C_{MeOH}$$

Illustrate (but not solve) a way of testing the above rate equation against the data graphically.

QUESTION #5

The catalytic partial oxidation of propylene (C_3H_6) to propylene oxide (C_3H_6O) was carried out in a continuous gas-sparged reactor.

$$C_3H_6 + \frac{1}{2} O_2 \rightarrow C_3H_6O$$

A gaseous mixture of propylene and oxygen was fed to an isothermal reactor that contained a solid supported catalyst Ag/SiO_2 in the form of very fine powder. The catalyst is suspended in liquid dibutyl phthalate. The unconverted propylene and oxygen, as well as the product propylene oxide and by-products such as CO_2 and H_2O, left the reactor as a gas. The catalyst and the liquid remained in the reactor. The reaction was carried out at four temperatures, using the same total pressure (1 atm), feed composition (21% mole O_2 and 79% mole C_3H_6), space velocity (35 cc of gas per gram of catalyst per hour), and the following data obtained:

Reactor Temperature (°C)	Propylene Conversion (%)
160	16
180	30
200	40
230	44

Assume that the reaction is first-order in propylene, zero-order in oxygen, and irreversible. Also, you may neglect volume change due to reaction.

(a) Which of the three ideal reactors (batch, mixed flow and plug flow) best matches the actual reactor described above? Explain your answer.

(b) Using your answer in part(a), calculate the value of the rate constant at each of the four temperatures listed in the data table.

(c) What is the average activation energy between 160 °C and 180 °C, 180 °C and 200 °C, and 200 °C and 230 °C?

(d) Explain the behavior of the activation energy in part (c) in terms rate-controlling steps.

10 MM/CM