

04-CHEM-A4, CHEMICAL REACTOR ENGINEERING

May 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) 12.5 points, b) 12.5 points
2. 25 points
3. 25 points
4. 25 points
5. 25 points

QUESTION 1

Consider the ideal gas reaction $2A \rightarrow B + 2C$ occurring at 170°C , starting with 2.25 kg moles of pure A at 10 atm. The reaction rate equation is given by

$$r_A = - (1/V) (dn_A/dt) = 1.122 \times 10^4 C_A^2 \text{ in kg mol}/(\text{m}^3 \cdot \text{hr})$$

Evaluate the following rates of change at the time when the rate of reaction is $r_A = 1.6 \text{ kg mol}/(\text{m}^3 \text{ hr})$:

- a) dn_A/dt , dN_A/dt , dp_A/dt , $d\pi/dt$, dV/dt and dX_A/dt for reaction proceeding at constant volume
- b) dn_A/dt , dN_A/dt , dp_A/dt , $d\pi/dt$, dV/dt and dX_A/dt for reaction proceeding at constant pressure

Here $n_A \rightarrow$ number of moles of A at any given time

$N_A \rightarrow$ mole fraction of A at any given time

$p_A \rightarrow$ pressure of A at any given time

$\pi \rightarrow$ total pressure of the system at any given time

$V \rightarrow$ total volume of the system at any given time

$X_A \rightarrow$ fractional conversion of A at any given time

QUESTION 2

For the consecutive reactions $2A \rightarrow B$ and $2B \rightarrow C$, concentrations were measured as functions of residence time in a continuous stirred tank reactor (CSTR). In all experiments, the initial concentration of A (C_{A0}) was 1 lb mol/ft³ and the volumetric flow rate was constant. The concentration data as a function of mean residence time obtained from the experiments were as follows:

<u>Mean Residence Time (t), in sec</u>	<u>C_A, in lb mol/ft³</u>	<u>C_B, in lb mol/ft³</u>
10	1.000	0.4545
20	0.780	0.5083
40	0.592	0.5028
100	0.400	0.400
450	0.200	0.1636

The proposed rate equations are

$$r_A = k_1 C_A^\alpha$$

$$r_B = -0.5k_1 C_A^\alpha + k_2 C_B^\beta$$

Using the experimental data provided, calculate the values of the two rate constants (k_1 and k_2) and the two exponents (α and β) in the proposed rate equations.

QUESTION 3

A reversible reaction $A \leftrightarrow B$ is conducted in a plug flow reactor (PFR). The rate equation for the reaction is given by the equation

$$r_A = kC_{A0} \{1 - x_A - (x_A/K_e)\}$$

where C_{A0} is the initial concentration of A, x_A is the fraction of A converted, and K_e is the chemical equilibrium constant. The equations for rate constant (k) and chemical equilibrium constant (K_e) are:

$$k = \exp \{17.2 - (5800/T)\} \quad \text{and} \quad K_e = \exp \{-24.7 + (9000/T)\}$$

where T is the temperature in Kelvin.

For $C_{A0} = 4$ and 80% conversion, find the temperature at which the minimum residence time in the PFR is obtained. What is the value of this minimum residence time? Do not worry about the units.

QUESTION 4

A mixture of 0.5 moles of steam per mole of butadiene is dimerized ($2A \leftrightarrow B$) in a tubular reactor at 640 °C and 1 atm. The forward specific rate constant (k) is 118 kg mol/(L hr atm²) and the equilibrium constant (K_e) is 1.27.

Find the length of a tubular reactor (internal diameter = 10 cm) for 40% conversion when the total feed rate is 9 kg mol/hr.

QUESTION 5

The irreversible gas-phase trimerization reaction $3A \rightarrow B$ is taking place at steady state in an ideal continuous stirred tank reactor (CSTR) that has a volume of 10,000 liters. The feed to the reactor is a 1:1 molar mixture of A and N_2 at 5 atm total pressure and a temperature of 50 °C. The reactor operates at 350 °C and 5 atm total pressure. The volumetric feed rate is 8000 liters/hr at feed conditions. The gas mixture is ideal at all conditions. The reaction is homogeneous and the rate of disappearance of A is given by the equation

$$r_A = kC_A$$

where the rate constant (k) is $4 \times 10^{-5} \text{ hr}^{-1}$ at 100 °C and the activation energy (E) is 90 kJ/mol.

What is the fractional conversion of A in the stream leaving the reactor?

