04 -Chem-A4, Chemical Reactor Engineering

DEC 2013

3 HOURS DURATION

NOTES:

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**

   - 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 work book.

3) Graph paper will be provided. Any linear graph paper will be suitable.

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) 16 marks, b) 4 marks.
2. 20 marks - a) 8 marks, b) 8 marks, c) 4 marks.
3. 20 marks - a) 2 marks, b) 10 marks, c) 4 marks, d) 4 marks.
4. 20 marks - a) 6 marks, b) 6 marks, c) 2 marks, d) 6 marks.
5. 20 marks - a) 8 marks, b) 12 marks.

1. Two CSTRs are placed in series; the first having a volume of 250 L and the second a volume of 2000 L. The first reactor is fed by two independent liquid streams. One stream contains reactant A in water, while the other contains reactant B in water. Reaction occurs irreversibly according to the stoichiometry A + B → C + D, where C and D are water-soluble, inert products. A feed stream containing Reactant A at a concentration of exactly 0.1 mol/L with a volumetric flow of 1.80 L/s enters the first reactor; B enters the first reactor in a second stream at an identical concentration and flowrate to that of A. The temperature in both reactors is maintained at 75°C and the reaction proceeds according to a rate law $(-r_A) = kC_AC_B$, where r_A has units of mol/s and k = 0.65 L/(mol•s).

a) Calculate the conversion of A in the outlet stream from the first reactor and second reactor. {16 marks}

b) If the order of the two reactors is reversed (i.e., the 2000-L vessel is placed before the 250-L one), the overall conversion of A changes by about two percentage points. Would you expect the new conversion to be higher or lower than in part (a) and why? {4 marks}

2. At a temperature of 25°C, a mixed alcohol-water solvent of alcohol (L) and water (W) contains a monobasic organic acid (A), i.e., an acid with only one replaceable hydrogen atom per molecule, the concentration of which is 0.0677 mol/L. A quantity of the inorganic acid, HCl, is injected as a catalyst at the start of the reaction. The HCl concentration in the reaction mixture is 0.01934 mol/L. The resulting esterification reaction is monitored by titration to yield variations in the organic acid concentrations with time. This data is reported in the table below. Initially no ester (E) is present. The stoichiometry of the reaction is as follows:

$$L + A \leftrightarrow E + W$$

During the reaction, the alcohol concentration remains greatly in excess of that of organic acid. The water concentration is likewise in large excess of that of the ester. Alcohol and water concentrations are in some constant (though unknown) ratio. Effectively, the reaction behaves as if:

$$A \leftrightarrow E$$

at the given [L]/[W] ratio, the square brackets representing the concentration of the material indicated within them.

a) By constructing an appropriate table or graph, show that the reaction can be described by a reversible pseudo-first order rate law. For A ↔ E, one of the integrated forms for such a rate law is given as

$$ln\ \{([A] - [A]_e)/([A]^\circ - [A]_e)\} = -(k_f + k_r)t$$

where [A] is the concentration of A in the solution at any time t, $[A]^\circ$ is the initial concentration of A and $[A]_e$ is its equilibrium concentration. The forward and reverse rate constants for the given esterification reaction are k_f and k_r, respectively. {8 marks}

b) Use the data below to calculate the values of the rate constants k_f and k_r for the given [L]/[W] ratio. {8 marks}

c) Calculate the pseudo-equilibrium constant, $K = k_f/k_r$, for this particular solvent ratio. {4 marks}

t, min	*Total acid concentration*, mol/L
0	0.08704
50	0.0808
100	0.0755
160	0.0702
290	0.06218
∞	0.04858

3. A first-order, homogeneous, liquid-phase reaction (**A → B**) occurs in a CSTR that operates adiabatically at steady state. The reaction itself is exothermic. Data are as follows and should be considered as exact quantities:

inlet A concentration = C_A°= 1.75 mol_A/L
heat capacity of the reacting fluid = C_p = 2.5 J/g·K (assumed constant at all conversions.)
enthalpy of reaction ΔH_r = -27 000 J/mol_A
flowrate into the CSTR = q° = 30 L/min
reaction rate $(-r_A) = 1.8\text{x}10^{13}\ e^{(-84000/RT)}C_A$ ([mol_A/L·s]; R = 8.314 [J/mol·K]; T is in [K]).
inlet temperature of feed = T° = 315 K
reactor volume = V = 28 L
conversion of A leaving reactor = X_A = 0.9
liquid density = ρ = 500 g/L (assumed constant throughout the reaction)

a) What are the units of the constant $1.8\text{x}10^{13}$ in the rate equation? {2 marks}

b) Calculate the temperature at which this reactor operates under steady operating conditions. {10 marks}

c) Calculate the rate constant for conditions within the CSTR. {4 marks}

d) Calculate the rate of heat evolved within this reactor (in J/s) during steady-state operation. {4 marks}

4. The conversion of pure A to B occurs in the gas phase. At a constant temperature of 280°C, the stoichiometry for the reaction is:

$$A \rightarrow 2\,B$$

Initially the gas phase contains pure A. Total pressure data for this reaction at 280°C are provided in the table below.

Time, s	Total pressure, atm
0.0000	0.01974
0.1389	0.02487
0.2222	0.02724
0.3611	0.03026
0.5000	0.03263

a) By fitting the data in a plot to the integrated form of a second order reaction, show that this model fails to fit the data. (Graphical or tabular solutions are equally acceptable.) {6 marks}

b) Show that a first-order rate law fits the data. {6 marks}

c) Report the mean rate constant with appropriate units. {2 marks}

d) If the rate constant at 255°C were half as large as the value reported in (c), what would the activation energy be for this process in kJ/mol? {6 marks}

5. An isothermal, irreversible, second-order reaction with the following stoichiometry

$$2A \rightarrow A_2$$

is carried out in the gas phase. The reaction is carried out in an isothermal, plug-flow reactor, the dimensions of which are 2.5 cm in internal diameter and 3.2 m in length. A pure stream of species A is fed to the reactor at a rate of 1.5 mol/h at 320°C and 101.3 kPa total pressure. The resulting conversion of A to A_2 is 58.0%.

a) Calculate the space time (in seconds) of the reactor if the pressure of the inlet stream is 101.3 kPa. {8 marks}

b) Calculate the rate constant of the above reaction. Hint: See Fogler's textbook for an integrated form of the necessary equation. {12 marks}

10 MM/CM