TY Chemical Engg
CRE II Question Bank

Unit I and Unit II

(***Reactor selection and operating conditions***) For each of the following sets of reactions describe your reactor system and conditions to maximize the desired product D. Make sketches where necessary to support your choices. The rates are in (mol/dm^3 · s), and concentrations are in (mol/dm^3).

(a) (1) $A + B \rightarrow D$ $\quad -r_{1A} = 10 \exp(-8{,}000\ K/T)C_A C_B$

(2) $A + B \rightarrow U$ $\quad -r_{2A} = 100 \exp(-1{,}000\ K/T)C_A^{1/2} C_B^{3/2}$

(b) (1) $A + B \rightarrow D$ $\quad -r_{1A} = 100 \exp(-1{,}000\ K/T)C_A C_B$

(2) $A + B \rightarrow U$ $\quad -r_{2A} = 10^6 \exp(-8{,}000\ K/T)C_A C_B$

(c) (1) $A + B \rightarrow D$ $\quad -r_{1A} = 10 \exp(-1{,}000\ K/T)C_A C_B$

(2) $B + D \rightarrow U$ $\quad -r_{2A} = 10^9 \exp(-10{,}000\ K/T)C_B C_D$

(1) What reactor and conditions would you choose to maximize S_{D/U_1U_2}?
(2) What temperature (300 K < T < 700 K) would you recommend to maximize the overall selectivity for $C_{A0} = C_{B0} = 1$ mol/dm^3 and $v_0 = 1$ dm^3/min?

(***Reactor selection and operating conditions***) For each of the following sets of reactions describe your reactor system and conditions to maximize the desired product D. Make sketches where necessary to support your choices. The rates are in (mol/dm^3 · s), and concentrations are in (mol/dm^3).

(f) Consider the following parallel reactions[12]

(1) $A + B \rightarrow D$ $\quad -r_{1A} = 10 \exp(-8{,}000\ K/T)C_A C_B$

(2) $A \rightarrow U$ $\quad -r_{2A} = 26 \exp(-10{,}800 K/T)C_A$

(3) $U \rightarrow A$ $\quad -r_{3U} = 10{,}000 \exp(-15{,}000\ K/T)C_U$

(g) For the following reactions (mol/dm^3/min)

(1) $A + B \rightarrow D$ $\quad -r_{1A} = 800\ e^{(-8{,}000\ K/T)} C_A^{0.5} C_B$

(2) $A + B \rightarrow U_1$ $\quad -r_{2B} = 10\ e^{(-300\ K/T)} C_A C_B$

(3) $D + B \rightarrow U_2$ $\quad -r_{3D} = 10^6\ e^{(-8{,}000\ K/T)} C_D C_B$

(1) What reactor and conditions would you choose to maximize S_{D/U_1U_2}?
(2) What temperature (300 K < T < 700 K) would you recommend to maximize the overall selectivity for $C_{A0} = C_{B0} = 1$ mol/dm^3 and $v_0 = 1$ dm^3/min?

The following liquid-phase reactions were carried out in a CSTR at 325 K.

$$3A \longrightarrow B + C \qquad -r_{1A} = k_{1A}C_A \qquad k_{1A} = 7.0\ \text{min}^{-1}$$

$$2C + A \longrightarrow 3D \qquad r_{2D} = k_{2D}C_C^2C_A \qquad k_{2D} = 3.0\ \frac{\text{dm}^6}{\text{mol}^2 \cdot \text{min}}$$

$$4D + 3C \longrightarrow 3E \qquad r_{3E} = k_{3E}C_DC_C \qquad k_{3E} = 2.0\ \frac{\text{dm}^3}{\text{mol} \cdot \text{min}}$$

The concentrations measured *inside* the reactor were $C_A = 0.10$, C_B = (
$C_C = 0.51$, and $C_D = 0.049$ all in mol/dm^3.

(a) What are r_{1A}, r_{2A}, and r_{3A}? ($r_{1A} = -0.7$ mol/dm$^3\cdot$min)
(b) What are r_{1B}, r_{2B}, and r_{3B}?
(c) What are r_{1C}, r_{2C}, and r_{3C}? ($r_{1C} = 0.23$ mol/dm$^3\cdot$min)
(d) What are r_{1D}, r_{2D}, and r_{3D}?
(e) What are r_{1E}, r_{2E}, and r_{3E}?
(f) What are the net rates of formation of A, B, C, D, and E?
(g) The entering volumetric flow rate is 100 dm^3/min and, the entering con tration of A is 3 *M*. What is the CSTR reactor volume? (*Ans.:* 4000 dm^3
(h) Write a Polymath program to calculate the exit concentrations when the ume is given as 600 dm^3.

Unit III

Derive Michaelis-Menten kinetic equation for the enzyme catalyzed reaction A→R.

Explain the mechanism of non-competitive inhibition in enzyme reactions and obtain the kinetic expression

The stoichiometry and kinetics of the fermentation reaction are given by:

$$A \to R, -r_A = \frac{2C_A^2 + 0.1C_A}{1 + 50C_A}$$

Where C_A is the concentration of reactant and varies in the range 0.5-50 mol/m^3. For very high concentrations of A, determine the reaction order.

The thermal decomposition of ethane to ethylene, methane, butane and hydrogen is believed to proceed in the following sequence. Use the PSSH to derive the rate law for formation of ethylene.

$$C_2H_6 \xrightarrow{k1} 2CH_3^*$$

$$CH_3^* + C_2H_6 \xrightarrow{k2} CH_4 + C_2H_5^*$$

$$C_2H_5^* \xrightarrow{k3} C_2H_4 + H^*$$

$$C_2H_6 + H^* \xrightarrow{k4} C_2H_5^* + H_2$$

$$2C_2H_5^* \xrightarrow{k5} C_4H_{10}$$

Propose a mechanism for the decomposition of Nitrous oxide ($N_2O \to N_2 + \frac{1}{2} O_2$) and show that the rate is given by:

$$-r_{N_2O} = \frac{k_1[N_2O]^2}{1 + k'[N_2O]}$$

Experimental analysis shows that the homogeneous decomposition of ozone

($2O_3 \rightarrow 3O_2$) proceeds with a rate $-r_{O3} = k[O_3]^2[O_2]^{-1}$. Devise a two step mechanism to explain this rate.

P7-4$_A$ The pyrolysis of acetaldehyde is believed to take place according to the lowing sequence:

$$CH_3CHO \xrightarrow{k_1} CH_3\cdot + CHO\cdot$$

$$CH_3\cdot + CH_3CHO \xrightarrow{k_2} CH_3\cdot + CO + CH_4$$

$$CHO\cdot + CH_3CHO \xrightarrow{k_3} CH_3\cdot + 2CO + H_2$$

$$2CH_3\cdot \xrightarrow{k_4} C_2H_6$$

(a) Derive the rate expression for the rate of disappearance of acetaldeh $-r_{Ac}$.
(b) Under what conditions does it reduce to Equation (7-2)?
(c) Sketch a reaction pathway diagram for this reaction.
(d) List ways you can work this problem incorrectly.
(e) How could you make this problem more difficult?

P7-22$_C$ Cell growth with uncompetitive substrate inhibition is taking place in a CSTR. The cell growth rate law for this system is

$$r_g = \frac{\mu_{max} C_s C_c}{K_s + C_s\,(1 + C_s/K_I)}$$

with $\mu_{max} = 1.5\ h^{-1}$, $K_s = 1\ g/dm^3$, $K_I = 50\ g/dm^3$, $C_{s0} = 30\ g/dm^3$, $Y_{c/s} = 0.08$, $C_{c0} = 0.5\ g/dm^3$, $V = 500\ dm^3$, and $D = 0.75\ h^{-1}$.

(a) Make a plot of the steady-state cell concentration C_c as a function of D. What is the volumetric flow rate (dm³/h) for which the cell production rate is a maximum?
(b) What would be the wash-out rate if $C_{c0} = 0$? What is the maximum cell production rate and how does it compare with that in part (a)?
(c) Plot C_s as a function of D on the same graph as C_c vs. D? What do you observe?

P7-11$_B$ Beef catalase has been used to accelerate the decomposition of hydrogen oxide to yield water and oxygen [*Chem. Eng. Educ.*, 5, 141 (1971)]. The centration of hydrogen peroxide is given as a function of time for a reac mixture with a pH of 6.76 maintained at 30°C.

t (min)	0	10	20	50	100
$C_{H_2O_2}$ (mol/L)	0.02	0.01775	0.0158	0.0106	0.005

(a) Determine the Michaelis–Menten parameters V_{max} and K_M.
(b) If the total enzyme concentration is tripled, what will the substrate centration be after 20 minutes?
(c) How could you make this problem more difficult?
(d) List ways you can work this problem incorrectly.

P7-13$_B$ The following data on bakers' yeast in a particular medium at 23.4°C and various oxygen partial pressures were obtained:

P_{O_2}	Q_{O_2} (no sulfanilamide)	Q_{O_2} (20 mg sulfanilamide/mL added to medium)
0.0	0.0	0.0
0.5	23.5	17.4
1.0	33.0	25.6
1.5	37.5	30.8
2.5	42.0	36.4
3.5	43.0	39.6
5.0	43.0	40.0

P_{O_2} = oxygen partial pressure, mmHg; Q_{O_2} = oxygen uptake rate, μL of O_2 per hour per mg of cells.

(a) Calculate the Q_{O_2} maximum (V_{max}), and the Michaelis–Menten constant K_M. (*Ans.:* $V_{max} \doteq 52.63$ μL O_2/h·mg cells.)
(b) Using the Lineweaver–Burk plot, determine the type of inhibition sulfanilamide that causes O_2 to uptake.
(c) List ways you can work this problem incorrectly.
(d) How could you make this problem more difficult?

1) Using PSSA how do we develop a rate equation from the proposed mechanism?

2)What is the Michaelis-Menten reaction mechanism for enzyme promoted reactions?

Unit IV

1) Discuss about determination of rate controlling step for fluid particle reaction

2)Write the limitations of the shrinking core model.

3) Differentiate between Progressive Conversion Model (PCM) and Shrinking Core Model (SCM) for fluid-particle r

4) Derive the time-conversion-radius relationship for shrinking-core model for spherical particles of unchanging size diffusion through gas film controls

5) Derive the time-conversion-radius relationship for shrinking-core model for spherical particles of unchanging chemical reaction controls.

6) What is effectiveness factor? Derive a relationship between effectiveness factor and Thiele Modulus for first c reaction.

Unit V

1) Discuss the various reasons due to which non-ideal behavior exists.

2)Differentiate between ideal flow reactors and non ideal flow reactors

3) Discuss in detail deviations from ideal flow pattern with examples.

4)What are Stimulus response (SR) techniques? List various possible SR techniques used to study the flow in vessels.

5)Explain stimulus-Response techniques commonly used to study the flow behavior in the vessels.

6)Discuss dispersion model for representing flow in real vessel (non ideal reactor).

7) Discuss in details the factors affecting the performance of a real reactors

8) Explain Micro fluid and Macro fluid in detail.

9) Discuss the types of non-ideal flow in process equipments with neat diagrams.

10) Explain the step input method and impulse input method for determining **C**, **E**, and **F** curves in non-ideal chemical reactors

Unit VI

1) **Discuss the classification of models for non ideal reactors**
2) Discuss the significance of tank in series model

3) Derive an equation for dispersion and chemical reaction tank in series model

4)Derive an equation for dispersion and chemical reaction

5) From a pulse input a vessel the following output signal is obtained

Time (min)	1	3	5	7	9	11	13	15
Conc.	0	0	10	10	10	10	0	0

We want to represent the flow through the vessel with tank in series model. Using the variance matching procedure determine the number of tanks to use?

6)

A sample of the tracer hytane at 320 K was injected as a pulse to a reactor, and the effluent concentration was measured as a function of time resulting in the data shown in Table.

t, min	0	1	2	3	4	5	6	7	8	9	10	12	14
C, g/m^3	0	1	5	8	10	8	6	4	3	2.2	1.5	0.6	0

The measurements represent the exact concentrations at the times listed and not average values between the various sampling tests. (a) Construct figures showing E(t) as functions of time. (b) Calculate the mean residence time and the variance for the reactor.