The University of Jordan
School of Engineering
Chemical Engineering Department

(0905422) Chemical Reaction Engineering II — **Second Semester – 2021/2022**

Second Exam

Name: ______________________ **ID #** ________________

Dear students:

Answer all questions to the best of your ability and knowledge.

Start with the easiest question first. Use only the available space.

Don't waste your time on the questions that you are not confident about.

You know that cheating is not accepted and you would not need it anyway!

Good Luck 😊

Question 1: [8 points]

(a) [4 pts] Choose the correct answer:

1- __________ inhibition occurs when the inhibitor deactivates the enzyme-substrate complex.

a. Competitive b. Uncompetitive c. Noncompetitive

2- In Lineweaver-Burk plot, as the inhibitor (I) concentration is increased the slope increases while the intercept remains fixed. This is true for ____________ inhibition.

a. competitive b. uncompetitive c. noncompetitive

3- The class of enzyme that catalyzes the reaction (A + B + E → AB + E) is called __________.

a. transferase b. lyase c. ligase

4- The following reaction steps describe the ________________________ enzyme inhibition.

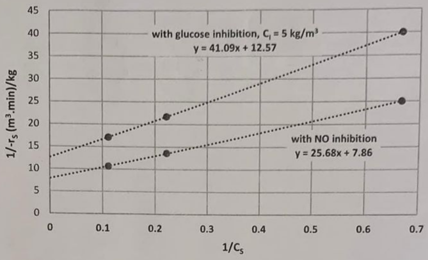
$$E + S \Leftrightarrow E{\bullet}S$$
$$E{\bullet}S \rightarrow P + E$$
$$I + E{\bullet}S \Leftrightarrow I{\bullet}E{\bullet}S$$

a. competitive b. uncompetitive c. noncompetitive

إذا جاوبه نفس جواب ١ شو ما كان
أعطيهم $\boxed{0.5}$

Question 3 [7 points] $cellulose \xrightarrow{cellulase} glucose$

Cellulose can be converted to glucose by cellulase, but glucose acts to inhibit this enzymatic attack! To study the reaction kinetics, a number of runs are made in a CSTR kept at 50°C and using a feed of finely shredded cellulose (C_{S0} = 25 kg/m³), and enzyme (C_{E0} = 0.01 kg/m³). The results are as follows:



1- As shown above, the enzyme follows Michaelis-Menten mechanism, evaluate V_{max}, k_{cat}, and K_M.

V_{max} = 0.5 0.127 k_{cat} = 12.7 0.5 K_M = 3.27 0.5

2- What type of inhibition does glucose possess? Evaluate K_I.

Inhibition type: Noncompetitive 1 K_I = 8.33 0.5

Show down your calculations ↓ and how you decided on the inhibition type.

0.5

$$\frac{1}{-r_S} = \frac{1}{V_{max}} + \frac{K_M}{V_m[S]} \quad , \text{ intercept} = \frac{1}{V_{max}} = 7.86$$

$$\Rightarrow V_{max} = 0.127$$

0.5

$$\text{slope} = \frac{K_M}{V_{max}} = 25.68 = 7.86 K_M \Rightarrow K_M = 3.27$$

0.5

$$V_M = k_{cat} E_{tot} \Rightarrow k_{cat} = \frac{0.127}{0.01} = 12.7$$

0.5

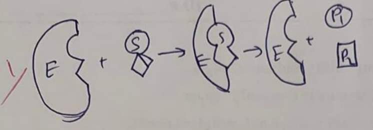
Both slope & intercept changed with the same ratio

$$\text{slope } \frac{41.09}{25.68} = 1.6 \;\; 0.5 \; , \quad \frac{12.57}{7.86} = 1.6 = 1 + \frac{C_I}{K_I} \;\; 0.5 \;\; 0.5$$

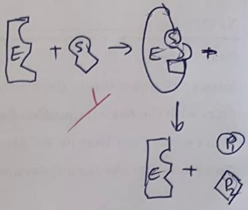
$$\Rightarrow K_I = \frac{5}{0.6} = 8.33$$

(b) [4 pts] There are two models for substrate-enzyme interactions, what are they? Draw a sketch to how each one works.

Lock - and - key



Induced fit



Question 2 [6 points]

A substrate inhibiting enzyme reaction $S \xrightarrow{enzyme} products$ is carried out in a CSTR with residence time τ. The inlet concentration of the substrate is C_{S0} = 40 mmol/dm³, and the rate law is defined as

$$v = \frac{V_m[S]}{K_m' + [S] + [S]^2/K_{SI}}$$

where $V_m = 1.8\ mmol/dm^3 \cdot min$, $K_m' = 16\ mmol/dm^3$, and $K_{SI} = 0.5\ dm^3/mmol$

(a) At what substrate concentration, C_S, will the rate be at its maximum value?

(b) What CSTR residence time is needed to operate this reaction at its maximum rate?

a) $\frac{dv}{d[S]} = \frac{(K_m' + [S] + [S]^2/K_{SI})V_m - V_m[S](1+2[S]/K_{SI})}{(\quad)^2} = 0$

3

$\Rightarrow K_M' V_m + V_m[S] + V_m[S]^2/K_{SI} = V_m[S] + 2V_m[S]^2/K_{SI}$

$\Rightarrow K_M' = [S]^2/K_{SI} \Rightarrow [S] = \sqrt{K_M' K_{SI}}$

$\Rightarrow [S] = \sqrt{16 \times 0.5} = \sqrt{8} = 2.82$

OR خطأ في السؤال $[S]_{max} = \sqrt{16/0.5} = 5.66$ mmol/dm³ $\tau =$

b) 3 $\tau = \frac{V}{v_0} = \frac{C_{A0}X}{-r_A} = \frac{C_{A0} - C_S}{-r_A}$, $-r_A =$ 0.146 → 255 min; 0.119 → 289 min

Question 4 [9 points] $CO + Cl_2 \rightarrow COCl_2$

Experimental observation for formation of phosgene, $COCl_2$, from chlorine, Cl_2, and carbon monoxide, CO, showed that the rate law is first order with respect to the CO concentration and independent of $COCl_2$ concentration. Also, it was observed that the rate law is three-halves order in Cl_2 at low Cl_2 concentrations, and one-half-order in Cl_2 at high Cl_2 concentrations.

(a) Suggest a rate law consistent with the experimental observations.

$$-r_{CO} = \frac{k_1 [CO] [Cl_2]^{3/2}}{1 + k_2 [Cl_2]}$$

0.5 0.5 0.5 0.5

(b) Consider the following chain reaction mechanism and answer the following questions:

$$Cl_2 \xrightarrow{k_1} 2Cl\cdot \quad \rightarrow \text{ initiation } 0.5$$

$$CO + Cl\cdot \underset{k_3}{\overset{k_2}{\rightleftarrows}} COCl\cdot$$

$$COCl\cdot + Cl_2 \xrightarrow{k_4} COCl_2 + Cl\cdot$$

propagation 0.5

$$2Cl\cdot \underset{k_6}{\overset{k_5}{\rightarrow}} Cl_2 \quad \rightarrow \text{ termination } 0.5$$

i. **What are $Cl\cdot$ and $COCl\cdot$ called?** active intermedrates 1

ii. **Label the initiation, propagation, and termination steps.**

iii. **Show that this mechanism can represent your suggested rate law in (a).**

$$-r_{CO} = r_{COCl_2} = k_4 [COCl\cdot][Cl_2] \quad 0.5$$

(PSSH)

$$\sum r_{COCl\cdot} = 0 = k_2 [CO][Cl\cdot] - k_3 [COCl\cdot] - k_4 [COCl\cdot][Cl_2] \quad 0.5 \quad -①$$

$$\Rightarrow [COCl\cdot] = \frac{k_2 [CO][Cl\cdot]}{k_3 + k_4 [Cl_2]} \quad 0.5$$

(PSSH)

$$\sum r_{Cl\cdot} = 0 = 2k_1 [Cl_2] - k_2 [CO][Cl\cdot] + k_3 [CO][Cl\cdot] + k_4 [COCl\cdot][Cl_2] - 2k_5 [Cl\cdot]^2 \quad 0.5 \quad -②$$

Adding ① + ②

$$0 = 2k_1 [Cl_2] - 2k_5 [Cl\cdot]^2 \quad 0.5 \Rightarrow [Cl\cdot] = \sqrt{\frac{k_1 [Cl_2]}{k_5}} \quad 0.5$$

$$\Rightarrow [COCl\cdot] = \frac{k_2 \left(\frac{k_1}{k_5}\right)^{1/2} [CO][Cl_2]^{1/2}}{k_3 + k_4 [Cl_2]} \quad 0.5$$

substitute

$$\Rightarrow r_{COCl_2} = \frac{\frac{k_2 k_4}{k_3} \left(\frac{k_1}{k_5}\right)^{1/2} [CO][Cl_2]^{3/2}}{1 + \left(\frac{k_4}{k_3}\right)[Cl_2]} \quad 0.5 \qquad \frac{k [CO][Cl_2]^{3/2}}{1 + k' [Cl_2]} \quad 0.5$$

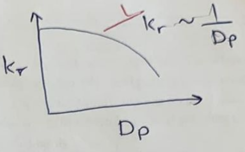
Start with ... questions to the h...

(c) **[3 pts]** What is the second step in a catalytic reaction? What does affect this step rate? Use a sketch to explain the relations between this factor and the rate.

1 Internal diffusion -

- Particle diameter 1

rate = $k_r C_{As}$



Question 2 [12 points] → 11 المجموع + العلامة تكل → الإذا موكاتب ولاشي

The reaction CO + Cl_2 → $COCl_2$ has been studied over an activated carbon catalyst. Experimental data show that the rate of this reaction is

$$r'_{COCl_2} = \frac{kP_{CO}P_{Cl_2}}{1 + K_1P_{Cl_2} + K_2P_{COCl_2}}$$

[k = 0.09 mol/atm²/kg cat/min, K_1 = 5 atm⁻¹ and K_2 = 1 atm⁻¹]

(a) Propose an adsorption-surface reaction-desorption mechanism and a rate-limiting step consistent with the rate law.

(b) What is the ratio of sites containing Cl_2 to those containing $COCl_2$ when the conversion is 20%? What fraction of total sites is vacant? The feed is equal molar in CO and Cl_2 with $P_{CO_0} = P_{Cl_{2_0}} = 2\ atm$.

(c) The molar feed rate of CO to a fluidized CSTR is 5 mol/min. The feed is equal molar in CO and Cl_2 with $P_{CO_0} = P_{Cl_{2_0}} = 2\ atm$. Determine the catalyst weight needed to reach 60% conversion of CO.

Remember, for "fluidized" catalytic CSTR: $W = \frac{F_{A0}X}{-r'_A}$

a) 1 $Cl_2 + S \rightleftharpoons Cl_2 \cdot S$ ads.

2 1 $Cl_2 \cdot S + CO \rightarrow COCl_2 \cdot S$ surf. rxn → rate limiting step 1

1 $COCl_2 \cdot S \rightleftharpoons COCl_2 + S$ des.

b) 0.5 $r_{ad} = k_a\left(P_{Cl_2}C_v - \frac{C_{Cl_2 \cdot S}}{K_1}\right)$ 0.5 & $\frac{r_{ad}}{k_a} \approx 0$ 0.5 ⇒ $C_{Cl_2 \cdot S} = K_1 P_{Cl_2} C_v$ 0.5

$r_d = k_d$ 0.5 $\left(C_{COCl_2 \cdot S} - K_2 P_{COCl_2} C_v\right)$, $\frac{r_d}{k_d} \approx 0$ 0.5 ⇒ $C_{COCl_2 \cdot S} = K_2 P_{COCl_2} C_v$ 0.5

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Good Luck ☺

Question 1: [8 points]

(a) [3 pts] Fill in the space:

0.5 1- Catalysis is the occurrence, study, and use of catalysts and catalytic processes.

0.5 2- Catalysts with so small pores that admit small molecules but prevent large ones from entering are called molecular sieves.

0.6 3- An active intermedrate is a high energy molecule that reacts virtually as fast as it is formed. أعطي علامة هذا السؤال للكل لأنه من خارج المادة.

0.5 4- Turnover frequency is the number of molecules reacting per active site per second at the conditions of the reaction.

0.5 5- Two models of reactant adsorption on catalyst surface are molecular (nondissociative) and dissociative adsorption.

(b) [2 pts] True or False? Correct the false statement!

0.5 1- Catalysts can accelerate the reaction rate but cannot change the equilibrium. (T)

2- Physisorption on the active site is what causes the reaction. 0.5 (F)

Chemisorptim 0.5

0.5 3- Adsorption equilibrium constant is the reciprocal of the desorption equilibrium constant. (T)

Question 3 [5 points]

The decomposition of cumene (C) to benzene (B) and propylene (P) on a Ni-Pt catalyst was studied using a differential reactor ($C \rightarrow P + B$). The reaction is /irreversible at the studied temperature. There were two inert species in the feed, X and Y, which may or may not be adsorbing. The following data was obtained.

Run	$-r'_A$ (mol/min.g cat)	P_C atm	P_B atm	P_P atm	P_X atm	P_Y atm
1	11.1	1	0	0	0	0
2	6.3	1	0	1	0.1	0
3	2.0	1	1	1	0	0
4	4.0	1	0.5	1	0	1
5	0.6	1	0	1	1	1
6	6.9	0.1	0	0	0	0
7	11.1	1	0	2	0	2
8	0.2	1	5	3	0	4
9	0.05	1	10	3	0	2
10	0.05	1	0	3	4	0
11	0.6	1	0	0	1	0
12	0.4	1	1	1	1	1
13	6.9	0.1	0	2	0	0

(a) Study the obtained data and complete the following sentences (if there is a bracket, then you need to choose one of the two options:

i. Comparing runs (6) and (13), we can see that P_P 0.5/ has no effect on the reaction rate.

ii. Comparing runs (1) and (7), we can see that P_Y 0.5/ also has no effect on the reaction rate.

iii. Comparing runs (3) and (9), we can see that when P_B is increased by a factor of 10 0.5/ the reaction rate (increases / decreases) 0.5/ by more than a factor of 10.

This means that P_B should be in (dominator / numerator) 0.5/ and raised to the power (1 / 2) 0.5/.

iv. Comparing runs (1) and (2), we can see that the presence of X 0.5/ decreases the reaction rate.

v. Comparing runs (1) and (6), we can see that the reaction rate decreases with decreasing P_C 0.5/.

(b) Based on your finding in part (a), suggest a rate law consistent with the above data.

$$-r_C = \frac{k P_C}{1 + K_B P_B^2 + K_X P_X}$$

1 → أصرتش
التربيع على P_B
و P_C في البسط

$$-r_C = \frac{k P_C}{(1 + K_B P_B + K_X P_X)^2}$$

$$-r_C = \frac{k P_C^{\alpha}}{(1 + K_B P_B + K_X P_X)^2}$$

? Use a

When $x = 0.2$

$$P_{Cl_2} = P_{Cl_2,0}\frac{(1-X)}{1+\varepsilon X} \quad 0.5 \qquad , \varepsilon = (1-1-1)\frac{1}{2} = \frac{-1}{2} \quad 0.5$$

$$\Rightarrow P_{Cl_2} = \frac{2(1-0.2)}{(1-\frac{1}{2}(0.2))} = \cancel{\frac{4}{8}} = \frac{16}{9}\ \text{atm} \quad 0.5$$

$$P_{COCl_2} = \frac{P_{Cl_2,0}(0+X)}{1+\varepsilon X} \quad 0.5 \quad = \frac{2(0.2)}{1-\frac{1}{2}(0.2)} = \frac{4}{9}\ \text{atm} \quad 0.5$$

$$\Rightarrow \frac{C_{Cl_2 \cdot S}}{C_{COCl_2 \cdot S}} = \frac{K_1 P_{Cl_2} \cancel{C_v}}{K_2 P_{COCl_2} \cancel{C_v}} \quad 0.5 \quad = \frac{5 \times \frac{16}{\cancel{9}}}{1 \times \frac{4}{\cancel{9}}} = 20 \quad 0.5$$

c) $F_{CO,0} = 5\ \text{mol/min}$ 2.5

$$W = \frac{F_{A0}X}{-r_A} \quad , \quad -r_A = \frac{k P_{Cl_2} P_{CO}}{1 + K_1 P_{Cl_2} + K_2 P_{COCl_2}}$$

at $x = 0.6$, $P_{Cl_2} = P_{CO} = \frac{2(1-0.6)}{1-\frac{1}{2}(0.6)} = \frac{8}{7}$ atm 0.5 0.5

$$P_{COCl_2} = \frac{2(0.6)}{1-\frac{1}{2}(0.6)} = \frac{12}{7}\ \text{atm} \quad 0.5$$

$$\Rightarrow W = \frac{5 \times 0.6}{\left[\frac{0.09(\frac{8}{7})^2}{1+5(\frac{8}{7})+1(\frac{12}{7})}\right]} = 223.8\ \text{kg cat.}$$