國立高雄大學 107 學年度研究所碩士班招生考試試題

科目：化工動力學
考試時間：100 分鐘

系所：化學工程及材料工程學系
（無組別）
本科原始成績：100 分

是否使用計算機：是

I. Single choice (4 points each, 48 points total)

1. Liquid A decomposes by first-order kinetics, and in a batch reactor 50% of A is converted to product in a 5-minute run. How much longer would it take to reach 75% conversion? (A) 5 min, (B) 10 min, (C) 15 min, (D) 20 min, (E) can not determine.
2. Repeat the above question for second-order kinetics. (A) 5 min, (B) 10 min, (C) 15 min, (D) 20 min, (E) can not determine.
3. If $-r_A$ = 0.2 mol/liter-sec when C_A = 1 mol/liter, what is the rate of reaction ($-r_A$) when C_A = 10 mol/l? (A) 1 mol/liter-sec, (B) 2 mol/liter-sec, (C) 20 mol/liter-sec, (D) 0.2 mol/liter-sec, (E) can not determine.
4. What is the half-life for a third-order reaction of reactant A? (A) 0.693/k, (B) k, (C) $1/(kC_{A0})$, (D) $C_{A0}/2k$, (E) $3/(2kC_{A0}^2)$. (k is the rate constant and C_{A0} is the initial concentration of A)
5. What is the half-life for a zero-order reaction of reactant A? (A) 0.693/k, (B) k, (C) $1/(kC_{A0})$, (D) $C_{A0}/2k$, (E) $3/(2kC_{A0}^2)$. (k is the rate constant and C_{A0} is the initial concentration of A)
6. A reaction $2A \longrightarrow 2B + C$ with the rate law $-r_A = k\,C_A^2$. What is the rate law for the reaction $A \longrightarrow B + 1/2\ C$? (A) $-r_A = k\,C_A$, (B) $-r_A = k\,C_A^2$, (C) $-r_A = k\,C_A^3$, (D) $-r_A = k\,C_A^{1/2}$.
7. For the reaction $A \longrightarrow$ products, if the plot of $1/C_A^2$ vs t is linear. What is the reaction order for the reaction? (A) 0, (B) 1, (C) 2, (D) 3, (E) 1/2.
8. For parallel reactions

   $A + B \longrightarrow D$, desired, $r_D = C_A^{0.4}C_B^{1.6}$

   $A + B \longrightarrow U$, undesired, $r_U = C_A^{1.0}C_B^{0.2}$

   Which of the following reactor types (or schemes) is the best for reducing C_U? (A) CSTR, (B) PFR, (C) Batch, (D) Semi-batch
9. For parallel reactions

   $A \longrightarrow D$, desired, $r_D = k_D\,C_A$

   $A \longrightarrow U$, undesired, $r_U = k_U\,C_A^2$

   Which of the following reactor types is the best for maximizing C_D? (A) CSTR, (B) PFR, (C) Batch.
10. An irreversible second-order liquid-phase reaction gave 80% conversion in a batch reactor in 200 min. What would be the conversion of this reaction in a CSTR with a 200 min space time? (A) 50%, (B) 61%, (C) 85%, (D) 90%, (E) can not determine.
11. Repeat the above question. What space time would be required for 80% conversion in a CSTR? (A) 100 min, (B) 200 min, (C) 500 min, (D) 1000 min, (E) can not determine.
12. An irreversible second order reaction $A \longrightarrow B$ is to be carried out isothermally in a plug-flow reactor (PFR). Calculate PFR reactor volumes necessary to consume 99 % of A (i.e., $C_A = 0.01\ C_{A0}$) when the entering molar flow rate (F_{A0}) is 5 mol/h and k is 3 dm^3/mol h. (A) 99 dm^3, (B) 128 dm^3, (C) 500 dm^3, (D) 660 dm^3, (E) 2750 dm^3.

II. (17 points)

Consider the following system of gas-phase reactions:

$$A \longrightarrow X \quad r_X = k_1 C_A^{1/2} \quad k_1 = 0.004(\text{mol/dm}^3)^{1/2}\cdot\text{min}$$

$$A \longrightarrow B \quad r_B = k_2 C_A \quad k_2 = 0.3\ \text{min}^{-1}$$

$$A \longrightarrow Y \quad r_Y = k_3 C_A^2 \quad k_3 = 0.25\ \text{dm}^3/\text{mol}\cdot\text{min}$$

B is the desired product, and X and Y are undesired products. The rate constants are at 27 ºC. The reaction system is to be operated at 27 ºC and 4 atm. Pure A enters the system at a volumetric flow rate of 10 dm^3/min.

(a) What is the instantaneous selectivity $S_{B/XY}$? (3 points)

(b) Determine the maximum $S_{B/XY}$? At which C_A, $S_{B/XY}$ is maximum? (6 points)

(c) If CSTR is used to carry out this reaction at this C_A as determined in (b), what is the volume of CSTR? (8 points)

III. (15 points)

(a) What is active intermediate? (3 points)

(b) What is pseudo-steady-state hypothesis (PSSH)? (2 points)

(c) Use the PSSH to derive the rate law for the reaction A $\longrightarrow$ P for the rate of the disappearance of A (i.e., $-r_A$). The reaction proceeds by first forming an active intermediate, A*, from the collision of the reactant molecule and an inert molecule of M. (10 points)

The mechanism consists of the three elementary reactions:

1. Activation $\quad A + M \xrightarrow{k_1} A^* + M$
2. Deactivation $\quad A^* + M \xrightarrow{k_2} A + M$
3. Decomposition $\quad A^* \xrightarrow{k_3} P$

IV. (20 points)

(a) The mechanism for carbon monoxide (CO) adsorption as molecules on the surface of the catalyst is

$$CO + S \rightleftarrows CO\cdot S$$

where *S* represents an active (vacant) site, CO•S represents that CO molecule is adsorbed on the site *S*. Derive the equilibrium isotherm equation (i.e.,$C_{CO\bullet S}$ as a function of P_{CO}) for this adsorption. ($C_{CO\bullet S}$ is the concentration of the adsorbed CO on S and P_{CO} is the partial pressure of CO.)

(b) The mechanism for dissociative carbon monoxide (CO) adsorption on the surface of the catalyst is

$$CO + 2S \rightleftarrows C\cdot S + O\cdot S$$

Derive the equilibrium isotherm equation (i.e.,$C_{C\bullet S}$ (or $C_{O\bullet S}$) as a function of P_{CO}) for this adsorption. ($C_{C\bullet S}$ is the concentration of the adsorbed C on S and P_{CO} is the partial pressure of CO.)