國立中正大學九十七學年度碩士班招生考試試題系所別:化學工程學系 科目:化工熱力學與化工動力學

第 3 節

第一頁,共型頁

Part I: Select the correct answer (or answers) for the following Questions (32%)

- For a heterogeneous reaction system, which of the following statements is (are) CORRECT?
  - reaction rate increases with total pressure if the reaction is controlled by adsorption.
  - reaction rate decreases with total pressure if the reaction is controlled by desorption.
  - assuming no catalyst deactivation, reaction rate may decrease with reaction temperature if the reaction is controlled by adsorption.
  - assuming no catalyst deactivation, reaction rate may decrease with reaction temperature if the reaction is controlled by desorption.

8%

- For a first-order irreversible reaction (A → R) occurs in an isothermal CSTR and PFR of equal volume and equal mass transfer rate, which of the following statements is (are) CORRECT?
  - a. the rate expression can be written as:  $-r_A = kC_A$
  - at the start of reaction CSTR gives higher reaction rate.
  - c. If the space time is the same in both reactors, at rather high conversion, in comparing with mixed flow, PFR gives the higher space-time yield.
  - d. If the space time is the same in both reactors, at rather low conversion, in comparing with mixed flow, CSTR gives the higher space-time yield.

- 3. Which of the following statements is are CORRECT for the features of chemisorption?
  - formation of covalent chemical bonds
  - b. more than single layer coverage are possible
  - c. coverage increases with increasing temperature.
  - d. coverage increase with increasing pressure

4%

- 4. One kilogram of air is heated reversibly at constant pressure from an initial state of 300 K 1bar to 5 times of its original volume. Assume that air obeys the relation PV/T = 8.314 bar cm<sup>3</sup> mol<sup>-1</sup> k<sup>-1</sup>; heat capacity of air,  $C_p$  = 29J mol<sup>-1</sup> k<sup>-1</sup> and that the molar mass of air  $M_{air}$  = 28.8 g mol<sup>-1</sup>. Calculate Q, W,  $\triangle U$ ,  $\triangle H$  for this process.
- 4-1. Q is equal to
  - a. 1208.2 kJ.
- b. 861.8 kJ
- c. -346.4 kJ
- d -1208.2 kJ
- e. None of the above answers are correct.
- 4-2 W is equal to
  - a. 1208.2 kJ.
- b. 861.8 kJ
- c. -346.4 kJ
- d -1208.2 kJ
- e. None of the above answers are correct.
- 4-3 △U is equal to
  - a. 1208.2 kJ.
- b. 861.8 kJ
- c. -346.4 kJ
- d -1208.2 kJ
- e. None of the above answers are correct.
- 4-4 △H is equal to
  - a. 1208.2 kJ.
- b. 861.8 kJ
- c. -346.4 kJ
- d -1208.2 kJ
- e. None of the above answers are correct.

Part II: Complete the following Questions by Calculation (68%)

 For the decomposition reaction (A → R), C<sub>A0</sub> =1 mol/liter, in a batch reactor conversion is 75% after 1 hour, and is just complete after 2 h. Find a rate equation to represent this kinetics.

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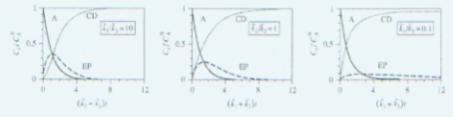
第 3 節

第三頁,共四頁

The following reactions are observed when an olefins is catalytically epoxidized with dioxygen:

Alkene (A) + 
$$O_2$$
 (O)  $\rightarrow$  epoxide (EP) (1)  
Epoxide +  $O_2$   $\rightarrow$   $CO_2$ (CD) +  $H_2$ O (2)  
Alkene +  $O_2$   $\rightarrow$   $CO_2$  +  $H_2$ O (3)  
 $\cap$  Alkene (A)  $\rightarrow$  coke (deposit on catalyst) (4)

- (i) derive the rate expression for this mixed-parallel series-reaction network and the expression for the present selectivity to the epoxide ( $S_{EP} = r_{EP}/(r_{EP} + r_{CD} + r_{coke})$ ). Where A: alkene, O: dioxygen, CD: carbon dioxide, EP: epoxide,  $r_{EP}$ : reaction rate of epoxide,  $r_{coke}$ : reaction rate of coke formation,and  $r_{CD}$ : total oxidation rate of alkene and epoxide. Note: you may use simple power rate law for each reaction path
- (ii) consult the figures attached below and calculate the maximum epoxide selectivity from equations derived from (i).
- (iii) in comparing other reactions, the reaction rate of alkene partial oxidation (eq. 1) is deactivated much faster with the coke formation what you expect about the trend of epoxide formation with respect to elapsed time when the reaction is performed at a fixed-bed reactor with constant space velocity.



Normalized concentration of species i as function of time for  $k_1=k_2$  and  $k_4=0$  (where  $k_1$ ,  $k_2$ ,  $k_3$ , and  $k_4$  are the rate constants for equation 1, 2, 3, and 4, respectively)

第3節

第四頁, 共四頁

- 3. A thermally isolated container is divided by a partition into two compartments with identical volume V. The first compartment contains n<sub>1</sub> mole of ideal gas at temperature T and pressure P, and the second compartment contains n<sub>2</sub> mole of ideal gas at temperature T and pressure P'. The partition is now removed to allowed gas mixing. Calculate
  - a. the final pressure of the gas mixture (in terms of  $n_1$ ,  $n_2$  and P) 8% b. the total change of entropy ( $\triangle S$ ) after the mixing. (in terms of  $n_1$ ,  $n_2$
  - b. the total change of entropy (△S) after the mixing. (in terms of n<sub>1</sub>, n<sub>2</sub> and R (gas constant)).
- 4. Nitrogen tetraoxide (mole fraction 40%) in nitrogen (60%) was heated at  $25^{\circ}$ C and 1 bar to initiate the dissociation reaction [  $N_2O_{4~(g)} < ----> 2NO_2$  (g)]. The standard Gibbs free energy of formation of  $N_2O_{4~(g)}$  and  $NO_{2~(g)}$  at  $25^{\circ}$ C are 97.9 and 51.3 KJ/mol respectively. Calculate
  - a. The chemical equilibrium constant for  $N_2O_4$  dissociation. 6% b. The extent of  $N_2O_4$  dissociation at equilibrium. 6%
  - c. The mole fraction of  $N_2O_{4\,(g)}$  and  $NO_{2\,(g)}$  at equilibrium. 6%