國立成功大學 106 學年度碩士班招生考試試題

系　　所：化學工程學系

考試科目：化學反應工程

考試日期：0213，節次：3

※ 考生請注意：本試題可使用計算機。　請於答案卷(卡)作答，於本試題紙上作答者，不予計分。

1.

(a) The rule of thumb that the rate of reaction doubles for a 10°C increase in temperature occurs only at a specific temperature for a given activation energy. Develop a relationship between the "temperature" and "activation energy" for which the rule of thumb holds. Neglect any variation of concentration with temperature. **(5%)**

(b) Determine the activation energy (Ea) and frequency factor (A) from the following data **(10%)**:

k (min^{-1})	0.005	0.12
T (°C)	10	100

2. The liquid phase reaction for conversion compound A to B was carried out in a CSTR. For an entering concentration of 2 mol/mL, the conversion was 40% when assume the reaction is 1st order. What's the conversion for the same reactor volume of PFR and entering conditions as the CSTR? **(10%)** However, if assuming the same conditions occurred in 2nd order reaction, what's the final conversion for PFR? **(8%)**

3. The elementary, reversible liquid-phase reaction (A + B ⇔ 2C) is performed in an adiabatic flow reactor without shaft work at steady-state. Reactants A and B enters at 500 K into the reactor simultaneously. The conversion was kept at 50%.

   Additional information:

   C_{PA} =80 cal/mol/K, C_{PB} = 90 cal/mol/K, C_{PC} = 85 cal/mol/K, ΔH = 12 kcal/mol, F_{A0} = 100 mol/min, C_{A0} = 10 mol/L, F_{B0} = 200 mol/min, k (300 K) = $1.6*10^{-6}$ L/mol/min, Kc (300 K) = 0.0014, E =15 kcal/mol.

(a) Please determine the volume if the flow reactor is CSTR type. **(8%)**

(b) Please determine the volume if the flow reactor is PFR type. **(8%)**

(c) Explain why operating a nonisothermal CSTR will frequently encounter multiple steady states, while not the case for operating a nonisothermal PFR? You may use Levenspiel plot to explain this. **(4%)**

4. The Michaelis-Menten model is the best-known approach to enzyme kinetics. It takes the form of an equation relating reaction velocity to substrate concentration for a system where a substrate (*S*) binds reversibly to an enzyme (*E*) to form an enzyme-substrate complex (*ES*), which then reacts irreversibly to generate a product (*P*) and to regenerate the free enzyme (*E*).

(a) Please derive the rate expression of product *P* as below: **(8 %)**

$$r_P = \frac{V_{max}\,[S]}{K_m + [S]}$$

where V_{max} represents the maximum velocity achieved by the system, while K_m (the Michaelis constant) is the substrate concentration at which the reaction velocity is 50% of the V_{max}.

(b) Please estimate the parameters, V_{max} and K_m, using the following data. **(5 %)**

	Trial 1	Trial 2	Trial 3	Trial 4
[S] (mM)	4.8	1.2	0.6	0.3
r_P (mmol/min)	0.081	0.048	0.035	0.020

5. The carbonation of allyl chloride (AC) was carried out over a Pd catalyst:

$$CH_2CHCH_2Cl + CO + NaOH \rightarrow C_3H_5COOH + NaCl$$

The rate law is of the form

$$-r_{AC} = \frac{kC_{CO}C_{AC}C_{NaOH}}{(1 + K_{AC}C_{AC})^2}$$

The reaction mechanism is believed to be

$$Pd + CO \leftrightarrow Pd{\cdot}CO$$

$$Pd{\cdot}CO + NaOH \leftrightarrow (Pd{\cdot}CO{\cdot}NaOH)^*$$

$$AC + Pd \rightarrow AC{\cdot}Pd$$

$$AC{\cdot}Pd + (Pd{\cdot}CO{\cdot}NaOH)^* \rightarrow C_3H_5COOH + NaCl + 2Pd$$

Is there a rate-limiting step for which the rate law is consistent with the mechanism? Please try to demonstrate or verify your thoughts. **(16%)**

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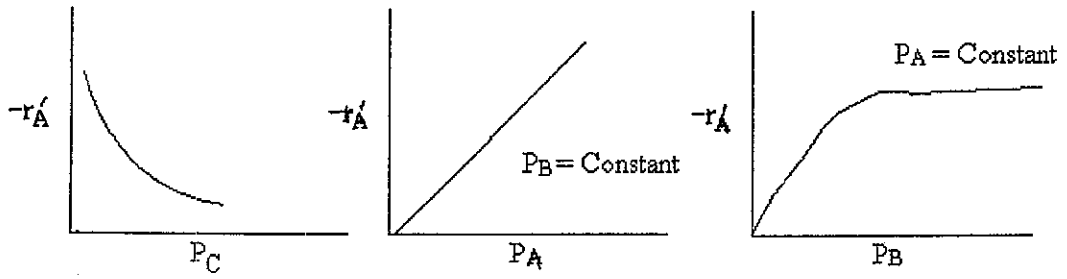
Single choice

6. The following figures were reported for the reaction A+B → C



Which description is **not appropriate**? **(8%)**

(a) Species A could be adsorbed on the surface but only very weakly adsorbed.

(b) Species A is not adsorbed on the surface.

(c) Species B is adsorbed on the surface.

(d) Species A is strongly adsorbed on the surface.

(e) Species C is adsorbed on the surface.

Single choice

7. Please choose the **incorrect** description. **(10%)**

(a) For overall effectiveness factor (Ω), the molar rate of mass transfer to the surface, M_A, is equal to the net (total) rate of reaction *on* and *within* the pellet.

(b) Overall effectiveness factor (Ω) can be defined as
Actual overall rate of reaction/rate that would result if the entire surface were exposed to the bulk conditions, C_{Ab}, T_b.

(c) The effective diffusivity D_e accounts for the fact that not all of the area normal to the direction of the flux is available for the molecules to diffuse.

(d) Large values of the Thiele modulus indicate surface reaction controls and a significant amount of the reactant diffuses well into the pellet interior without reacting.