PRINCE OF SONGKLA UNIVERSITY
FACULTY OF ENGINEERING

Midterm Examination: Semester I — Academic Year: 2006

Date: August 3, 2006 — Time: 9:00-12:00

Subject: 230-620 Advanced Engineering Kinetics and Chemical Reactor Design — Room: A401

อนุญาตให้นำเอกสารและเครื่องคำนวณทุกชนิดเข้าห้องสอบได้

ทุจริตในการสอบโทษขั้นต่ำคือปรับตกในรายวิชาที่ทุจริต

และพักการศึกษา 1 ภาคการศึกษา

Please do all 4 questions. Show all your work to receive full or partial credit. Total score is 160. (Total page 3, including first page)

Question #	Total Score	Score
1	50	
2	40	
3	40	
4	30	
Total	160	

สุกฤทธิรา รัตนวิไล

ผู้ออกข้อสอบ

Micro kinetics and Catalysis

1. Propose the mechanisms and find out reaction rate for the following reaction: **Please define all parameters that you need (50 scores)**

   1.1 $A \rightarrow B + C$:Using Langmuir Hinshelwood Model **(10 scores)**

   1.2 $A + 2B_{(g)} \rightarrow C$:Using Eley-Rideal Mechanism Model **(10 scores)**

   1.3 Using Pseudo Steady State Hypothesis: **(10 scores)**

$$A + (S) \underset{k_2}{\overset{k_1}{\longleftrightarrow}} A(S)$$
$$C_2 + 2(S') \underset{k_4}{\overset{k_3}{\longleftrightarrow}} 2C(S')$$
$$A(S) + C(S') \xrightarrow{k_5} P(S) + (S')$$
$$P(S) \underset{k_7}{\overset{k_6}{\longleftrightarrow}} P + (S)$$

   S and S′ are different active sites
   k_1, k_3, k_5, k_6 as forward reaction rate constant
   k_2, k_4, k_7 as backward reaction rate constant

   1.4 $A \rightarrow B + C$:Propose **ONE mechanism** which can explain reaction rate of A at both law and high pressures **(20 scores)**

   a. at low pressure, $r_A = k[A]^2$

   b. at high pressure, $r_A = k'[A]$

Macro kinetics and analysis data

2. A study of methane oxidation over iron phosphate with hydrogen present in a feed gas. High selectivity to methanol was observed under these conditions at low conversions. The role of H_2 was thought to be in generation of new surface sites active for methanol formation. **(40 scores)**

$$CH_4 \xrightarrow{O_2,k_1} CH_3OH \xrightarrow{O_2,k_2} CH_2O \xrightarrow{O_2,k_3} CO \xrightarrow{O_2,k_4} CO_2$$

   Oxygen is a feed gas in all reactions. Consider only data taken in the presence of hydrogen, propose and defend a reaction network for all species in a plug flow reactor. Using data in Tables A evaluate all of the parameters in the first reaction at 713 K.

Table A. Effect of methane partial pressure on methane conversion rate, T = 713K, Pressure of H_2 = 50 kPa, Pressure of O_2 = 8.4 kPa, W/F = 0.208 g h/dm^3.

Pressure of CH_4 (kPa)	Rate x 10^3 mol (g h)$^{-1}$
8.3	2.0
12.4	2.5
17.2	2.8
25.5	4.1
34.5	4.7
42.8	5.3

Catalyst and reaction rate

3. Using differential reactor to study the formation of methane from H_2 and CO over nickel catalysts showed reaction rate as following: **(40 scores)**

$$r_{CH_4} = \frac{0.0183 P_{H_2}^{0.5} P_{CO}}{1 + 1.5 P_{H_2}} \text{ mole/(g.cat s)}$$

Propose a mechanism and rate determination step that is consistent with experimental data. Reactor is desired to produce 20 tons/day of CH_4. Calculate the catalyst weights necessary to achieve 80% conversion in CSTR. The feed consists of 75% H_2 and 25% CO at a temperature of 500°F and a pressure of 10 atm.

Suggested mechanism is:

$$H_2 + (S) \underset{k_2}{\overset{k_1}{\rightleftarrows}} H_2(S)$$
$$H_2(S) + (S) \underset{k_4}{\overset{k_3}{\rightleftarrows}} 2H(S)$$
$$H(S) + CO \underset{k_6}{\overset{k_5}{\rightleftarrows}} CHO(S)$$
$$CHO(S) + H(S) \underset{k_8}{\overset{k_7}{\rightleftarrows}} C(S) + H_2O + (S)$$
$$C(S) + 2H_2 \underset{k_{10}}{\overset{k_9}{\rightleftarrows}} CH_4 + (S)$$

k_1, k_3, k_5, k_7, k_9 as forward reaction rate constant
k_2, k_4, k_6, k_8, k_{10} as backward reaction rate constant

Conceptual knowledge

4. Answer the following questions in THAI LANGUAGE based on your understanding: **(30 scores)**

4.1 In class, we discussed a lot about how to find out an actual reaction rate from experimental data. Now you have a bimolecular molecule reaction in a batch reactor and would like to correct data to get reaction rate parameter. Please suggest:
- How you correct the data from experiment?
- Which analytical method you expect to use?
- How do you solve for these parameters?
- Can I use method of half-lives to solve? Explain **(20 scores)**

4.2 Write an algorithm for determining reaction mechanism and rate-determining step **(10 scores)**