PRINCE OF SONGKLA UNIVERSITY
FACULTY OF ENGINEERING

Midterm Examination: Semester I — Academic Year: 2005

Date: August 3, 2005 — Time: 9:00-12:00

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

อนุญาตให้นำเอกสารและเครื่องคำนวณทุกชนิดเข้าห้องสอบได้
ทุจริตในการสอบโทษขั้นต่ำคือปรับตกในรายวิชาที่ทุจริตและพักการศึกษา 1 ภาคการศึกษา

Please do all 5 questions. Show all your work to receive full or partial credit. Total score is 100.

Question #	Total Score	Score
1	15	
2	20	
3	20	
4	25	
5	20	
Total	100	

สุกฤทธิรา รัตนวิไล
ผู้ออกข้อสอบ

1. If the irreversible reaction was elementary as written,

$$aA + bB \xrightarrow{K} cC + dD \qquad (1)$$

the rate expression was $-r_A = kC_A^a C_B^b$

If take A as our basis and divide thoroughly equation (1) by the stoichiometric coefficient of A so that the equation is expressed as

$$A + (b/a)\,B \xrightarrow{k} (c/a)\,C + (d/a)\,D \qquad (2)$$

Will the kinetic rate expression then become? Explain in detail. **(15 points)**

$$-r_A = kC_A C_B^{b/a}$$

Macro kinetics

2. The gas phase homogeneous oxidation of nitrogen monoxide (NO) with oxygen (O_2) to nitrogen dioxide (NO_2) is known to have a form of third order kinetics which suggests that the reaction is elementary, at least for low partial pressure of nitrogen oxides. However, starting from the fact that an active intermediate species, NO_3, is sometimes observed. In addition, NO_3 is a participant in some other known reactions that involve oxides of nitrogen. What reaction mechanism is suggested based on the above information in reaction of nitrogen monoxide and oxygen? **(20 points)**

$$2NO + O_2 \xrightarrow{K} 2NO_2$$

Micro kinetics and Catalysis

3. The catalytic oxidation of ethanol has been carried out over a tantalum oxide catalyst. **(20 points)**

Overall reaction

$$CH_3CH_2OH + \tfrac{1}{2}\,O_2 \longrightarrow CH_3CHO + H_2O$$

The overall reaction is believed to proceed by the following mechanism in which ethanol is adsorbed on one type of site, **S**, and oxygen is adsorbed on a different type of site, **S'**. Ethanol undergoes dissociative adsorption on two **S** sites:

$$C_2H_5OH + 2S \longleftrightarrow C_2H_5O{\cdot}S + H{\cdot}S; \quad k_1 \text{ forward, } k_{-1} \text{ reverse}$$

Oxygen also undergoes dissociative adsorption on two **S'** sites:

$$O_2 + 2S' \longleftrightarrow 2O{\cdot}S'; \quad k_2 \text{ forward, } k_{-2} \text{ reverse}$$

Assuming that the rate-limiting step is

$$C_2H_5O{\cdot}S + O{\cdot}S' \longrightarrow C_2H_4O + OH{\cdot}S' + S; \quad k \text{ forward}$$

Modeling diffusion with reaction

5. The elementary reaction as written,

$$A \xrightarrow{k} B + D$$

Species A is diffusing at steady state from the bulk fluid through the external surface of catalyst. Develop a mathematical model in term of differential equation based on concentration of A and distance Z for chemically reacting systems in which diffusional effects are important, develop only ODE, no need to solve. **(20 points)**

assume: mole fraction of A = $y_A = C_A/C_T$, C_T constant total concentration.

BULK

and the adsorbed hydroxyl may be converted into water by

$$OH\cdot S' + H\cdot S \quad \longleftrightarrow \quad H_2O + S + S';\ k_3 \text{ forward, } k_{-3} \text{ reverse}$$

Show that the initial rate law is

$$-r_{A0} = \frac{KP_A^{1/2}P_{O_2}^{1/2}}{\left(1+K_{O_2}P_{O_2}^{1/2}\right)\left(1+2K_A^{1/2}P_A^{1/2}\right)}$$

Note: $[H\cdot S] = [A\cdot S]$, where $A \equiv C_2H_5OH$, $A\cdot S \equiv C_2H_5O\cdot S$, $W \equiv H_2O$

Rate data

4. The ethane hydrogenolysis over a commercial nickel catalyst was studies in a stirred contained solids reactor. Only hydrogen and ethane are fed to reactor at 300°C

$$H_2 + C_2H_6 \rightarrow 2CH_4$$

Determine the rate law parameter from the data below. **(25 points)**

Total Pressure of Feed (atm)	Pressure Fraction of Ethane and Hydrogen in Feed Stream		Reaction Rate (disappear of Ethane, g mole/h)
	Ethane	Hydrogen	$-r_{Ethane}$
0.95	0.5	0.5	1.0625
0.93	0.5	0.5	1.0500
0.84	0.5	0.5	1.2000
0.84	0.4	0.6	0.6000
1.08	0.5	0.5	0.9375
0.94	0.6	0.4	2.0625

Modeling diffusion with reaction

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assume: mole fraction of A = $y_A = C_A/C_T$, C_T constant total concentration.