系所組別： 化學工程學系甲組
考試科目： 化學反應工程

※ 考生請注意：本試題 ☑可 ☐不可 使用計算機

$Q - W_s - F_{A0}X[\Delta H_R°(T_R) + \Delta C_p(T - T_R)] - F_{A0}\Sigma\Theta_i C_{pi}(T - T_{i0}) = 0$
$\ln[\boldsymbol{K}(T)/\boldsymbol{K}(T_1)] = \Delta H_R°(T_R)\,[1/T_1 - 1/T]\,/\,R$
$[R = 8.314\ J/(mol\ K)]$

1. A 5 liter CSTR is used to carry out a liquid-phase reaction A → 2R. Reactant A is fed to the reactor at a concentration of 1 mol/liter. We intend to find a rate expression for this reaction by conducting experiments at different conditions. The experimental results are summarized as follows.

Run No.	Feed Rate (cm^3/sec)	Reaction Temperature (°C)	Concentration of R in Effluent (mol/liter)
1	2	13	1.8
2	15	13	1.5
3	15	84	1.8

Please find the reaction order and activation energy for this reaction. (20%)

2. A PFR operating isothermally at 773 K is used to conduct the following reaction: A → B + C. If a feed of pure A enters at 5 atm and at a flow rate of 0.193 ft^3/s, what length of pipe with a cross-sectional area of 0.0388 ft^2 is necessary for the reaction to achieve 90 percent conversion?
Data: $k = 7.8\times10^9 \exp[-19200/T]\ s^{-1}$ (13%)

3. The catalytic reaction, $A \rightarrow B$, takes place within a fixed bed containing spherical porous catalyst. Figure 1 shows the overall rates of reaction at a point in the reactor as a function of temperature (T) for various entering total molar flow rates, F_{T0}.

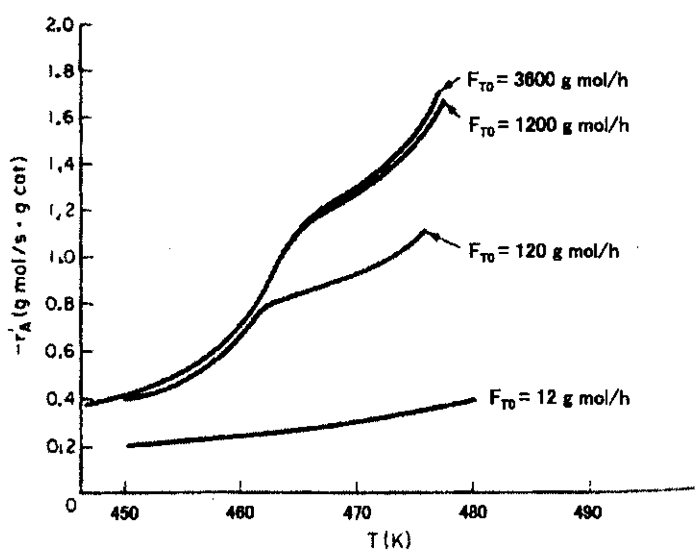

Figure 1

Under what conditions of those shown (i.e., T, F_{T0}) is the reaction limited by the rate of (a) the surface reaction, (b) internal diffusion and (c) external diffusion? (7%)

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

$$CH_2CHCH_2Cl\,(AC) + CO + NaOH \xrightarrow{Pd} C_3H_5COOH + NaCl$$

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 proposed 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? (15%)

5. (a) For a first order, gas-solid (catalyst) reaction, $A_{(g)} \rightarrow Product_{(s)}$, the isothermal overall effectiveness factor (η_0) is related to the catalyst effectiveness factor (η) by

$$\frac{1}{\eta_0} = \frac{k_A}{k_g} + \frac{1}{\eta}$$

where k_A is the reaction rate constant, and k_g is the gas-film mass transfer coefficient. Complete the table below ((i)-(v)) for the cases of (I) the surface reaction is rate controlling and (II) gas-film mass transfer is rate controlling. (8%)

Case	k_g vs. k_A	$C_{As} \rightarrow ?$	$\eta \rightarrow ?$	$\eta_0 \rightarrow ?$	$(-r_A) \rightarrow ?$
(I)	$k_g >> k_A$	C_{Ag}	(i)	1	$k_A C_{Ag}$
(II)	(ii)	(iii)	(ident.)	(iv)	(v)

Where C_{Ag} and C_{As} are the concentrations of A in bulk gas and on exterior surface of the catalyst, respectively, and $(-r_A)$ is the reaction rate.

(b) Under what circumstances does the calculation of catalyst effectiveness become independent on catalyst geometry? Explain. (3%)

6. (a) Give three factors that determine the selectivity in a chemical reaction. How and why do they affect the selectivity? (8%)

(b) Give the reason that we always find a mechanism for a chemical reaction? Describe the steps to find a satisfied mechanism for a chemical reaction? (6%)

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7. The elementary gas-phase reaction $A \xrightarrow{k} B$ is to be carried out in a CSTR adiabatically. The feed consists of 80% of A and the remainder inerts. The concentration of A in the feed at 27°C is 0.5 mol/*l*. The volumetric flow rate entering the reactor is 100 *l*/min. Calculate the reactor volume for 80% of the adiabatic equilibrium conversion. You do not need to obtain the final answer, but you **should**

   (a) write down all **equations** ready for solution, which mean no known variable or parameter is included.

   (b) describe **how** to obtain the answer. (20%)

   Additional Data: Heat capacity: C_{pA} = 12 J/mol·K, C_{pB} = 10 J/mol·K, C_{pI} = 15 J/mol·K
   Equilibrium constant: $\boldsymbol{K}$ = 70,000 at 300K,
   Rate constant: $k_1 = 0.217\ \text{min}^{-1}$ at 300K and $k = 0.324\ \text{min}^{-1}$ at 340K.
   The heat of reaction is a function of temperature, and its value at 300K is -57,000 J/mole of A.