1. For the elementary liquid-phase reaction $A \rightarrow B$, many combinations of CSTR, PFR and recycle reactors may be considered. The total volume of the reactors is 10 liters. The rate constant is $1 \cdot min^{-1}$ and pure A is fed at 5 $liter \cdot min^{-1}$. Please find the maximum conversion. (8%)

2. A long plug flow reactor was used to carry out an exothermic reaction with inlet temperature To. The temperature out side of the reactor, Ta, remains constant. (6%)
   (a) Sketch the temperature profiles inside of the reactor along the reactor length for:
      i. To > Ta,
      ii. To < Ta.
   (b) What is the major difference between these two profiles?

3. A first order reaction $2A \rightarrow B$ is carried out in an isothermal plug flow reactor. The inlet gas contains 50% A, 5% B and 45% inert. The feed flow rate of A is 1 $mole \cdot min^{-1}$. The feed temperature is 100 °C and the total pressure is 10 atm. At this temperature, the rate constant is 0.1 min^{-1}. What is the reactor volume to give outlet gas containing 10% A? (20%)

4. (a) The reaction $2NO + O_2 \rightarrow 2NO_2$ is third order. Assuming that a small amount of NO_3 exists in rapid reversible equilibrium with NO and O_2 and that the rate-determining step is the slow bimolecular reaction $NO_3 + NO \rightarrow 2NO_2$, derive the rate equation for this mechanism. (4%)
   (b) Another possible mechanism for the reaction $2NO + O_2 \rightarrow 2NO_2$ is
      (1) $NO + NO \xrightarrow{k_1} N_2O_2$
      (2) $N_2O_2 \xrightarrow{k_2} 2NO$
      (3) $N_2O_2 + O_2 \xrightarrow{k_3} 2NO_2$
   Apply the pseudo-steady-state hypothesis (PSSH) to obtain the rate law.
   If only a very small fraction of the N_2O_2 formed in (1) goes to form products in reaction (3), while most of the N_2O_2 reverts to NO in reaction (2), and if the activation energies are E_1, E_2, and E_3 for reactions (1), (2) and (3), respectively, what is the overall activation energy? (8%)
   (c) How would you distinguish experimentally between the mechanisms suggested in parts (a) and (b)? (3%)

(背面仍有題目,請繼續作答)

5. Calculate the selectivities of forming B in CSTR and PFR reactors at 70% conversion of A starting with C_{A0} = 5 moles/liter in the parallel reactions

$$A \xrightarrow{k_1} B \qquad r_1 = k_1 = 2$$
$$A \xrightarrow{k_2} C \qquad r_2 = k_2 C_A = C_A$$

where rate are in moles/liter-min. (8%)

6. A case of noncompetitive inhibition in enzyme reaction is represented in the following mechanism:

$$E + S \underset{k_{-1}}{\overset{k_1}{\longleftrightarrow}} ES \qquad (1)$$
$$E + I \underset{k_{-2}}{\overset{k_2}{\longleftrightarrow}} EI \quad (inactive) \qquad (2)$$
$$ES + I \underset{k_{-3}}{\overset{k_3}{\longleftrightarrow}} EIS \quad (inactive) \qquad (3)$$
$$ES \xrightarrow{k_r} E + P \qquad (4)$$

where E is the enzyme, S is a substrate, I is the inhibitor and P is a product.
Show the steady-state rate equation is the form

$$r_p = \frac{V_{\max} C_S}{C_S(1 + C_I / K_3) + K_m(1 + C_I / K_2)}$$

where V_{max} is the maximum initial rate $r_{po,\ max}=k_r C_{E0}$ and K_m is the Michaelis constant ($K_m = (k_{-1} + k_r)/k_1$). (10%)

7. Hydrogen (H) and toluene (T) are reacted over a solid mineral catalyst containing clinoptilolite (a crystalline silica-alumina) to yield methane (M) and benzene (B):

$$C_6H_5CH_{3\,(g)} + H_{2\,(g)} = C_6H_{6\,(g)} + CH_{4\,(g)}$$

The reaction sequence for this hydrodemethylation is

$T_{(g)} + S \rightleftharpoons T \cdot S$	Adsorption of toluene on the surface ($K_A = k_a / k_{-a}$)	(1)
$H_2 + T \cdot S \rightleftharpoons B \cdot S + M_{(g)}$	Surface reaction between adsorbed toluene and gaseous hydrogen ($K_S = k_s / k_{-s}$)	(2)
$B \cdot S \rightleftharpoons B_{(g)} + S$	Desorption of benzene from the surface ($K_D = k_d / k_{-d}$)	(3)

Assume that the surface reaction is the rate-determining step.

(a) Derive the rate law in terms of partial pressures of species present and the total concentration of sites (C_t). (10%)

(b) For an equal molar feed consisting only of toluene and hydrogen, express the initial rate in terms of total pressure (P_o). (5%)

8. The isomerization A → B is taking place on the surface of a solid sphere. The surface reaction follows a Langmuir-Hinshelwood single-site mechanism for which the rate law is

$$-r''_{As} = \frac{k_r C_{As}}{1 + K_A C_{As} + K_B C_{Bs}} \qquad (4)$$

and the molar flux to the surface is equal to the rate of reaction on the surface, i.e.,

$$W_A = -r''_{As} = k_c (C_A - C_{As}) \qquad (5)$$

where k_r = rate constant,

k_c = mass-transfer coefficient,

C_A, C_{As} = concentrations of component A in the bulk phase and at surface, respectively.

(a) Assuming that only very weak adsorption of A and B is needed to consider as the temperature is sufficiently high, show that the rate of reaction on the surface is (6%)

$$W_A = -r''_{As} = \frac{k_c k_r C_A}{k_r + k_c} \qquad (6)$$

(b) What is the rate of reaction for a rapid reaction? How would be the effects of velocity and particle size of catalyst on the reaction rate? (6%)

(c) What is the rate of reaction for a slow reaction? How would be the effects of velocity and particle size of catalyst on the reaction rate? (6%)