※ 考生請注意：本試題可使用計算機

1、A reactor system is to be designed for 85% conversion of A in a second-order liquid-phase reaction, A → products; $k_A = 0.075$ L mol^{-1}, $v_0 = 25$ L min^{-1} (volumetric flow rate), and $C_{A0} = 0.04$ mol L^{-1}. The cost of a vessel is \$ 0.29 L^{-1}, but a 10% discount applies if both vessels are of the same size and geometry. The design options are:

(A) two equal-sized stirred tanks in series; what is the capital cost of this design? (11%)

(B) two stirred tanks in series to provide a minimum total volume: what is the capital cost of this design? (11%)

(Hint: the solutions may be obtained by trial & error.)

2、Calculate the ratio of the volumes of a CSTR and a PFR (V_{ST}/V_{PF}) required to achieve a fractional conversion of 0.99 for the reactant A with an identical feed rate for each reactor, if the liquid-phase reaction A → products is

(A) first-order with respect to A (please find the value of V_{ST}/V_{PF}?) (5%)

(B) second-order with respect to A (please find the value of V_{ST}/V_{PF}?) (7%)

3、An enzyme Glucose 6-phosphatase has a K_M value of 10^{-4} M and a k_3 value of 10^4 min^{-1} at 37°C. The reaction catalyzed is the following:

$$\alpha\text{-D-Glucose 6-phosphate} \xrightarrow{Glucose\ 6-phosphatase} \text{D-Glucose}$$

Which can be represented as

$$E + S \underset{k_2}{\overset{k_1}{\rightleftharpoons}} ES \xrightarrow{k_3} E + P$$

Where S is α-D-Glucose 6-phosphate and P is D-glucose, E is the enzyme Glucose 6-phosphatase. The enzyme is not stable at 37 °C and the amount of active enzyme will decrease along time:

$$E = E_0 e^{-k_d t}$$

Where E_0 is the initial enzyme concentration and $k_d = 0.1$ min^{-1}. In an experiment, a certain amount of enzyme and 0.02M of α-D-Glucose 6-phosphate is added into a batch reactor and incubated at 37°C. After 12 hours, the concentration of D-glucose is found to be 0.002M. What is the initial concentration of enzyme (E_0)? (8%)

（背面仍有題目，請繼續作答）

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4、Cyclohexanol was passed over a catalyst to form water and cyclohexene:

cyclohexanol ⟶ water + cyclohexene

The following data were obtained:

Run	Reaction rate $(mol/dm^3 \cdot s) \times 10^5$	Partial pressure of cyclohexanol	Partial pressure of cyclohexene	Partial pressure of steam (H_2O)
1	3.30	1	1	1
2	1.05	5	1	1
3	0.57	10	1	1
4	1.83	2	5	1
5	1.49	2	10	1
6	1.36	3	0	5
7	1.08	3	0	10
8	0.86	1	10	10
9	0.00	0	5	8
10	1.37	3	3	3

It is suspected that the reaction may involve a dual-site mechanism. Please suggest a reaction mechanism and corresponding rate law for the above data. Detailed rationales and supporting calculations are required. (12%)

5、Reactant A at P_{A0} = 500kPa is to be passed through a packed bed catalytic reactor where it will decompose into either R or S. To maximize the formation of R, determine:

(A) Should the reactor operated in the strong pore diffusion regime or reaction rate limited regime? Please state your reason in detail and provide equations to validate your statement. (5%)

(B) Following (A), what is the length of the reactor if the conversion of A is 90%? (8%)

Additional information:

without the diffusion limitation, the reaction rates of R and S are: $A \nearrow R,\ r_R = 0.02C_A$; $A \searrow S,\ r_S = 0.03C_A$

Effective diffusivity of A: $2.66 \times 10^{-8}\ m^2/s$

Catalyst pellet diameter: 0.4 cm

（背面仍有題目，請繼續作答）

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Catalyst pellet density: $2 \times 10^6\ {}^{g}/_{m^3}$

Internal surface area of the catalyst pellet: $400\ {}^{m^2}/_{g}$

Linear velocity of A: $3\ {}^{m}/_{s}$
Inlet temperature: 250 °C

6、The following liquid-phase reactions were carried out in a 100-dm^3 PFR at 300K. The entering volumetric flow rate was 10 dm^3/min, with equal molar feed of A and B of $C_{A0} = C_{B0} = 2$ mol/dm^3.

$A + 2B \rightarrow 2C + 3D$	$r_{1D} = k_{1D}C_AC_B^2$	$k_{1D} = 0.25\ (dm^3/mol)^2/min$
$2D + 3A \rightarrow C + 2E$	$r_{2E} = k_{2E}C_AC_D$	$k_{2E} = 0.1\ (dm^3/mol)/min$
$B + 2C \rightarrow 3D + 4F$	$r_{3F} = k_{3F}C_BC_C^2$	$k_{3F} = 5.0\ (dm^3/mol)^2/min$

(A) Please list out all the equations you need to input into a computer software in order to obtain the species concentrations and the instantaneous selectivity $S_{C/DEF}$ (i.e. C is the desired product and D~F are undesired products) as a function of reactor volume. (10%)

(B) Please qualitatively describe how to enhance the selectivity and which type of reactor would be suitable. (3%)

7、Please explain the phenomenon of "multiple steady state" in a nonisothermal CSTR running an exothermic and first-order reaction and define the condition of runaway point mathematically. (20%)

Hint: By neglecting the shaft work and assuming $\Delta C_P = 0$,

$$-X\Delta H_{Rx}^{o} = C_{P0}(1 + \kappa)(T - T_c)$$

where $C_{P0} = \Sigma\Theta_iC_{Pi}$; $\kappa = (UA/C_{P0}F_{A0})$; $T_c = (\kappa T_a + T_0)/(1 + \kappa)$

(X: conversion; ΔH_{Rx}^{o} : heat of reaction; U: overall heat transfer coefficient; A: heat transfer area; T_a: coolant temperature)