國立臺灣科技大學103學年度碩士班招生試題

系所組別： 化學工程系碩士班

科　　目： 化工熱力學與動力學

（總分為100分）

PART I. 化工熱力學 (50%)

1. The heat of mixing for the *n*-octanol + *n*-decane liquid mixture at atmospheric pressure is approximately fit by

$$\Delta_{\text{mix}}\underline{H} = x_1 x_2 (A + B(x_1 - x_2)) \qquad \text{J/mol}$$

where A = 2477.5 and B = -1455.9 at T = 300 K and x_1 being the *n*-octanol mole fraction. Compute the difference between the partial molar and pure-component enthalpies of n-octanol and n-decane at x_1 = 0.5 and T = 300 K. (15%)

2. A gas with a heat capacity $C_P = 28.87\ \text{JK}^{-1}\text{mol}^{-1}$ obeys the equation of state, $P\underline{V} = RT + BP$, where B is a function of temperature:

T(K)	200	250	300	400
B(cm^3/mol)	-35.2	-16.2	-4.2	+9.0

Determine the Joule-Thomson coefficient of the gas at 2°C. (15%)

3. A catalyst has been found which gives adequate rate of reaction at 500°C in the reaction CO + 2H_2 = CH_3OH. The feed contains CO and H_2 only with a molar ratio CO/H_2=1/2. Estimate the pressure required to obtain 10% CO conversion. The free energy and heat of formation are as follows (cal/mol)

	$\Delta_f G^0_{298}$	$\Delta_f H^0_{298}$
CO	-32810	-26420
CH_3OH	-38690	-48080

Assuming the heat of reaction at standard state, ΔH^0_T, is independent of temperature and the gases at the reaction condition obey ideal gas law. (20%)

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PART II. 化工動力學 (50%)

1. (20%)

The adiabatic exothermic irreversible gas-phase reaction

$$2A + B \rightarrow 2C$$

is to be carried out in a flow reactor for an equimolar feed of A and B. The following data for this reaction are shown below, where $F_{A0}/(-r_A)$ is the ratio of molar flow rate of reactant A in the feed and the rate of consumption of reactant A per unit volume at conversion X.

Conversion X	0	0.1	0.3	0.5	0.6	0.7	0.8
$F_{A0}/(-r_A)$ (m^3)	50	42	26	10	70/3	110/3	50

(a) What PFR (Plug Flow Reactor) volume is necessary to achieve 50% conversion? (5%)

(b) What CSTR (Continuous Stirred Tank Reactor) volume is necessary to achieve 50% conversion? (5%)

(c) What conversion can be achieved if an $8m^3$ CSTR is followed in a series by an $8\ m^3$ PFR? (10%)

Hint: Useful formula for this problem

(1) The five-point quadrature formula for the integration $\int_{x0}^{x4} f(x)dx = h/3(f_0+4f_1+2f_2+4f_3+f_4)$,

where f_i is the function value at x_i, and $h = (x_4-x_0)/4$

(2) For $ax^2 + bx + c = 0$, the roots, p and q, are $\frac{-b \pm \sqrt{b^2-4ac}}{2a}$

Show All Your Work.

2. (15%)

Pharmacokinetics (藥物動力學) concerns the ingestion (攝取), distribution, reaction, and elimination (移除) reaction of drugs in the body. Consider the application of pharmacokinetics to one of the major problems in Taiwan, drinking and driving (酒醉開車). Here, we shall model how long one must wait to drive after having a tall martini (一高杯的馬丁尼酒). In Taiwan, the legal intoxication limit (法定酒醉限值) is 0.3 g of ethanol (酒精) per liter of body fluid. (In the United States, it is 0.8 g/L, in Sweden it is 0.2 g/L, and in Eastern Europe and Russia it is any value above 0.0 g/L.) The ingestion of ethanol into the bloodstream(血液) and subsequent elimination can be modeled as a series reaction. The rate of absorption from the gastrointestinal tract (腹部的腸道) into the bloodstream and body is a first-order reaction with a specific reaction rate constant of

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$10\ h^{-1}$. The rate at which ethanol is broken down in the bloodstream is limited by regeneration of a coenzyme. Consequently, the process may be modeled as a zero-order reaction with a specific reaction rate of 0.192 g/h·L of body fluid.

(a) How long would a person have to wait to drive in Taiwan if they drank two tall martinis immediately after arriving at a party? (10%)

(b) Suppose that one went to a party, had one and a half tall martinis right away, and then received a phone call saying an emergency had come up and the person needed to drive home immediately. How many minutes would the individual have to reach home before he/she became legally intoxicated (超出法定酒醉限值), assuming that the person had nothing further to drink? (5%)

(Hint: Base all ethanol concentrations on the volume of body fluid. Calculate and plot the concentration of ethanol in the blood as a function of time.)

Additional information:

Ethanol in a tall martini: 40 g

Volume of body fluid: 40 L

Show All Your Work.

3．(15%)

For the elementary reversible solid-catalyzed liquid-phase reaction

$$A \Leftrightarrow B$$

(a) Make a plot of equilibrium conversion as a function of temperature. (5%)

Hint 1: Prepare a table of equilibrium constant K_e and equilibrium conversion X_e as a function of temperature at 298, 350, 400, 425, 450, 475, and 500 K first, and then make a plot of X_e vs. T in (a).

Hint 2: $K_e(T) = K_e(T_1)\ \exp[\Delta H^0_{RX}/R\ (1/T_1 - 1/T)]$

(b) Determine the adiabatic equilibrium temperature and conversion when pure A is fed to the reactor at a temperature of 300 K. (10%)

Additional information:

H_A^0 (298 K) = -40,000 cal/mol, H_B^0 (298 K) = -60,000 cal/mol, C_{PA} = 50 cal/mol.K, C_{PB} = 50 cal/mol.K, K_e = 100,000 at 298 K, and R (gas constant) = 1.987 cal/mol.K.

Show All Your Work.