國立中正大學八十七學年度碩士班考試試題

所　別：化學工程學系　　科　目：化工熱力學與化工動力學

(化工動力學部份　　)

1. An ester is formed in aqueous solution by reacting an acid with an alcohol. Assuming this reaction is an irreversible, second order reaction over the conversion range,

(1) prove that in any instant

$$\ln\frac{[acid]}{[alcohol]} = \left([acid]_o - [alcohol]_o\right) k\, t + \ln\frac{[acid]_o}{[alcohol]_o}$$

where k is the rate constant, t is the reaction time, and the subscript o represents the initial condition.

(10 points)

(2) Suppose the initial acid concentration is 0.1 molal and the alcohol concentration is 0.2 molal, calculate the rate constant based on the following experimental data

time (min)	acid conversion (%)
10	17.05
20	30.17
30	40.55
40	48.91

(10 points)

2. The following isothermal reversible reaction occurs in a tubular reactor at 760 ℃ with an equilibrium constant of 0.312

$$2A \underset{k_r}{\overset{k}{\Leftrightarrow}} B + C$$

where the second order rate constant k for the forward reaction follows the Arrhenius law

$$k = 15.31 \times 10^5\, e^{-\frac{15200}{T}} \quad ft^3 / lb\ mole \cdot hr$$

(a) What is the maximum achievable conversion of reactant A ?
(10 points)

(b) What is the reactor volume required to achieve 50% conversion of A at a feed rate of 150 lb mole/hr?
(10 points)

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3. A liquid phase, first order reaction was carried out isothermally in three CSTR reactors in series. It was known that the second reactor was as large as the first reactor, and the third reactor was χ times larger than the first one. It was also assumed that the density was constant throughout the system. If 30% conversion was achieved in the first reactor, what should the χ be in order to achieve a total conversion of 81.95% ?
(10 points)

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4. The virial equation of state for gases has a sound theoretical foundation and is free of arbitrary assumptions. It can be written as:

$$Z = \frac{PV}{RT} = 1 + B/V + C/V^2 + D/V^3 + \cdots$$

It is usually said that a virial equation, when truncated after the third term (*i.e.*, Z = 1 + B/V), can be used with good accuracy at pressures up to *ca.* 15 atms. At higher pressures, however, the second and even higher virial coefficients may be required in the calculation. Explain why? **(10 points)**

5. One method for manufacturing synthesis gas is the catalytic reforming of CH_4 with steam at high temperature and atmospheric pressure:

$$CH_4(g) + H_2O(g) \rightarrow CO(g) + 3\,H_2(g)$$

The only other reaction which occurs to a significant extent is the water-gas-shift reaction:

$$CO(g) + H_2O(g) \rightarrow CO_2(g) + H_2(g)$$

If the reactants are supplied at a rate of 3 mol s^{-1} in the ratio, 2 moles steam to 1 mole CH_4 in a steady-flow process at 1 atm, and if heat is supplied to the reactor so that the products reach a temperature of 1,300 K, the CH_4 is completely converted and the product stream contains 17.4 mole percent CO. If the reactants are preheated to 600 K, calculate the rate of heat requirement for the reactor in J s^{-1}. **(20 points)**

Table 1　Standard heat of formation

Chemical species		State	$\triangle H^o_{298}$ (J mol^{-1})
Methane	CH_4	g	-74,520
Carbon monoxide	CO	g	-110,525
Carbon dioxide	CO_2	g	-393,509
water	H_2O	g	-241,818

Table 2　Constants for $C_p^{ig} / R = A + BT + CT^2 + D / T^2$

Chemical species	A	10^3B	10^6C	10^{-5}D
Methane	1.702	9.081	-2.164	---------
Carbon monoxide	3.376	0.557	---------	-0.031
Carbon dioxide	5.457	1.045	---------	-1.157
Water	3.470	1.450	---------	0.121
Hydrogen	3.249	0.422	---------	0.083

6. The enthalpy of a binary liquid system of ethanol (1) and water (2) at fixed temperature and pressure is represented by following:

$$H = 200x_1 + 300x_2 + x_1x_2(60x_1 + 30x_2)$$

where H is in J mol^{-1}. Determine expressions for $\overline{H}_1$ and $\overline{H}_2$ as functions of x_1, numerical values of enthalpy for pure ethanol and pure water, and numerical values of partial molar enthalpy for ethanol and water at infinite dilution. **(20 points)**

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