國立臺北科技大學

九十四學年度化學工程研究所入學考試

化工熱力學與反應工程試題

填准考證號碼　　　　　　　　　　　　　第一頁　共二頁

注意事項：
1. 本試題共 4 題，配分共100分。
2. 請按順序標明題號作答，不必抄題。
3. 全部答案均須答在答案卷之答案欄內，否則不予計分。

1. For a second order gas phase reaction, $2A_{(g)} \rightarrow B_{(g)}$, the rate is reported as

$$-\frac{dC_A}{dt} = k\,C_A^{\,2}\ , \qquad \frac{\text{mol}}{\text{liter} \cdot \text{hr}}$$

For an elementary reactions, theory predicts that the rate constant should be temperature-dependent in Arrhenius' law or collision theory. The data of partial pressure of A in Table (1) are the kinetic study of this gas phase reaction system.

(1). What are the units of the rate constant? (5%)

(2). What are the rate constant of each temperature? (15%)

(3). For the case of Arrhenius' law, what is the activation energy of this gas reaction system? (10%)

Table (1) The experimental data of the gas reaction, $2A_{(g)} \rightarrow B_{(g)}$

T/K	400	450	500
time/hr		P_A / bar	
0.0	2.000	2.250	2.500
0.1	1.415	0.842	0.409
0.2	1.095	0.518	0.223
0.3	0.893	0.374	0.153
0.4	0.754	0.293	0.116
0.5	0.652	0.240	0.094

2. For the isomeric reaction of $A \rightarrow R$, $k_c = 0.02\ \text{min}^{-1}$. It is desired to product 2,376 mol of R for one-batch operation, and 99% of A entering the reactor is to be converted. To charge the reactor and to heat it to reaction temperature requires 0.28 hr. To discharge the reactor and to prepare it for the next run takes 0.95 hr. Pure A with molar density of 8 mol/liter is charged to the reactor and the products with molar density of 10 mol/liter is identify at the ending of reaction.

(1). Calculate the total cycle time [hr] of one batch operation required. (10%)

(2). Calculate the minimum volume [m^3] of the reactor required. (10%)

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3. The data in Table (2) are molar volume of carbon dioxide at 423.15 K. The fugacity coefficient ($\phi_i = f_i/P$), a dimensionless property, is a measure of the ideal gas behavior, which may will calculated from the volumetric data. According to the definition, the fugacity coefficient is given by residual Gibbs free energy as

$$\ln\phi_i = \frac{G_i^R}{RT} \quad \text{at constant T.}$$

(1). Derive the equation of fugacity coefficient in terms of PVT properties. (10%)

(2). Calculate the fugacity coefficient of carbon dioxide at pressure of 300 bar. (10%)

Table(2) Molar volume of carbon dioxide at 423.15 K

P/bar	$\underline{V}$/cm^{3}mol^{-1}	P/bar	$\underline{V}$/cm^{3}mol^{-1}
10	3,465.3	100	305.7
20	1,706.3	200	134.6
40	827.6	300	89.4
60	535.3	400	72.5
80	390.5	500	64.0

4. The heat of mixing data for a binary liquid mixture at atmospheric pressure as approximately fit by

$$\Delta \underline{H}_{mixing} = x_1 x_2 [A + B(x_1 - x_2)] \qquad \text{J/mol}$$

where

$$A = -12{,}974 + 51.505T$$

and

$$B = +8{,}782.8 - 34.129T$$

The molar enthalpy of pure components are $\underline{H}_1 = 10{,}250$ J/mol and $\underline{H}_2 = 8{,}850$ J/mol, respectively.

(1). Derive the formula of $\overline{H}_2 = f(x_1)$ at T = 300 K. (10%)

(2). Calculate the $\overline{H}_2$ at $x_1 = 0.3$ and T = 300 K. (10%)

(3). Calculate the $\overline{H}_2^{\infty}$ at T = 300 K. (10%)