八十六學年度 化學工程學系 系(所) 甲 組碩士班研究生入學考試

科目 化工熱力學及化學反應工程 科號 1602 共 3 頁第 1 頁 *請在試卷【答案卷】內作答

Problem 1 (20%)

在炎炎的夏日午季中,喝杯冰鎮紅茶是一件很愉快的事。除了那沁透身心的涼意外,看著那晶瑩剔透的冰塊,於紅茶中載浮載沉,也是一件賞心悅目的事。 冰塊一般是由室溫的純水,於約攝氏零下五度的冷凍室中凝結而成,其環境的壓力則為一標準大氣壓。請問:

(a) 此從純水凝結成冰塊的反應,是否為自發(spontaneous)反應? 何謂自發反應?

(b) 此從純水凝結成冰塊的反應,是否為可逆(reversible)的反應? 何謂可逆反應?

(c) 當此純水系統(system)凝結成冰塊時,此系統(僅指純水與冰塊,不含環境)的亂度(entropy),則因此作何改變(增加、不變、還是減少)?為什麼?

(d) 當純水凝結成冰塊時,整個宇宙(universe)(含系統與環境)的焓(enthalpy),則因此作何改變?為什麼?

(e) 當純水凝結成冰塊時,整個宇宙(universe)(含系統與環境)的亂度(entropy),則因此作何改變?為什麼?

Problem 2 (20%)

VLE in the benzene-toluene system is well represented by Raoult's law at low and moderate pressure. Vapor-pressure data [in(atm)] for benzene (1) and toluene (2) are:

| T(°C) | $P_1^{sat}$ | $P_2^{sat}$ | T(°C) | $P_1^{sat}$ | $P_2^{sat}$ |
|---|---|---|---|---|---|
| 80.1 | 1.000 | 0.384 | 98 | 1.683 | 0.689 |
| 84 | 1.126 | 0.439 | 100 | 1.777 | 0.732 |
| 88 | 1.268 | 0.501 | 104 | 1.978 | 0.825 |
| 90 | 1.343 | 0.535 | 108 | 2.196 | 0.928 |
| 94 | 1.506 | 0.608 | 110.6 | 2.347 | 1.000 |

(i) What are the bubble point pressure and vapor phase composition at 90°C with $x_1 = 0.3$ (in liquid)?

(ii) What are the dew point pressure and liquid phase composition at 100°C with $y_1 = 0.3$ (in vapor)?

(iii) What is the bubble point temperature at 1 atm total pressure and $x_1 = 0.3$ (in liquid)?

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Problem 3 (20%)

The dimethylether decomposition at 504°C is studied in an isothermal constant volume reactor. Only pure dimethylether is initially in the reactor. Ideal gas behavior is assumed

$$CH_3OCH_3 \rightarrow CH_4 + H_2 + CO$$

| Time (s) | P ($kP_a$) |
|---|---|
| 0 | 41.6 |
| 390 | 54.4 |
| 777 | 65.1 |
| 1195 | 74.9 |
| 3155 | 103.9 |
| ∞ | 124.1 |

(i) Determine the order of the reaction. (8%)

(ii) Determine the rate constant at this temperature. (8%)

(iii) If this reaction is studied in an isothermal constant pressure reactor with the same initial condition as above, how long will it take to double the volume of the reactor? (4%)

Problem 4 (20%)

The gas-phase reaction $A + 2B \rightarrow 2D$ is to be carried out in an isothermal plug-flow reactor at 5.0 atm. The mole fractions of the feedstream are: A = 0.20, B = 0.50, and inerts – 0.30.

(4%) (a) Derive an expression for the steady-state volumetric flow rate as a function of conversion (based on A) at any point in the reactor if the pressure drop due to fluid friction can be ignored.

(4%) (b) Derive the expressions for the concentrations of A, B, and D as a function of conversion at any point along the reactor.

(4%) (c) Calculate the feed concentration (units: $mol/dm^3$) of A if the feed temperature is 55 °C. Assume ideal-gas behavior.

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(8%) (d) If a plug-flow reactor has achieved a conversion (based on A) of 0.70, how large (unit: $dm^3$) would a CSTR have to be to take the effluent from the plug-flow reactor and achieve a conversion of 0.85 (based on the feed of A to the plug-flow reactor)? The temperature of the CSTR is 55 °C, the volumetric feed rate is 50 $dm^3$ / min, and the rate law at 55 °C is

$$-r_A = 2.5\, C_A^{1/2}\, C_B \quad kmol / m^3 \cdot min$$

Problem 5(20%)

The elementary reversible gas-phase reaction

$$A \rightleftharpoons B$$

is to be carried out adiabatically to achieve 45% conversion of A. Pure A is to be fed to the reactor at a rate of 10 g-mole/min at a pressure of 2.87 atm and a temperature of 77°C. Calculate the temperature of the exit stream and reactor volume for a CSTR.

Additional data:

specific reaction rate at 0°C: 0.001 $h^{-1}$ (first order)

activation energy: 10,000 cal/g-mole

exothermic heat of reaction at 27°C: -20,000 cal/g-mole A

equilibrium constant at 127°C: 25,000

heat capacity of A: 20 cal/g-mole · K

heat capacity of B: 30 cal/g-mole · K