國立台灣科技大學九十八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

（總分爲 100 分）

PART I 化工熱力學 (50%)

1. "A reaction that results in more order in the system ($\Delta S_{system} < 0$) can never be spontaneous." Is the above statement correct or incorrect? Without explanation you will receive no points. (5)

2. An ideal gas is contained in a rigid tank of volume V initially at P_1 and T_1. Heat is supplied to the contents until a pressure P_2. The gas can escape as the pressure reaches P_2, which is the set pressure of the relief valve on the tank.
   (a) Derive an expression for the heat transfer in terms of V, P_1 and P_2 during the change from P_1 to P_2. (5)
   (b) Derive an expression for the heat transfer in terms of V, T and P_2 when gas start to escape from the tank. (10)

3. (a) Use the Clayperon equation, $\frac{dP}{dT} = \frac{\Delta H}{T\Delta V}$, to calculate the pressure (in kPa) at which ice would melt at -5 °C. Data: ice melts at 273.15 K at 101.3 kPa, ΔH_{fusion} = 6.01 kJ/mol, the density of ice is 920 kg/m^3, the density of liquid water is 997 kg/m^3, and the molar mass of water is 18.02 g/mol. (10)
   (b) Assume an ice skater weighs 60 kg, and she uses skates that have a length of 30 cm. What should be the width of her skates to make ice melt at -5 °C? Describe in details what happen to the ice during her ice skating. (5)

4. Calculate the heat exchange of (i) one mole of a gas following the equation of state of P(V - b) = RT, and (ii) one mole of Ni during (a) a reversible process of isothermal change in pressure from 1 atm to 1000 atm at 300 K and (b) a sudden release of pressure from 1000 atm, 300 K back to 1 atm. (Hint: Find the thermodynamic relationship of reversible heat.) The needed data for the gas: b = 0.04 m^3/kmol and C_P = 35.56 J/mol/K, and for Ni: $C_P = 16.99 + 2.95\cdot10^{-2}$ T in J/mol/K, density = 8.9 g/cm^3, MW = 58.7 g/mol, $\alpha_P = 40\cdot10^{-6}$ K^{-1}, and $\kappa_T = 1.5\cdot10^{-6}$ atm^{-1}. (15)

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PART II 化工動力學 (50%)

(1) The catalytic liquid-phase reactions in an isothermal batch reactor are shown as following. In the beginning, the values of C_A, C_B, C_C and C_D are C_{A0}, C_{B0}, 0 and 0, respectively.

$$A + B \xrightarrow{k_1} C + D$$

$$C + A \xrightarrow{k_2} P$$

$$D \xrightarrow{k_3} B$$

Where k_3 is very large and $k_2 >> k_1$. All reactions are elementary and please express the conversion of A species by time, rate constant and C_B. (10%)

(2) The homogeneous gas decomposition of phosphine, 4 $PH_3(g) \rightarrow P_4(g) + 6\ H_2(g)$, proceeds isothermally at 649°C with a rate constant of 10 hr^{-1}.

(a) What size plug-flow reactor (PFR) operating at 460 kPa can produce 70% conversion of a pure feed consisting of 40 mol/h of pure phosphine? (10%)

(b) What is the size of continuous-stirred tank reactor (CSTR) in the same operating conditions for 80% conversion? (10%)

Hint: gas constant (R) = 8.3 Pa-m^3/mol-K,

$$\int_0 \frac{1+ax}{1-x} = (1+a)\ln\frac{1}{1-x} - ax$$

(3) Make your sketches to get maximum selectivity of product D. Please describe the proper operation conditions, such as temperature, concentration. (5%)

A+B→D $-r_{1A}=10\exp(-1000/T)C_A^{1.5}C_B$

A+B→U $-r_{2A}=10^9\exp(-10000/T)C_A^{0.5}C_B^{1.5}$

(4) The following liquid-phase reaction is carried out in an **adiabatic** CSTR without shaft work.

$$A \underset{k_2}{\overset{k_1}{\rightleftharpoons}} B$$

Please calculate the reactor volume necessary to achieve 90% conversion. The formula obtained from energy balance of reactor temperature and conversion is: T (K) = T_0 + 40 X.

Additional information:

Feed = 300 kmol/h at 330K, C_{A0}= 20 M, C_{B0}=0,

E (activation energy) = 60000 J/mol, k_1 (rate constant at 360K) = 30 h^{-1},

K_c (concentration equilibrium constant at 330 K) = 3

ΔH_{Rxn} (Heat of reaction at 298K) = -7000 J/mol-A, R=8.3 J/mol-K

Van't - Hoff Relationship $\frac{d\ln K_c}{dT} = \frac{\Delta H_{Rxn}(T)}{RT^2}$ (15%)