國立中央大學 112 學年度碩士班考試入學試題

所別： 化學工程與材料工程學系碩士班

科目： 化工熱力學及化學反應工程

計算題與問答題請在答案卷內作答，計算題請詳列計算過程。

1. **(15 pts)** An empirical relation is proposed to describe the fugacity of a pure gas for a pressure ranging from 0 to 20 bar and a temperature region of 30 to 120 °C:

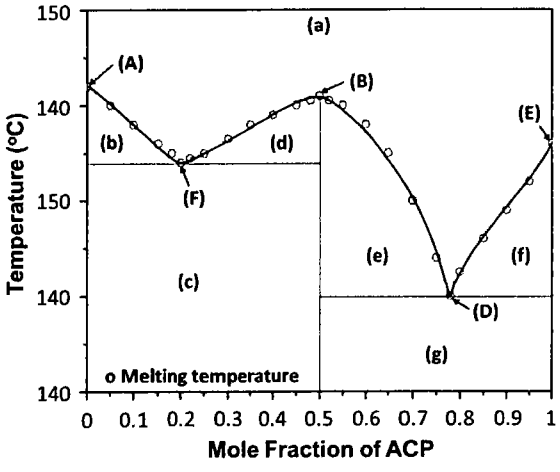
$$\ln\left(\frac{f}{P}\right)=-\left(-0.07+\frac{28.70}{T}\right)P-\left(0.0011-\frac{0.420}{T}\right)P^2$$

where P is the pressure in bar and T is the temperature in K. Please use the Gibbs-Helmholtz equation to determine the molar enthalpy ($\underline{H}^{\text{real}}$) of the gas at 60 °C and 10 bar relative to that of the ideal gas at the same temperature, i.e., $\Delta\underline{H}$.

Hint: (1) The Gibbs-Helmholtz equation: $\dfrac{\partial\left(\frac{\Delta\underline{G}}{T}\right)}{\partial\left(\frac{1}{T}\right)}=\Delta\underline{H}=\underline{H}^{\text{real}}-\underline{H}^{\text{ideal}}$

(2) The definition of fugacity: $f=P\exp\left[\dfrac{\underline{G}^{\text{real}}(T,P)-\underline{G}^{\text{ideal}}(T,P)}{RT}\right]$

2. **(15 pts)** Understanding phase diagrams of solid-liquid equilibrium is essential for a chemical engineer. According to the solid-liquid equilibrium phase diagram for 2-amino-5-chloropyridine (ACP) + 3-nitrobenzoic acid (NBA) at room pressure [adapted from U. Neupane and R.N. Rai, *J. Chem. Thermodyn.*, 161, 106513 (2021)], please answer the following questions:



(1) How many eutectic points exist on the melting temperature curve? Where are they? **(5 pts)**

(2) Which regions represent the solid-liquid equilibrium? **(5 pts)**

(3) In which region can solid ACP be observed? **(5 pts)**

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3. (1) **(10 pts)** The expression for excess Gibbs energy of the van Laar model is as follows:

$$\frac{G^{ex}}{RT}=\frac{\alpha x_1 \beta x_2}{\alpha x_1+\beta x_2}$$

Please derive the activity coefficient equations for both components of a binary mixture in the following form:

$$\ln\gamma_1=\frac{\alpha}{A} \text{ and } \ln\gamma_2=\frac{\beta}{B}$$

What is the expression for A and B?

(2) **(10 pts)** The values of the parameters in the activity coefficient equations are usually found by fitting these equations to experimental activity coefficient data over the whole composition range. Alternatively, if only limited data are available, the van Laar equations can be written as

$$\alpha=\left(1+\frac{x_2\ln\gamma_2}{x_1\ln\gamma_1}\right)^2\ln\gamma_1 \text{ and } \beta=\left(1+\frac{x_1\ln\gamma_1}{x_2\ln\gamma_2}\right)^2\ln\gamma_2$$

Please use these two equations to determine the values of binary interaction parameters for a vapor-liquid mixture of furfural and water at 1.013 bar and 109.5 °C. It is observed that at equilibrium the water content of the liquid is 10 mol% and that of the vapor is 81 mol%. Assuming that the vapor phase is ideal. The vapor pressures of furfural and water at 109.5 °C are 0.169 and 1.41 bar, respectively.

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4. The gas phase reaction

$A + B \rightarrow C + D$ (the stoichiometric coefficients, for A, B, C, and D, are 1)

is carried out in a packed-bed catalytic reactor. As a chemical engineer, you are assigned to design this reaction system. Please answer the following questions based on your reaction engineering knowledge.

(1) **(6 pts)** When the catalyst particle size was decreased by 10%, the conversion remained unchanged. When the particle size was decreased by 15%, the conversion decreased. When the original particle size was increased by 10%, the conversion also decreased. In all cases, the temperature, the total catalyst weight, and all other conditions remained unchanged. What is the suitable explanation?

(2) **(10 pts)** Please develop an algebraic rate law based on the experimental observations shown below.

(3) **(16 pts)** Find a mechanism consistent with experimental observations and identify the rate-limiting step. Assume Eley-Rideal mechanism applies for this reaction, while A will adsorb on the catalyst surface. Explain how to determine the model parameters of the rate law derived in (2).

(4) **(18 pts)** The molar feed rate of A to the reactor is 40 mol/min, and the reactor inlet is at 20 atm and 627 °C. This gas phase reaction is carried out in a packed-bed reactor isothermally. The feed consists of 25% A, 40% B, and 35% inert. The pressure drop parameter α is 10^{-4} kg^{-1}. Plot, schematically, the conversion, and the pressure ratio, y, as a function of PBR catalyst weight. Please write down the balance equation and the detailed procedures.

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Run	$-r_A' \times 10^{10}$ $\left(\frac{\text{g mol A}}{\text{g cat.} \cdot \text{s}}\right)$	*Partial Pressure* (atm) P_A	P_B	P_C	P_D
Set A					
1	35.0	1	1	1	0
2	35.7	1	1	4	0
Set B					
3	20.8	1	1	0	1
4	9.8	1	1	0	4
5	21.0	1	1	1	1
6	8.5	1	1	0	5
Set C					
7	36.0	1	1	0	0
8	71.0	1	2	0	0
9	142.0	1	4	0	0
Set D					
10	23.5	0.5	1	0	0
11	35.5	1	1	0	0
12	58.5	5	1	0	0
13	63.5	10	1	0	0
14	65.7	15	1	0	0
15	66.3	20	1	0	0
16	20.9	1	1	1	1

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