Problem 1 (20%)

(a) A vessel, divided into two parts by a partition, contains 2 moles of ideal gas A at one side at 300 K and 10^5 Pa and 3 moles of ideal gas B at 400 K and 4×10^5 Pa. What is the volume of the ideal gas A? (b) The gas A is first compressed isothermally to 2×10^5 Pa by following a reversible process. Please calculate Q, W, ΔU, and ΔH for the process. (c) The partition is then removed. The gases A and B mix adiabatically and completely. What is the temperature of the gas mixture? What is the pressure of the gas mixture? What is the change in ΔS? The heat capacities of the two gases are $C_p = 3.5R$ and $C_v = 2.5R$. R is the universal gas constant and is 8.314 J mol^{-1} K^{-1}(8.314 m^3 Pa $mol^{-1}K^{-1}$). $\ell n\,2$=0.6931, $\ell n\,3$=1.0986, $\ell n\,5$=1.6094, $\ell n\,7$=1.9459.

Problem 2 (20%)

(i) Draw the $p-x_1-y_1$ phase diagrams of a binary mixture at constant temperature: (a) $T_a < T_{c1}, T_{c2}$, (b) $T_{c1} < T_b < T_{c2}$, and (c) $T_d > T_{c1}, T_{c2}$.

T_{c1} and T_{c2} are critical temperatures of components 1 and 2, respectively.

(ii) Write $\frac{\Delta G}{RT}, \frac{P\Delta V}{RT}, \frac{\Delta H}{RT}$, and $\frac{\Delta S}{R}$ in terms of activities and find the corresponding expressions for ideal solutions.

Note: ΔM is the property change of mixing.

Problem 3 (20%)

$$H_2 + CO_2 = CO + H_2O$$

1. (4%) Write down the stoichiometric coefficient of H_2, CO_2, CO, H_2O
2. (2%) Define the extent of this reaction
3. (4%) If there are 0.5 mole of H_2 and 0.5 mole of CO_2 initially, what are the mole fraction of H_2, CO_2, CO, H_2O when the extent of reaction is 0.2.
4. (2%) The Gibbs free energy of formation at 1000 K of CO_2, CO, H_2O are -192,420, -200,240 and -395,790 J mol^{-1} respectively. Find the initial Gibbs free energy of the system
5. (6%) Find Gibbs free energy when the extent of reaction are 0.2 and 0.4
6. (2%) Which extent of reaction is closer to equilibrium

The following data are given to facilitate calculations：

$R = 8.314 \frac{J}{K \cdot mol}$ $RT = 8314 \frac{J}{mol}$

x	ln(x)
0.1	-2.30259
0.2	-1.60944
0.3	-1.20397
0.4	-0.91629
0.5	-0.69315
0.6	-0.51083
0.7	-0.35667
0.8	-0.22314
0.9	-0.10536

Problem 4 (20%)

The overall reaction for the thermal decomposition of acetaldehyde is

$$CH_3CHO \rightarrow CH_4 + CO$$

A chain-reaction sequence of elementary steps proposed to explain the decomposition is as follows:

Initiation

$$CH_3CHO \xrightarrow{k_1} CH_3^{\cdot} + CHO^{\cdot}$$

Propagation

$$CH_3^{\cdot} + CH_3CHO \rightarrow CH_3CO^{\cdot} + CH_4$$

$$CH_3CO^{\cdot} \rightarrow CH_3^{\cdot} + CO$$

Termination

$$CH_3^{\cdot} + CH_3^{\cdot} \xrightarrow{k_4} C_2H_6$$

Use the stationary-state approximation to derive an expression for the overall rate of decomposition.

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Problem 5 (20%)

Compound A undergoes a reversible reaction $A \rightleftharpoons B$ in a plug flow reactor. The feed to the reactor is pure A and the reaction is elementary. A and B are liquid, miscible, and of nearly indentical density. The product from the plug flow reactor are separated and only the unconverted A is fed to a second, identical reactor.

(5%) (1) Derive the equation for the conversion of A in the first reactor, x_1.

(10%) (2) Derive the equation for the conversion of A in the second reactor, x_2, in terms of x_1 and K_{eq}.

(5%) (3) Find the overall conversion X.

Notation:

k	:forward reaction rate constant
K_{eq}	:equilibrium constant for the reaction
F_{AO}	:molar flow rate of A to the first reactor
C_{AO}	:concentration of A in the feed to the first reactor
V:	:reactor volume