Problem 1 (20%)

A gas mixture of one mole C_2H_2 and three moles N_2O was ignited at 300 K. A gas mixture which contains two moles CO, one mole H_2O, and three moles N_2 is then formed corresponding to the following reaction: $C_2H_2 + 3N_2O = 2CO + H_2O + 3N_2$. Assume that the gas mixture is contained at 1 atm in an insulated container, the combustion process is isobaric, the gases behave ideally, and their heat capacities are all 10 cal/degree/mole. (a) What is the enthalpy change of the gas mixture before and after combustion ? (b) What is temperature of the gas mixture after combustion ? (c) What is the entropy change of the gas mixture before and after combustion ?

Given:

$\Delta H^o_{300K,(C_2H2)} = 54.23 kcal/mole$, $\Delta H^o_{300K,(N_2O)} = 19.70 kcal/mole$

$\Delta H^o_{300K,(CO)} = -26.42 kcal/mole$, $\Delta H^o_{300K,(H_2O)} = -57.80 kcal/mole$

$C_{p,(C_2H_2)} = C_{p,(N_2O)} = C_{p,(CO)} = C_{p,(H_2O)} = C_{p,(N_2)} = 10 cal/degree/mole$

Logarithms to Base e (Natural logarithms)

N	.0	.1	.2	.3	.4	.5	.6	.7	.8	.9
1	0.000	0.095	0.182	0.262	0.336	0.405	0.470	0.531	0.588	0.642
2	0.693	0.742	0.788	0.833	0.875	0.916	0.956	0.993	1.030	1.065
3	1.099	1.131	1.163	1.194	1.224	1.253	1.281	1.308	1.335	1.361
4	1.386	1.411	1.435	1.459	1.482	1.504	1.526	1.548	1.569	1.589
5	1.609	1.629	1.649	1.668	1.686	1.705	1.723	1.740	1.758	1.775
6	1.792	1.808	1.825	1.841	1.856	1.872	1.887	1.902	1.917	1.932
7	1.946	1.960	1.974	1.988	2.001	2.015	2.028	2.041	2.054	2.067
8	2.079	2.092	2.104	2.116	2.128	2.140	2.152	2.163	2.175	2.186
9	2.197	2.208	2.219	2.230	2.241	2.251	2.262	2.272	2.282	2.293
10	2.303	2.313	2.322	2.332	2.342	2.351	2.361	2.370	2.380	2.389

Problem 2 (20%)

(i) 10% For a separations process it is necessary to determine the VLE compositions of a mixture of ethyl bromide and n-heptane at 30℃。 At this temperature the vapor pressure of pure ethyl bromide is 0.7569 bar, and the vapor pressure of pure n-heptane is 0.0773 bar. Calculate the bubble pressure and the composition of the vapor in equilibrium with a liquid containing 47.23 mol % ethyl bromide assuming ideal solution behavior.

(ii) 10% The values of H and S for steam at 400℃ are listed below. Use them to calculate the fugacity of steam at 400℃ and 15 Mpa.

State 1 (low pressure)	State 2
T_1=400℃	T_2=400℃
P_1=0.01 MPa	P_2=15 MPa
H_1=3279.9 KJ/kg	H_2=2975.7 KJ/kg
S_1=9.6094 KJ/kg·K	S_2=5.8819 KJ/kg·K

Problem 3 (20%)

The formation and decomposition of phosgene can be described by the following rate expressions:

$$CO + Cl_2 \rightarrow COCl_2$$

Forward reaction: $r = k_1[Cl_2]^{1.5}[CO]$
Reverse reaction: $r = k_2[Cl_2]^{0.5}[COCl_2]$

Determine which of the following mechanisms is consistent with these rates. Also, state how you are going to further test this mechanism.

Mechanism I:
- $Cl_2 \rightarrow 2Cl^*$ — fast, at equilibrium
- $Cl^* + CO \rightarrow COCl^*$ — fast, at equilibrium
- $COCl^* + Cl_2 \rightarrow COCl_2 + Cl^*$ — slow, rate limiting

Mechanism II:
- $Cl_2 \rightarrow 2Cl^*$ — fast, at equilibrium
- $Cl^* + Cl_2 \rightarrow Cl_3^*$ — fast, at equilibrium
- $Cl_3^* + CO \rightarrow COCl_2 + Cl^*$ — slow, rate limiting

Problem 4 (20%)

A first-order irreversible gas-phase reaction $A \rightarrow B + 2C$ takes place in a CSTR with a constant volume. The operation is isothermal and isobaric. The reaction rate constant is 0.2 min^{-1}, and the reactor volume is 500 L. The feed contains a 60 mol% of A and a 40 mole % of an inert compound. The molar flow rate of the reactant A is 400 mol/min and the concentration of A in the feed is 4 mol/L. What is the conversion at the exit of this CSTR?

Problem 5 (20%)

Methane can be produced from hydrogen and carbon monoxide according to the reaction

$$CO + 3H_2 \rightleftharpoons CH_4 + H_2O$$

Laboratory investigations using a nickle catalyst resulted in the following expression for the forward reaction rate at a particular temperature

$$r = \frac{1.1 P_{CO} P_{H_2}{}^{0.5}}{1 + 1.5 P_{H_2}}, \frac{\text{lb moles CH}_4}{\text{hr - lbm catalyst}}, T = 400^\circ K$$

With partial pressures in atmospheres.

At the temperature of the study

$$\Delta G^\circ = -34{,}000 \quad \text{cal/gm-mole}$$

$$\Delta H^\circ = -49{,}300 \quad \text{cal/gm-mole}$$

(a) Calculate the chemical reaction equilibrium constant. (8%)

(b) Write the expression for the backward rate. (8%)

(c) What principle of catalysis did you use to determine your answer to part b? (4%)