KATHMANDU UNIVERSITY
End Semester Examination [C]
November, 2023

Marks Scored:

Level : B.E.
Year : II
Course : CHEG 211
Semester : II

Exam Roll No. : Time: 30 mins. F. M. : 10

Registration No.: Date 28 NOV 2023

SECTION "A"

[20 Q. × 0.5 = 10 marks]

Encircle the most appropriate alternative from the given set of choices.

1. Pick out the correct statement.
   a. The absolute value of standard entropy for elementary substances is 0
   b. Maximum work is done under reversible conditions
   c. Melting of ice involves increase in enthalpy and decrease in randomness
   d. Internal energy of an ideal gas depends only on its pressure

2. Two substances are in equilibrium in a reversible chemical reaction. If the concentration of each substance is doubled, then the value of the equilibrium constant will be
   a. Doubled
   b. Same
   c. Halved
   d. One third of its original value

3. According to the Gibbs/Duhem equation for a binary mixture
   a. The activity coefficients of the two components are the same
   b. The activity coefficient of a component increases with its mole fraction
   c. An increase in the activity coefficient of a component results in a decrease in activity coefficient of the other component.
   d. The activity coefficient of a component is maximum at a mole fraction of 1.

4. 5 kg of water and 5 kg of alcohol are put in a container in vapor liquid equilibrium. How many extensive variables does this system have?
   a. 0
   b. 1
   c. 2
   d. 3

5. The activity coefficient of a component in a liquid mixture
   a. Approaches to 1 as its mole fraction approaches to 0
   b. Is the ratio of actual partial pressure to the partial pressure predicted by Raoult's law
   c. Varies significantly with the system pressure
   d. Is the ratio of actual fugacity to the fugacity predicted by assuming ideal solution

6. If the equilibrium constant for the reaction $2H_2O \rightarrow 2H_2 + O_2$ is $1/K^2$, the equilibrium constant for the reaction $H_2 + 1/2O_2 \rightarrow H_2O$ at the same temperature is
   a. K
   b. 1/2K
   c. 2K
   d. $1/K^2$

7. If the Emf of the cell is 1.184 volts, the Gibbs free energy of a reaction for a hydrogen fuel cell is
   a. -228,512 $J.mol^{-1}$
   b. 228,512 $J.mol^{-1}$
   c. 268,572 $J.mol^{-1}$
   d. -268,572 $J.mol^{-1}$

8. The fugacity coefficient of a gas at constant pressure ___ with the decrease of temperature.
   a. Increases
   b. Decreases
   c. Remains the same
   d. Fugacity coefficient doesn't depend on temperature

9. If temperature of a two phase system in equilibrium is changed, the ___ must also change for the two phases to continue to coexist in equilibrium.
   a. Volume b. Enthalpy
   c. Chemical potential d. Pressure

10. The partial pressure of a component in the vapor phase for vapor liquid equilibrium of ideal mixtures at low pressures can be calculated by
   a. Ideal gas law b. Clapeyron equation
   c. Raoult's law d. Antoine equation

11. Calculate the internal energy change when 290 kg of air is cooled from 70 to 40 C in a constant volume process. The constant volume heat capacity of air is 2×10^4 J/kgmol.C.
   a. 6 MJ b. - 6 MJ c. - 50 MJ d. 60 MJ

12. For the stoichiometric reaction CO (g) + $2H_2$ (g) → CH_3OH (g), what is the value of equilibrium constant K at 298 K if the Gibbs free energy for CO and CH_3OH are -137,169 and -161,960 J/mol respectively.
   a. 10000 b. 15250 c. 18347 d. 22051

13. For the problem in question 12, what is the reaction coordinate (ε) ?
   a. 0.83 b. 0.89 c. 0.94 d. 0.98

14. For the problem in question 12, if the equilibrium methanol mole fraction is equal to 0.5, what is the equilibrium constant?
   a. 15 b. 22 c. 27 d. 32

15. One mole of an ideal gas is compressed isothermally but irreversibly at 100 C from 2.5 bar to 6.5 bar. What is the entropy change of the gas?
   a. -8 J/K b. -9 J/K c. 10 J/K d. 11 J/K

16. For ideal gas state, the enthalpy change of mixing is
   a. 0 b. 1 c. 2 d. 3

17. For the reaction, H_2 + $0.5O_2$ → H_2O, what is the mole fraction of O_2 molecule if stoichiometric amounts of reactants are initially present?
   a. $0.5 - 0.5\varepsilon / 1.5 - 0.5\varepsilon$ b. $\varepsilon / 5 + 0.5\varepsilon$
   c. $0.5\varepsilon / 5 + 0.5\varepsilon$ d. $1 + \varepsilon / 5 + 0.5\varepsilon$

18. Air is compressed from an initial state of 3 bar and 600 K to a final state of 8 bar and 600 K by three different mechanically reversible processes in a closed system. What is the ΔU for the process?
   a. 1267 J b. 1621 J c. 2421 J d. 0 J

19. 1 mol of 1-butene liquid with normal boiling point of 267 K is vaporized. Estimate the latent heat for the phase change based on Trouton's rule.
   a. 20,157 J b. 22,198 J c. 25,143 J d. 32,587 J

20. How may phase rule variables must be specified to fix the thermodynamic state for liquid water in equilibrium with its vapor?
   a. 0 b. 1 c. 2 d. 3

KATHMANDU UNIVERSITY
End Semester Examination [C]
November, 2023

28 NOV 2023

Level : B.E.
Year : II
Time : 2 hrs. 30 mins.

Course : CHEG 211
Semester : II
F. M. : 40

SECTION "B"
[8Q × 5 = 40 marks]

Attempt *ALL* questions

1. Air at 1 bar and 300 K is compressed to 5 bar and 300 K by heating at constant volume followed by cooling at constant pressure. The C_p and C_v of air, assumed independent of temperature, is 20.785 and 29.1 J/mol.K. Assume PV/T remains constant for air and the volume of air at 300 K and 1 bar is 0.02479 m^3/mol. Calculate the total heat and work requirements for the process. [5]

2. A natural gas fuel contains 85 mol% methane, 10% ethane and 5% and nitrogen. The fuel is supplied to a furnace with 50% excess air. Fuel and air both enter at 25 °C and the products leave at 600 °C. If the combustion is complete, what is the ΔH for the process? The heat of formation of methane, ethane, carbon dioxide and water are -74520, -83820, -393509 and -241818 J/mol respectively. [5]

$Cp/R = A + BT + CT^2 + DT^{-2}$				
Components	A	10^3B	10^6C	$10^{-5}D$
CO_2	5.457	1.045	-	-1.157
H_2O	3.47	1.45	-	0.121
N_2	3.28	0.593	-	0.04
O_2	3.639	0.506	-	-0.227

3. An inventor has devised a flow process with 1 mol/s of air as working fluid that was expanded from 200 °C and 5 bar to 50 °C and 1 bar. The cold reservoir temperature is 30 °C and $C_p/R = 3.5$ is assumed for air. The inventor claimed that 5000 J/s of work was produced.
   a. Determine whether the claimed performance is consistent with the second law of thermodynamics. [2.5]
   b. What would be the maximum work obtained theoretically? [2.5]

4. Estimate H^R and S^R for a 40-60% mixture of oxygen and nitrogen at 100 K and 50 bar using the Lee/Kesler correlation. [5]

5. Calculate the fraction and the composition of liquid that will remain at equilibrium when a mixture of 68.6% hexane and the balance toluene is flashed at 80 °C and 1 atm. The vapor pressures of hexane and toluene are 1020 and 290 mm Hg respectively. [5]

6. The following set of VLE data for methanol (1) / water (2) system at 60 C is given

P/kPa	x_1	y_1
19.953	0	0
39.223	0.1686	0.5714
42.984	0.2167	0.6268
48.852	0.3039	0.6943
52.784	0.3681	0.7345
56.652	0.4461	0.7742
60.614	0.5282	0.8085
63.998	0.6044	0.8383
67.924	0.6804	0.8733
70.229	0.7255	0.8922
72.832	0.7776	0.9141
84.562	1	1

a. At $x_1 = 0.2167$, determine the activity coefficients of methanol and water? [1]
b. Calculate excess Gibbs energy G^E at $x_1 = 0.2167$ [2]
c. Show that as x_1 approaches 1, the activity coefficient of component 1 approaches 1 using Gibbs Duhem equation. [2]

7. Determine the equilibrium constant for the reaction $H_2 + 0.5O_2 \Leftrightarrow H_2O$ at 2000K. [5]
The following data is provided.

Component	ΔH_{f298} (J/mol)	ΔG_{f298} (J/mol)	Cp/R
H_2	0	0	$3.249 + 0.422 \times 10^{-3}T + 0.083 \times 10^5T^{-2}$
O_2	0	0	$3.639 + 0.506 \times 10^{-3}T - 0.227 \times 10^5T^{-2}$
H_2O	-241,818	-228,572	$3.470 + 1.45 \times 10^{-3}T + 0.121 \times 10^5T^{-2}$

8. For the cracking reaction C_3H_8 (g) → C_2H_4 (g) + CH_4 (g), if the feed is in stoichiometric proportion, and assuming ΔH_{rxn}^o is independent of temperature
a. Determine the fractional conversion of propane at 500 K and 1 bar. [2.5]
b. The temperature at which the fractional conversion is 85%. Assume a pressure of 10 bar for this part. [2.5]

Component	ΔH_{f298} (J/mol)	ΔG_{f298} (J/mol)
C_3H_8	-104,680	-24,290
C_2H_4	52,510	68,460
CH_4	-74,520	-50,460

Useful Equations and Tables (To be provided with the questions):

$$\Delta S = \int_{T_1}^{T_2} \frac{C_p}{T} dT - nR\ln\frac{P_2}{P_1}$$

$$\frac{H^R}{RT_c} = \frac{(H^R)^0}{RT_c} + \omega\frac{(H^R)^1}{RT_c} \qquad \frac{S^R}{R} = \frac{(S^R)^0}{R} + \omega\frac{(S^R)^1}{R} \quad Z = Z^0 + \omega Z^1$$

$$\frac{\Delta G^\circ}{RT} = \frac{\Delta G_0^\circ - \Delta H_0^\circ}{RT_0} + \frac{\Delta H_0^\circ}{RT} + \frac{1}{T}\int_{T_0}^{T}\frac{\Delta C_P^\circ}{R}dT - \int_{T_0}^{T}\frac{\Delta C_P^\circ}{R}\frac{dT}{T}$$

$$\ln K = -\Delta G^\circ/RT.$$

$$\ln\left(\frac{K_2}{K_1}\right) = -\frac{\Delta H_{rxn}{}^o}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

$$\prod_i (y_i\phi_i)^{v_i} = \left(\frac{P}{P^0}\right)^{-v}K$$

$$\sum_i \frac{z_i K_i}{1 + V(K_i - 1)} = 1$$

	Molar mass	ω	T_c/K	P_c/bar	Z_c	V_c $cm^3 \cdot mol^{-1}$	T_n/K
Ethylene glycol	62.068	0.487	719.7	77.00	0.246	191.0	470.5
Acetic acid	60.053	0.467	592.0	57.86	0.211	179.7	391.1
Hydrogen	2.016	−0.216	33.19	13.13	0.305	64.1	20.4
Oxygen	31.999	0.022	154.6	50.43	0.288	73.4	90.2
Nitrogen	28.014	0.038	126.2	34.00	0.289	89.2	77.3
Air†	28.851	0.035	132.2	37.45	0.289	84.8	[illegible]

Table D.7: Values of $(H^R)^0/RT_c$

$P_r =$	1.0000	1.2000	1.5000	2.0000	3.0000	5.0000	7.0000	10.000
T_r								
0.30	−5.987	−5.975	−5.957	−5.927	−5.868	−5.748	−5.628	−5.446
0.35	−5.845	−5.833	−5.814	−5.783	−5.721	−5.595	−5.469	−5.278
0.40	−5.700	−5.687	−5.668	−5.636	−5.572	−5.442	−5.311	−5.113
0.45	−5.551	−5.538	−5.519	−5.486	−5.421	−5.288	−5.154	−5.950
0.50	−5.401	−5.388	−5.369	−5.336	−5.279	−5.135	−4.999	−4.791
0.55	−5.252	−5.239	−5.220	−5.187	−5.121	−4.986	−4.849	−4.638
0.60	−5.104	−5.091	−5.073	−5.041	−4.976	−4.842	−4.794	−4.492
0.65	−4.956	−4.949	−4.927	−4.896	−4.833	−4.702	−4.565	−4.353
0.70	−4.808	−4.797	−4.781	−4.752	−4.693	−4.566	−4.432	−4.221
0.75	−4.655	−4.646	−4.632	−4.607	−4.554	−4.434	−4.393	−4.095
0.80	−4.494	−4.488	−4.478	−4.459	−4.413	−4.303	−4.178	−3.974
0.85	−4.316	−4.316	−4.312	−4.302	−4.269	−4.173	−4.056	−3.857

Table D.8: Values of $(H^R)^1/RT_c$

$P_r =$ / T_r	1.0000	1.2000	1.5000	2.0000	3.0000	5.0000	7.0000	10.000
0.30	−11.062	−11.055	−11.044	−11.027	−10.992	−10.935	−10.872	−10.781
0.35	−10.640	−10.637	−10.632	−10.624	−10.609	−10.581	−10.554	−10.529
0.40	−10.121	−10.121	−10.121	−10.122	−10.123	−10.128	−10.135	−10.150
0.45	−9.525	−9.527	−9.531	−9.537	−9.549	−9.576	−9.611	−9.663
0.50	−8.888	−8.892	−8.899	−8.909	−8.932	−8.978	−9.030	−9.111
0.55	−8.238	−8.243	−8.252	−8.267	−8.298	−8.360	−8.425	−8.531
0.60	−7.596	−7.603	−7.614	−7.632	−7.669	−7.745	−7.824	−7.950
0.65	−6.980	−6.987	−6.997	−7.017	−7.059	−7.147	−7.239	−7.381
0.70	−6.388	−6.395	−6.407	−6.429	−6.475	−6.574	−6.677	−6.837
0.75	−5.824	−5.832	−5.845	−5.868	−5.918	−6.027	−6.142	−6.318
0.80	−5.285	−5.293	−5.306	−5.330	−5.385	−5.506	−5.632	−5.824
0.85	−4.763	−4.771	−4.784	−4.810	−4.872	−5.000	−5.149	−5.358
0.90	−4.249	−4.255	−4.268	−4.298	−4.371	−4.530	−4.688	−4.916
0.93	−3.934	−3.937	−3.951	−3.987	−4.073	−4.251	−4.422	−4.662
0.95	−3.712	−3.713	−3.730	−3.773	−3.873	−4.068	−4.248	−4.497

Table D.11: Values of $(S^R)^0/R$

$P_r =$ / T_r	1.0000	1.2000	1.5000	2.0000	3.0000	5.0000	7.0000	10.000
0.30	−7.099	−6.935	−6.740	−6.497	−6.180	−5.847	−5.683	−5.578
0.35	−6.663	−6.497	−6.299	−6.052	−5.728	−5.376	−5.194	−5.060
0.40	−6.275	−6.109	−5.909	−5.660	−5.330	−4.967	−4.772	−4.619
0.45	−5.924	−5.757	−5.557	−5.306	−4.974	−4.603	−4.401	−4.234
0.50	−5.608	−5.441	−5.240	−4.989	−4.656	−4.282	−4.074	−3.899
0.55	−5.324	−5.157	−4.956	−4.706	−4.373	−3.998	−3.788	−3.607
0.60	−5.066	−4.900	−4.700	−4.451	−4.120	−3.747	−3.537	−3.353
0.65	−4.830	−4.665	−4.467	−4.220	−3.892	−3.523	−3.315	−3.131
0.70	−4.610	−4.446	−4.250	−4.007	−3.684	−3.322	−3.117	−2.935
0.75	−4.399	−4.238	−4.045	−3.807	−3.491	−3.138	−2.939	−2.761
0.80	−4.191	−4.034	−3.846	−3.615	−3.310	−2.970	−2.777	−2.605
0.85	−3.976	−3.825	−3.646	−3.425	−3.135	−2.812	−2.629	−2.463
0.90	−3.738	−3.599	−3.434	−3.231	−2.964	−2.663	−2.491	−2.334
0.93	−3.569	−3.444	−3.295	−3.108	−2.860	−2.577	−2.412	−2.262
0.95	−3.433	−3.326	−3.193	−3.023	−2.790	−2.520	−2.362	−2.215

Table D.12: Values of $(S^R)^1/R$

$P_r =$ / T_r	1.0000	1.2000	1.5000	2.0000	3.0000	5.0000	7.0000	10.000
0.30	−16.586	−16.547	−16.488	−16.390	−16.195	−15.837	−15.468	−14.925
0.35	−15.278	−15.251	−15.211	−15.144	−15.011	−14.751	−14.496	−14.153
0.40	−13.896	−13.877	−13.849	−13.803	−13.714	−13.541	−13.376	−13.144
0.45	−12.496	−12.482	−12.462	−12.430	−12.367	−12.248	−12.145	−11.999
0.50	−11.153	−11.143	−11.129	−11.107	−11.063	−10.985	−10.920	−10.836
0.55	−9.914	−9.907	−9.897	−9.882	−9.853	−9.806	−9.769	−9.732
0.60	−8.799	−8.794	−8.787	−8.777	−8.760	−8.736	−8.723	−8.720
0.65	−7.810	−7.807	−7.801	−7.794	−7.784	−7.779	−7.785	−7.811
0.70	−6.933	−6.930	−6.926	−6.922	−6.919	−6.929	−6.952	−7.002
0.75	−6.155	−6.152	−6.149	−6.147	−6.149	−6.174	−6.213	−6.285
0.80	−5.458	−5.455	−5.453	−5.452	−5.461	−5.501	−5.555	−5.648
0.85	−4.826	−4.822	−4.820	−4.822	−4.839	−4.898	−4.969	−5.082
0.90	−4.238	−4.232	−4.230	−4.236	−4.267	−4.351	−4.442	−4.578
0.93	−3.894	−3.885	−3.884	−3.896	−3.941	−4.046	−4.151	−4.300
0.95	−3.658	−3.647	−3.648	−3.669	−3.728	−3.851	−3.966	−4.125