National Exams May 2010

98-met-A1, Metallurgical Thermodynamics

3 hours duration

NOTES:

1. <u>Answer only **five** questions</u>. Any five questions(out of seven) constitute a complete paper. Only the first five questions as they appear in your answer book will be marked.

2. All questions are of equal value(20 marks each out of 100).

3. If doubt exists as to the interpretation of any question, the candidate is urged to submit with the answer paper a clear statement of any assumptions made.

4. Candidates may use one of two calculators, the Casio or Sharp approved models. This is a closed book exam.

Question 1: (a) 12, (b) 8

Question 2: (a) 12, (b) 8

Question 3:   (a) 6, (b) 6, (c) 8

Question 4:   (a) 5, (b) 5, (c) 5, (d) 5

Question 5: (a) 20

Question 6:   (a) 20

Question 7:   (a) 4, (b) 4, (c) 4, (d) 4, (e) 4

Problem No. 1(20 marks): Pure CH_4 gas at 25 °C is fully combusted with 100% excess amount of air. The air(assume 21 mole% O_2 and 79 mole% N_2) is pre-heated to 500 °C before it reacts with the methane.
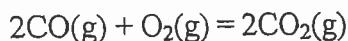
a) Determine the resulting flame composition(mole %)
b) Calculate the adiabatic flame temperature

Table of Data

	Molecular Mass g/mole	Standard Enthalpy of Formation (kJ/mole)	Average Heat Capacity (J/mole·°C)
$CH_4(g)$	16	-75	38
$H_2O(g)$	18	-242	39
$CO_2(g)$	44	-394	51
$O_2(g)$	32	0	34
$N_2(g)$	28	0	32

Problem No. 2(20 marks):

a) Calculate the enthalphy of the reaction

$$2CO(g) + O_2(g) = 2CO_2(g)$$

at 1100 K.

b) Is the entropy change positive or negative for that reaction ? Justify your answer.

Given the following data:

Standard Heat of Formation(kJ/mol)
1) $CO(g)$, $\Delta H^o_{298\,K} = -111.4$ kJ/mol
2) $CO_2(g)$, $\Delta H^o_{298\,K} = -393.5$ kJ/mol

Heat Capacity(J/molxK)
3) $O_2(g)$: $Cp = 34.6 + 0.001xT - 7.85x10^5/T^2$
4) $CO(g)$: $Cp = 27.61 + 0.005xT$
5) $CO_2(g)$: $Cp = 43.26 + 0.011xT - 8.2x10^5/T^2$

Problem No. 3(20 marks): Use the data in the table below to solve the following problems

a) What is the enthalpy change(kJ/mol) at 25 °C for the following reaction:
$CH_4(g) + CO_2(g) = 2CO(g) + 2H_2(g)$

b) What is the enthalpy change(kJ/mol) at 1500 °C for the following reaction:
$CH_4(g) + CO_2(g) = 2CO(g) + 2H_2(g)$

c) How much cooling water(mol) is required to cool 100 mol of a gas from 1200 °C to 250 °C. The gas consists of 45 mol% N_2, 20 mol% H_2O and 35 mol% CO_2. The cooling water enters at 10 °C and leaves at 35 °C.

Table of Data

	Molecular Mass g/mole	Standard Enthalpy of Formation (kJ/mole)	Heat Capacity (J/mole·°C)
$CH_4(g)$	16	-75	38
$H_2O(g)$	18	-242	39
$CO_2(g)$	44	-394	51
$CO(g)$	28	-111	43
$H_2(g)$	2	0	28
$O_2(g)$	32	0	34
$N_2(g)$	28	0	32
$H_2O(l)$	18	-286	$62 + 0.5 \times T(°C)$

Note: Standard enthalpy of formation refers to 25 °C.

Problem No. 4(20 marks): The standard Gibbs Free energy of the following reaction

$$2Cr(s) + 3H_2O(g) = Cr_2O_3 + 3H_2(g)$$
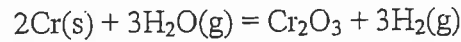
is given by

$$\Delta G^\circ(kJ/mol) = -408.6 + 0.12 \times T(K)$$

a) find the equilibrium constant at 1500 K(use data given, not Ellingham diagram)
b) what is the maximum partial pressure(atm) of water vapour in otherwise pure H_2 in which chromium can be heated to 1500 K without oxidizing. The total pressure is 1 atm
c) in a particular chromium alloy, the activity of chromium is 0.35. What is the maximum partial pressure(atm) of water vapour in otherwise pure H_2 in which this alloy can be heated to 1500 K without oxidizing the chromium. The total pressure is 1 atm
d) in terms of activities of components in a solution, describe Raoult's and Henry's laws

Problem No. 5(20 marks): Construct the predominace area diagram(also called stability diagram) for the $Pb - O_2 - SO_2$ system at 1500 K. As x-axis use $\log(P-O_2)$ and as y-axis use $\log(P-SO_2)$. The x-scale should go from -10 to +2 and the y-axis from -8 to +8. Use the graph paper at the end of this exam booklet. Put your name and student number on it and hand it in together with your other answers.

Thermodynamic Data at 1500 K(R = 8.314 J/molxK)

	Species	$\Delta G^\circ(kJ/mol)$
1	Pb	0.0
2	PbO	-79.0
3	PbS	-36.7
4	PbSO$_4$	-295
5	O$_2$(g)	0.0
6	SO$_2$(g)	-253

Problem No. 6(20 marks): Calculate the entropy of molten aluminium at 1050 K.

Given the following data:

$S^{\circ}_{298\,K} = 28.33$ J/molxK

Heat of melting of aluminium: 10,460 J/mol, Melting temperature at 933 K.

Heat Capacity(J/molxK)
   Al(solid): $Cp = 20.67 + 0.012xT$
   Al(molten): $Cp = 29.29$

Problem No. 7(20 marks): Use the Ellingham Diagram to answer

a) What is ΔG°(kJ/mol) at 1000 °C for the reaction: $Ti + 2MnO = TiO_2 + 2Mn$
b) What is the CO/CO_2 ratio in equilibrium with Ni and NiO at 1400 °C and what does this tell you about the possible efficiency of using CO gas to reduce NiO to metallic Ni
c) What is ΔG°(kJ/mol) for the reaction: $3TiO_2 + 4Al = 2Al_2O_3 + 3Ti$ at 1600 °C
d) A small sealed container at 1200 °C contains metallic chromium(Cr) as well as chromium oxide(Cr_2O_3). What is the equilibrium oxygen pressure in that system.
e) Use the Ellingham diagram to explain why solid carbon becomes a very good reductant at high temperature. Give an example.
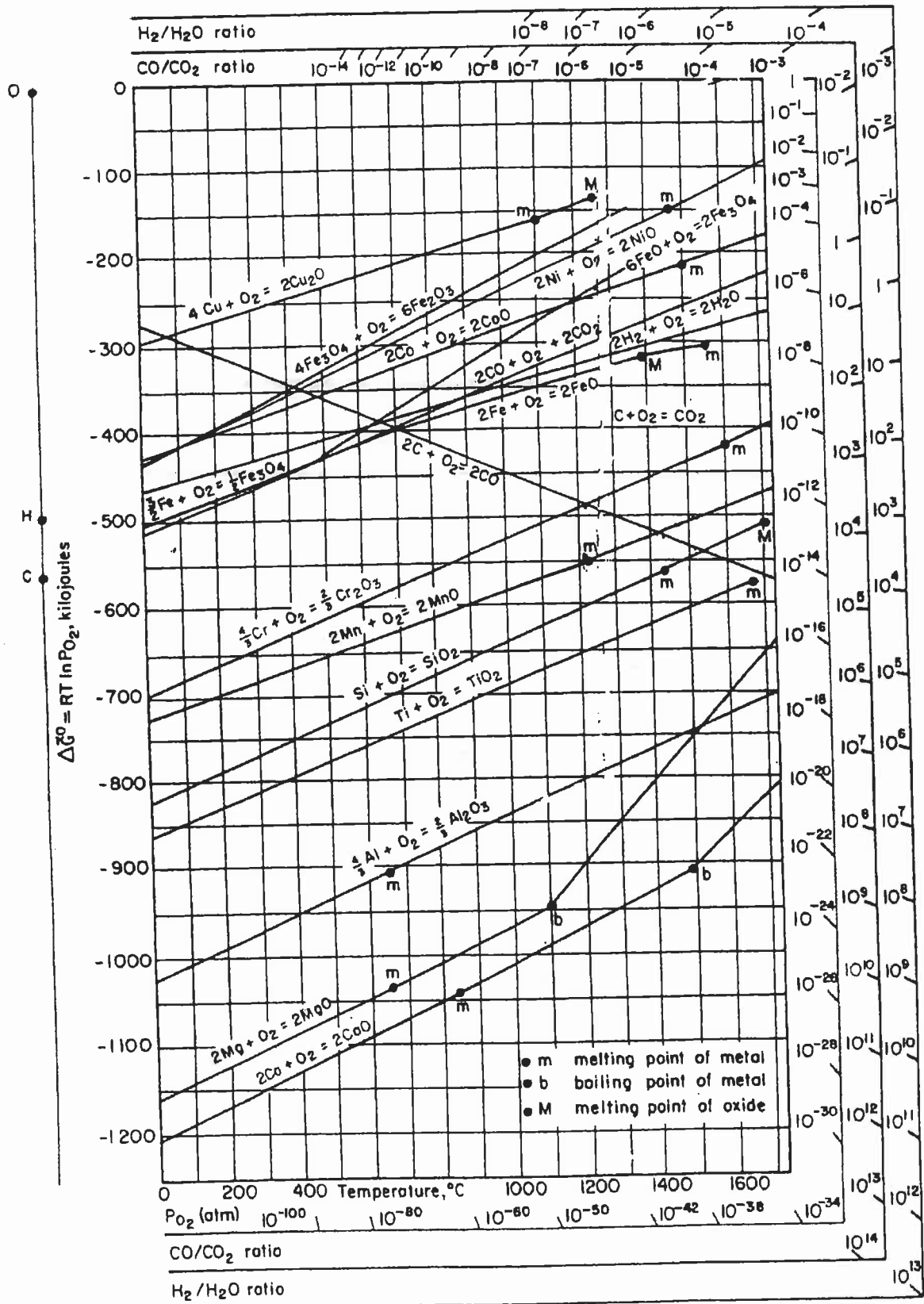
Figure 9−3. Ellingham diagram for some oxides; Richardson nomographic scales are included. (Adapted from D. R. Gaskell, *Introduction to Metallurgical Thermodynamics*, 2nd ed., Hemisphere Publishing, New York, 1981.)