National Exams December 2009

98-met-A1, Metallurgical Thermodynamics

3 hours duration

NOTES:

1. Answer only **five** questions. 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.

5. The exam consists of seven pages including graph paper and Ellingham diagram

Question 1: (a) 4, (b) 4, (c) 4, (d) 4, (e) 4
Question 2: (a) 5, (b) 15
Question 3: (a) 20
Question 4: (a) 10, (b) 10
Question 5: (a) 5, (b) 5, (c) 5, (d) 5
Question 6: (a) 20
Question 7: (a) 4, (b) 4, (c) 4, (d) 4, (e) 4

Problem No. 1(20 marks): Use the data in the table below to solve the following problems

a) One mole of CH_4 is fully combusted with 50% excess air. What is the composition of the off-gas(mol%)

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

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

d) What is the adiabatic flame temperature when CO(g) is combusted with 100% excess air, when both the CO and the air enter at 25 °C

e) 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 + 0.5xT(°C)

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

Problem No. 2(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. 3(20 marks): Calculate the entropy of molten aluminium at 1100 K.

Given the following data:

$S^{o}_{298\,K}$ = 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. 4(20 marks): Hematite(Fe_2O_3) is reduced to metallic iron by carbon, and the resulting gaseous reaction product is a mixture of CO and CO_2 with two parts of CO to one part of CO_2 per volume.

a) calculate the heat of reaction at 25 °C per mole of iron(Fe) produced
b) calculate the heat of reaction at 1000 °C per mole of iron(Fe) produced

	ΔH^o_f(25 °C) kJ/mol	Cp(J/mol·K)
Fe_2O_3	-1207	141
Fe	0	$16.32 + 28.4\text{x}10^{-3}\ T$
C	0	$11.2 + 9.5\text{x}10^{-3}\ T$
CO(g)	-110.5	$28.4 + 4.1\text{x}10^{-3}\ T - 0.46\text{x}10^{5}/T^2$
CO_2(gas)	-394	37.2

!Heat capacities are given as a function of temperature in Kelvin
K = 273.15 + °C

Problem No. 5(20 marks): The standard Gibbs Free energy of the following reaction

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

is given by

$$\Delta G^o(\text{kJ/mol}) = 408.6 - 0.12\text{x}T(K)$$

a) find the equilibrium constant at 1500 K
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) derive from the data whether the oxidation of chromium metal with water vapour is exothermic or endothermic
d) indicate in general terms how the equilibrium for the above reaction is affected by a change in the total pressure from 1 to 2 atm(explain)

Constant: R = 8.314 J/molxK

Problem No. 6(20 marks): Construct the predominace area diagram(also called stability diagram) for the $Zn - O_2 - SO_2$ system at 1173 K. As x-axis use $\log(P\text{-}O_2)$ and as y-axis use $\log(P\text{-}SO_2)$. The scale on the x-axis should go from -25 to +5, and the y-axis from -20 to + 10.

The following data are given at 1173 K. The data represents the Gibbs energy of formation when the compounds are formed from the elements in their standard state.

ZnO: ΔG^o(kJ/mol) = -229.0
ZnS: ΔG^o(kJ/mol) = -151.6
$ZnSO_4$: ΔG^o(kJ/mol) = -544.3
SO_2: ΔG^o(kJ/mol) = -276.3

Constant: R = 8.314 J/molxK

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

a) What is ΔG^o(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^o(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.

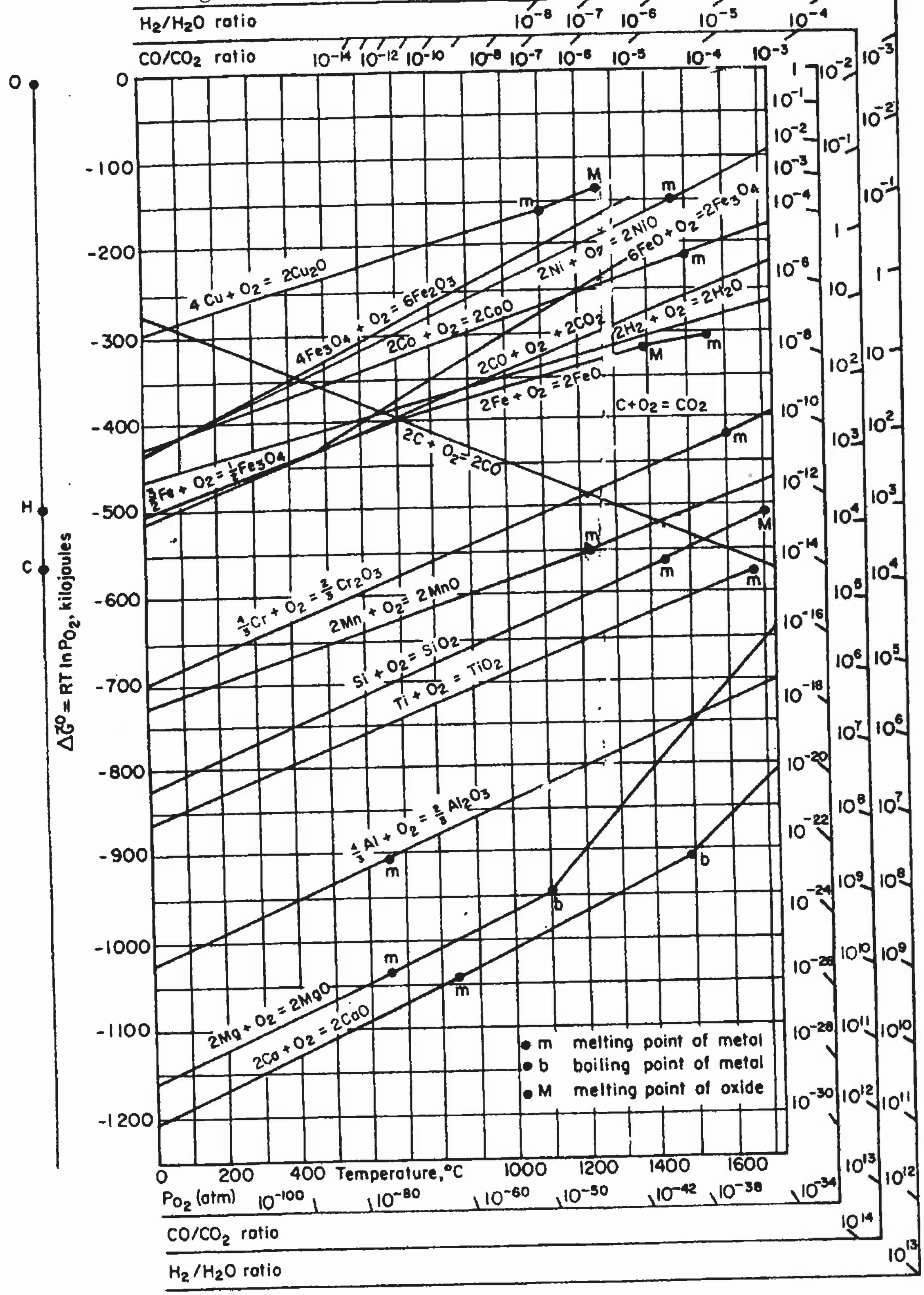

Figure 9–3. Ellingham diagram for some oxides; Richardson nomographic scales are included. (Adapted from D. R. Gaskell, *Introduction to Metallurgical Thermodynamics*, 2nd ed., Hemisphere Publishing, New York, 1981.)