National Exams May 2015

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 5 pages including Ellingham diagram.

Question 1: (a) 6, (b) 6, (c) 6, (d) 2
Question 2: (a) 10, (b) 10
Question 3: 20
Question 4: (a) 8, (b) 12
Question 5: (a) 8, (b) 8, (c) 4
Question 6: (a) 8, (b) 12
Question 7: (a) 4, (b) 4, (c) 4, (d) 4, (e) 2, (f) 2

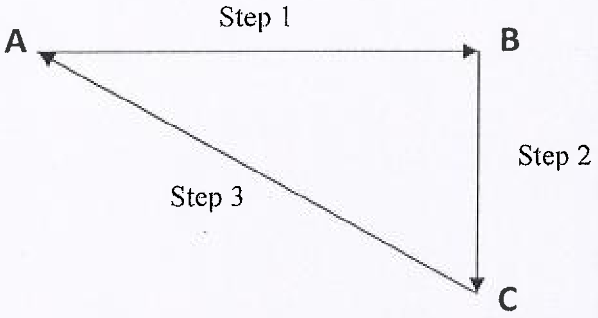
Problem No. 1 (20 marks):

1 mol of a monatomic ideal gas is taken through following steps as shown below:

Step 1: Constant pressure process: from state A (T_A, P_A = 100 kPa, V_A= 25 L) to state B (T_B, P_B = 100 kPa, V_B= 100 L)

Step 2: Constant volume process: from state B (T_B, P_B = 100 kPa, V_B= 100 L) to state C (T_A = T_C, P_C, V_C= 100 L)

Step 3: Constant temperature process: back to State A from State C



(a) Calculate heat flow in the system (q), work done on the system (w), change in internal energy of the system (ΔE) and change in enthalpy of the system (ΔH) for Step 1. (6 marks)

(b) Calculate heat flow in the system (q), work done on the system (w), change in internal energy of the system (ΔE) and change in enthalpy of the system (ΔH) for Step 2. (6 marks)

(c) Calculate heat flow in the system (q), work done on the system (w), change in internal energy of the system (ΔE) and change in enthalpy of the system (ΔH) for Step 3. (6 marks)

(d) Calculate heat flow in the system (q), work done on the system (w), change in internal energy of the system (ΔE) and change in enthalpy of the system (ΔH) for the cycle. (2 marks)

Assume that $C_v = 20.8\ J\ K^{-1}\ mol^{-1}$ for the ideal gas.

Problem No. 2 (20 marks):

(a) Prove that $P_i V_i^{\gamma} = P_f V_f^{\gamma}$ for the reversible adiabatic expansion of an ideal gas. Assume that C_v is constant over temperature range and $C_p - C_v = R$. (10 marks)

(b) An ideal gas underwent reversible adiabatic expansion from 80 kPa to 60 kPa. If the initial temperature of the gas was 300 K, what was its final temperature? Assume that $C_p = 28.9\ J\ K^{-1}\ mol^{-1}$ for the ideal gas. (10 marks)

Problem No. 3 (20 marks):

Calculate ΔS^o_R for the reaction $CO(g) + \frac{1}{2} O_2(g) = CO_2(g)$ at 500 K given the following data:

S^o_{298K} (CO, g) = 197.7 $J\ K^{-1}\ mol^{-1}$

S^o_{298K} (CO_2, g) = 213.7 $J\ K^{-1}\ mol^{-1}$

S^o_{298K} (O_2, g) = 205.1 $J\ K^{-1}\ mol^{-1}$

C_p (CO, g) in $J\ K^{-1}\ mol^{-1} = 31.1 - 1.5 \times 10^{-2}\ T + 3.1 \times 10^{-5}\ T^2 - 1.5 \times 10^{-8}\ T^3$

C_p (CO_2, g) in $J\ K^{-1}\ mol^{-1} = 18.9 + 7.9 \times 10^{-2}\ T - 6.8 \times 10^{-5}\ T^2 + 2.4 \times 10^{-8}\ T^3$

C_p (O_2, g) in $J\ K^{-1}\ mol^{-1} = 30.8 - 1.2 \times 10^{-2}\ T + 2.4 \times 10^{-5}\ T^2$

Assume that T is in K for heat capacity data.

Problem No. 4 (20 marks):

Acetylene (C_2H_2) is combusted at 298 K according to the following reaction:

$$C_2H_2 + 2\tfrac{1}{2}\, O_2 = 2CO_2 + H_2O$$

Standard enthalpy of formation at 25°C is given in the following table:

Compound	Standard enthalpy of formation
C_2H_2	+226.7 kJ mol^{-1}
CO_2	-393.5 kJ mol^{-1}
H_2O	-241.8 kJ mol^{-1}

Heat capacity data is as follows:

$C_p(CO_2)$ in J K^{-1} mol^{-1} = $18.9 + 7.9 \times 10^{-2}$ T
$C_p(H_2O)$ in J K^{-1} mol^{-1} = $31.4 + 0.4 \times 10^{-2}$ T
$C_p(N_2)$ in J K^{-1} mol^{-1} = $27.9 + 0.4 \times 10^{-2}$ T

Assume that T is in K for heat capacity data.

(a) Calculate the adiabatic flame temperature when acetylene is combusted with stoichiometric amount of oxygen. (8 marks)

(b) Calculate the adiabatic flame temperature when acetylene is combusted in air (containing 21% O_2, rest being N_2) containing stoichiometric amount of oxygen. (12 marks)

Problem No. 5 (20 marks):

Calculate the ΔG of mixing at 298 K and 1 atm pressure for the following cases:

(a) Mixing of 1 mole of O_2 and 1 mole of N_2. (8 marks)

(b) Mixing of 1 mole of O_2 and 2 mole of N_2. (8 marks)

(c) Mixing of 1 mole of O_2 to a mixture of 1 mole of O_2 and 1 mole of N_2. (4 marks)

Problem No. 6 (20 marks):

(a) A tank contains pure oxygen at a total pressure of 1 atmosphere. Oxygen exists primarily in the diatomic form, but it can exist in monatomic state as well. The equilibrium is governed by the following reaction:

$$\tfrac{1}{2}\, O_2 = O$$

If the standard Gibbs energy for the reaction is 187,800 J/mol of monatomic oxygen at 1000 K, what is the composition of the gas at 1000 K? (8 marks)

(b) A tank contains oxygen, hydrogen and water vapor at a total pressure of 1 atmosphere. The equilibrium is governed by the following reaction:

$$H_2 + \tfrac{1}{2}\, O_2 = H_2O;\ \Delta G^\circ = -246{,}000 + 54.84T$$

If partial pressure of oxygen is maintained at 1×10^{-10} atmosphere at 1750 K, what is the composition of the gas at 1750 K? (12 marks)

Problem No. 7 **(20 marks):** Use the attached Ellingham Diagram to answer the following questions:

a) What is the partial pressure of oxygen in equilibrium with Cu and Cu_2O at 500 °C? (4 marks)

b) What is the ratio of partial pressures of CO to CO_2 for equilibrium of Cr and Cr_2O_3 in a CO-CO_2 atmosphere at 400 °C? (4 marks)

c) What is the ratio of partial pressures of H_2 to H_2O for equilibrium of Ti and TiO_2 in a H_2-H_2O atmosphere at 600 °C? (4 marks)

d) What is ΔG° (kJ/mol) at 1500 °C for the reaction: $Ti + SiO_2 = TiO_2 + Si$? (4 marks)

e) Explain why the line for reaction $C(s) + O_2 (g) = CO_2 (g)$ runs nearly horizontally on the chart. (2 marks)

f) Explain why the line for reaction $2C(s) + O_2 (g) = 2CO (g)$ runs downward on the chart. (2 marks)

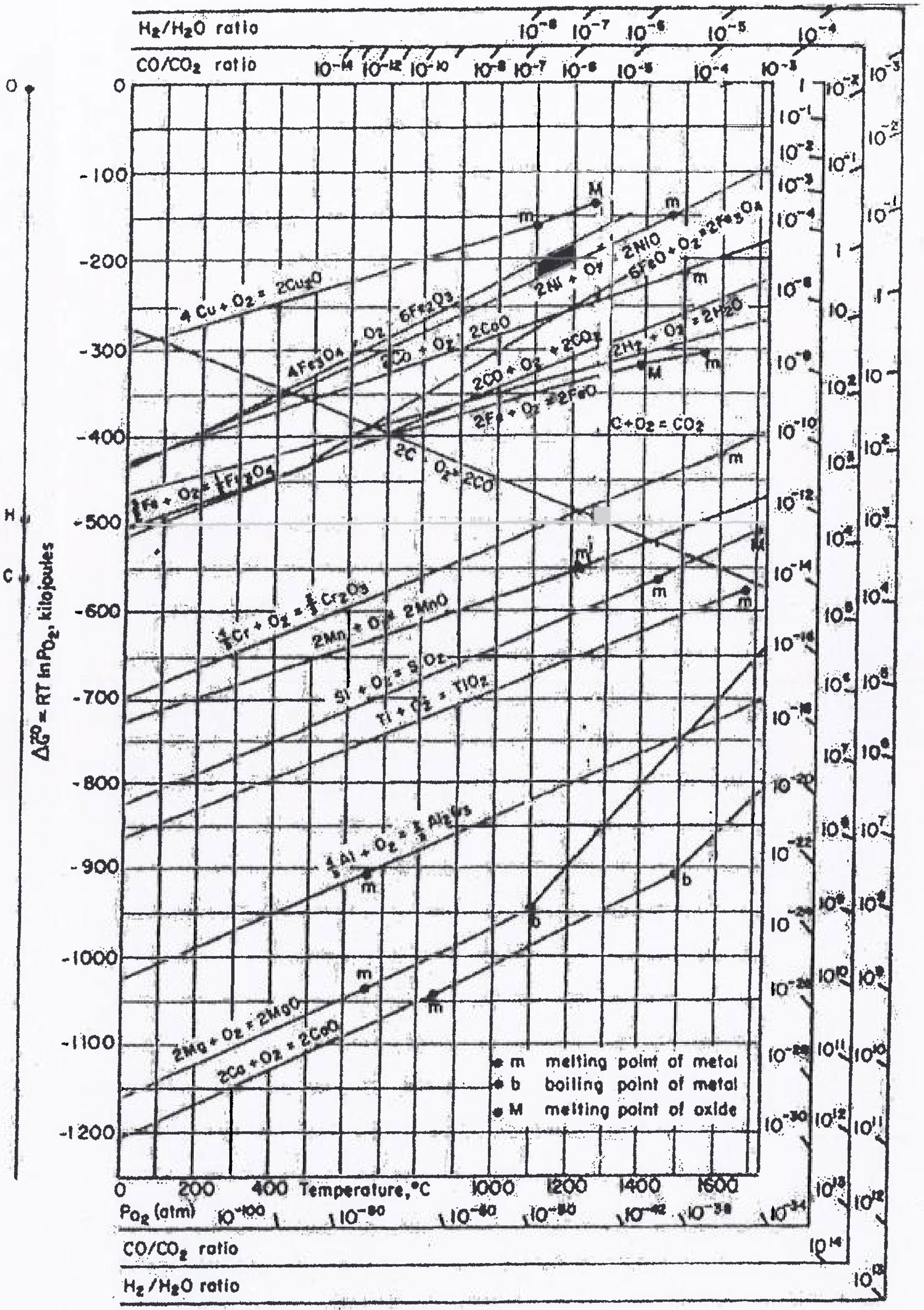


Figure 9–3. Ellingham diagram for some oxides; Richardson nomographic scales are included. (Adapted from D. R. Gaskell, *Introduction to Metallurgical Thermodynamics*, 2nd ed., Hemisphere Publishing, New York, 1981.)