CE 329 Fall 2015

Assignment 3

Background

The following problem was solved in class as Activity 3.1: If a system initially contains 3 moles of H_2O and 1 mole of CO at 1 atm and the isobaric water-gas shift, reaction (1), proceeds to equilibrium, what is the CO conversion if the temperature is (a) 150 °C, (b) 250 °C and (c) 350 °C?

$$CO + H_2O \rightleftarrows CO_2 + H_2 \qquad (1)$$

The expression for the heat of reaction (1) as a function of temperature given in equation (2) and a value of -6810 cal mol^{-1} for $\Delta G_1^0\left(298\text{ K}\right)$ can be generated as described in Unit 2. They are being provided here so that you can focus on the analysis of the equilibrium composition. Expressions for the heat capacities of the reagents are provided in Table 1.

$$\Delta H_1^0\left(T\right) = -9437 - 3.863T + 0.01118T^2 - 9.620\times10^{-6}T^3 + 2.455\times10^{-9}T^4 \qquad (2)$$

Table 1. Heat capacity expressions

Species	***ΔH$_f$(298 K) (kcal/mol)***	***$\hat{C}_p$ (cal/(mol K) with T in K)***
CO	-26.42	$7.373 - 3.07 \times 10^{-3}\ T + 6.662 \times 10^{-6}\ T^2 - 3.037 \times 10^{-9}\ T^3$
H_2O (g)	-57.8	$7.701 + 4.595 \times 10^{-4}\ T + 5.521 \times 10^{-6}\ T^2 - 0.859 \times 10^{-9}\ T^3$
CO_2	-94.05	$4.728 + 1.754 \times 10^{-2}\ T - 1.338 \times 10^{-5}\ T^2 + 4.097 \times 10^{-9}\ T^3$
H_2	0.0	$6.483 + 2.215 \times 10^{-3}\ T - 3.298 \times 10^{-6}\ T^2 + 1.826 \times 10^{-9}\ T^3$

Problem Statement

Continuing from Activity 3.1, supposing that the reaction occurs at 260 ºC and proceeds to thermodynamic equilibrium, what partial pressure of methanol would be produced if reaction (3) simultaneous occurs and reaches equilibrium, and what would the percent conversion of CO equal?

$$CO + 2\ H_2 \rightleftarrows CH_3OH \qquad (3)$$

You may use the equations in Example 3.1 and Activity 3.1 to calculate the equilibrium constants for reactions (1) and (3); you do not need to derive them.