A First Course on Kinetics and Reaction Engineering

Activity 3.1

Problem Purpose

This problem will help you determine whether you have mastered the learning objectives for this unit.

Problem Statement

If a system initially contains 3 moles of H2O 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	$6.483 + 2.215 \times 10^{-3}\, T - 3.298 \times 10^{-6}\, T^2 + 1.826 \times 10^{-9}\, T^3$

Worksheet

1. Show how to calculate the value of the equilibrium constant at 298 K.

2. Show how to calculate the value of the equilibrium constant at any other temperature, T.

3. Write the equilibrium expression in terms of thermodynamic activities. Then express the thermodynamic activities in terms of moles, assuming ideal gas behavior

4. Express the moles in terms of the extent of reaction.

5. Substitute the value of the equilibrium constant at T and the expressions for the mole fractions in terms of the extent of reaction into the equilibrium expression and solve for the equilibrium extent of reaction.

6. Compute the equilibrium CO conversion using the equilibrium extent of reaction.