Chapter Problems

Problem 4

Given data arrays of $\Delta h_o(kJ/mol)$ and $\Delta s_o(J/mol*K)$ versus δ for Ceria, fit a third degree poynomical function suitable for describing Δh_o and Δs_o as a function of δ using the _curve*fit* function from the *scipy.optimize* library.

NOTE: For this we will use Python and import tabulated data from a *.csv* file.

Problem 5

Given a temperature of operation $T = 1273K$ for Ceria and an initial amount of moles of water $n_{H_2O,i} = \delta_f = 0.1$. Solve for δ using an iterative approach.

Background: The partial molar Gibbs free energy for Ceria Δg_o, which is a function of both nonstoichiometry and temperature, is expressed as two equations below:

$$\Delta g_o(\delta, T) = -RT \ln p_{O2}(\delta, T)^{1/2} \qquad (1.50)$$
$$\Delta g_o(\delta, T) = \Delta h_o(\delta) - T\Delta s_o(\delta) \qquad (1.51)$$

Also, the oxygen partial pressure p_{O2} can be obtained from the reaction equilibrium analysis of the dissociation of H_2O. From (1.33) we recognize that the reaction coordinate ϵ is equal to $\delta_f - \delta$,

$$K_{H_2O} = \frac{(\frac{\epsilon}{n_{total}}) * {p_{O2}}^{1/2}}{(\frac{n_{H_2O,i} - \epsilon}{n_{total}})} = \frac{(\delta_f - \delta) * {p_{O2}}^{1/2}}{n_{H_2O,i} - (\delta_f - \delta)}$$

$${p_{O2}}^{1/2} = \frac{n_{H_2O,i} - (\delta_f - \delta)}{(\delta_f - \delta) * K_{f,H_2O}}$$

NOTE: For this we will use Python, and import data for the equilibrium constant of formation of water K_{f,H_2O} from the NIST-JANAF website. A curve fitting procedure needs to be applied, similar to Problem 4.

Problem 6

Given a temperature of operation $T = 1273K$ for Ceria and an initial amount of moles of water $n_{H_2O,i} = \delta_f = 0.1$. Solve for δ and the H_2 yield. Create a solver/minimizer using the *minimize* function from the *scipy.optimize* library.

NOTE: For this we will use Python, and remember that $H_2 = \delta_f - \delta$, which is the difference between the final and initial nonstoichiometries.

Problem 7

Given 6 different temperatures of reduction $T_H = 1573, 1673, 1773, 1873, 1973, 2073K$, temperature of oxidation $800K < T_L < 1200K$, and oxygen partial pressure $p_{O2} = 0.00001$ for Ceria. Compute H_2 yield to reproduce data from Chueh et al. **Figure 17.a**

NOTE: For this we will use Python, and remember that $n_{H_2O,i} = \delta_f$ (initial moles of water is equal to the nonstoichiometry after reduction).

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