EECE 503 **Spring 2015**

HOMEWORK #2

Due January 27

PROBLEM #1

The reaction between nitrogen and oxygen can occur at very high temperature with the following stoichiometry:

$$1/2\, N_2 + 1/2\, O_2 = NO$$

and leads to pollutant *NO* formation.

a. Is this reaction exothermic or endothermic? Calculate the standard heat of reaction.
b. Find the equilibrium constant for the above reaction as a function of temperature.
c. Evaluate the equilibrium mole fraction of *NO* at *298 K*, *1000 K* and *3000 K* in:

   i. air with *N/O = 3.76*, and
   ii. mixture of combustion flue gases with *N/O = 40*.

For case ii, report the equilibrium concentration of *NO* also in ppm.

PROBLEM #2

Estimate the equilibrium mole fraction of NO_2 in a combustion mixture with 3.3% oxygen and 76% nitrogen at *298 K*, *1273 K* and *1873 K*. Reactions to be considered are:

$$1/2\, N_2 + 1/2\, O_2 = NO$$
$$NO + 1/2\, O_2 = NO_2$$

Based on the above findings, which is the dominant nitrogen oxide, NO or NO_2?

PROBLEM #3

Consider the reaction system consisting of the reactions listed below which commonly occur in gasification of coal and/or biomass. Consider the equilibrium composition over the temperature range from 600 to 1600 K. The reactions occur at atmospheric pressure.

$C + 2H_2O = CO_2 + 2H_2$
$C + H_2O = CO + H_2$
$C + CO_2 = 2CO$
$C + 2H_2 = CH_4$
$CO + H_2O = CO_2 + H_2$

a) How many chemical species do you have in that reaction system (S=?)?
b) What is the number of independent reactions in the system (R=?)?
c) List the independent reactions you chose (Hint: start from the top of the list and use as many reactions as needed).
d) For each independent reaction compute the standard Gibbs free energy, the standard heat of reaction and the thermodynamic equilibrium constant at standard conditions. Then plot the equilibrium constants as a function of temperature (600 to 1600K). List the thermodynamic properties that you used in your calculations and the reference for their source. Assume that you have great excess of carbon with respect to steam initially (what can you assume then

about the activity of carbon?). Do the problem by assuming heat of reaction as constant and repeat by accounting for the temperature variation in the heat of reaction. Comment on the difference in the results.

e) Use as basis 1 mole of water (steam) initially and calculate the molar extent of each independent reaction and plot as function of temperature. Since the set of equations is nonlinear show what constraints must acceptable solutions satisfy?

f) Plot the mole fractions of all gaseous species as a function of temperature.

g) Describe how increased pressure would affect this reaction system.

HOMEWORK #2: APPENDIX

DATA FOR PROBLEM #1

Standard State: 25°, 1 atm, ideal gas

Specific Heat (Heat Capacity) $\dfrac{C_p\left(cal/mol\ ^\circ K\right)}{T\ \underline{in}\left(^\circ K\right)}$

$C_p = a + bT + cT^2 + dT^3$

NITROGEN, $N_2(g)$

$\Delta H_f = \Delta G_f = 0$

$a = 6.529$ $b = 0.1488\times10^{-2}$ $c = -0.02271\times10^{-5}$ $d = 0$

OXYGEN, $O_2(g)$

$\Delta H_f = \Delta G_f = 0$

$a = 6.732$ $b = 0.1505\times10^{-2}$ $c = -0.01791\times10^{-5}$ $d = 0$

NITRIC OXIDE, $NO(g)$

$\Delta H_f = 21.600\ (kcal/mol)$ $\Delta G_f = 20.719\ (kcal/mol)$

$a = 6.461$ $b = 0.2358\times10^{-2}$ $c = -0.07705\times10^{-5}$ $d = 0.08729\times10^{-9}$

NITROGEN DIOXIDE, $NO_2(g)$

$\Delta H_f = 7.960\ kcal/mol$ $\Delta G_f = 12.26\ kcal/mol$

$a = 5.480$ $b = 1.365\times10^{-2}$ $c = 0.841\times10^{-5}$ $d = 1.88\times10^{-9}$