AME 513	**Assigned: Tuesday 9/11/2012**
Problem Set #1	• **Due Wednesday 9/19/2012 at 12:00 pm in the drop box in OHE 430N (Xerox room)** • **Email to the grader (Thada Suksila) at ame513_fall2012@yahoo.com or fax to 213-740-8071 if you're off campus** • **DEN students submit through the usual channels**

Note: You can find most of the needed thermodynamic data from Turns or from http://ronney.usc.edu/AME513F12/GasThermoData.xls. The rest can be found from external sources, e.g. http://webbook.nist.gov/chemistry/.

Problem #1 (10 points)

a) For an equivalence ratio $\Phi = 0.6$, what are the fuel mass fractions (f) for methane, propane and decane ($C_{10}H_{22}$) burning in air?

b) For some "reforming" applications, it is desirable to burn very rich so that the products of combustion are CO, H_2 and N_2 rather than the usual CO_2, H_2O and N_2, and the CO / H_2 mixture (called "syngas" among other names) is then used in other chemical processes. Repeat part (a) for assumed products of CO, H_2 and N_2 but in this case assume a **stoichiometric mixture** with the assumed CO, H_2 and N_2 products.

Problem #2 (10 points)

a) Assuming "complete" combustion (i.e. all C $\rightarrow$ CO_2, all H $\rightarrow$ H_2O, all N $\rightarrow$ N_2), determine the stoichiometric fuel-to-air mole ratio for an arbitrary oxygenated compound $C_xH_yO_z$.

b) Determine the stoichiometric fuel mass fraction (f) for an arbitrary oxygenated compound.

c) Determine the heating values of ethanol (C_2H_5OH) and dimethyl ether (CH_3OCH_3) burning in air.

Problem #3 (30 points)

Nitrous oxide (N_2O) is used as an oxidant in some racing cars instead of air. But, is it better than using oxygen (O_2)?

a) Compute the stoichiometric fuel-to-oxidant mole and mass ratios of iso-octane (C_8H_{18}) burning with air, N_2O and O_2 oxidants. Note that for air, the "oxidant" is O_2 + 3.77 N_2, not just O_2.

b) Compute the heating value of iso-octane (per unit mass of **fuel only**) with each of these 3 oxidants.

c) Compute the heating value of iso-octane **per unit volume of fuel-oxidant mixture** with each of these 3 oxidants.

d) Estimate the constant-pressure adiabatic flame temperatures of iso-octane (C_8H_{18}) burning with air, N_2O and O_2. Assume that the values of C_P at 298K can be used in this estimate. **Note that the thermodynamic tables give C_P per mole, not per mass, whereas the relation $T_{ad} = T_\infty$**

+ fQ_R/C_P requires the mass-based C_P. (How does one know that formula requires the mass-based C_P? Check the units!)

e) Repeat part (d) using the values of C_P at the **average temperature** between 298K and the adiabatic flame temperatures computed in part (d).

f) In part (c) you should have found that O_2 yields the highest heating value per volume, with N_2O the second highest. Thus, O_2 should be a better oxidant than air or N_2O for racing applications, where the volume of reactants that can be ingested per unit time is what limits power. Can you explain why is N_2O rather than O_2 used in racing applications?

Problem #4 (30 points)

For a carbon monoxide-oxygen (not air!) mixture with equivalence ratio 0.6, initial temperature 500K and initial pressure 5 atm:

a) Assuming constant specific heats and all CO burns to form CO_2, determine the constant volume adiabatic flame temperature for this mixture.

b) Determine the final pressure.

c) Repeat Problem 4a assuming the combustion products are CO, O, O_2, O_3 and CO_2 using GASEQ. The procedure is as follows:

1. At the top of the page, under "Problem type" select "adiabatic T and composition at const v"
2. Under "Reactants" enter "CO" and hit return
3. Under "Reactants" enter "O2" and hit return
4. In the list of reactants click on "CO" then enter the number of moles of CO needed to obtain an equivalence ratio of 0.6
5. In the list of reactants click on "O2" then enter the number of moles of O_2 needed to obtain an equivalence ratio of 0.6
6. In the box below the reactants box, enter the reactant temperature and pressure (500K, 5 atm in this case)
7. Under "Products" enter "CO" and hit return; repeat for O, O_2, O_3 and CO_2
8. Click on the "calculate" button

d) Why is the flame temperature and pressure so much lower in part c) than in a)? (There are two main reasons, both of which were discussed in class).

e) Show that the equilibrium concentrations of CO, O_2 and CO_2 predicted by GASEQ are consistent with a hand calculation (Lecture 3 notes).

f) Using the property data in the Excel spreadsheets, calculate the internal energy per unit mass of the reactants and compared this calculation to the value reported by GASEQ.

g) Using the property data in the Excel spreadsheets, calculate the internal energy per unit mass of the products and compared this calculation to the value reported by GASEQ. (Note that the internal energy per unit mass is the same before and after combustion, which must be the case for constant-volume combustion.)

h) Calculate the entropy per unit mass of these combustion products and compare this calculation to the value reported by GASEQ.

i) Using GASEQ, expand these products back to 5 atm. The procedure is as follows:

1. Click the “R<<P” button to make the products of combustion become the reactants for the expansion
2. At the top of the page, under "Problem type" select "Adiabatic compression/expansion"
3. Uncheck “Frozen chemistry”
4. In the products property list, enter “5” in the pressure box
5. Click on the "calculate" button

j) Calculate the entropy per unit mass of these expanded products and compare this calculation to the value reported by GASEQ. (Note that of course it’s the same as the entropy per mass before expansion).

<u>Problem #5 (20 points)</u>

Hydrogen peroxide (H_2O_2) is a liquid rocket fuel that decomposes exothermically to form a mixture of gaseous H_2, O_2 and H_2O:

$$H_2O_2 \text{ (liquid)} \rightarrow ??? \ H_2 \text{ (gas)} + ??? \ O_2 \text{ (gas)} + ??? \ H_2O \text{ (gas)}$$

Note that there is no H_2O_2 in the products.

For H_2O_2 you only need Δh_f^o(liq) = -187.8 kJ/mole and its molecular weight = 0.0340 kg/mole.

a) What is the heating value of hydrogen peroxide “fuel” in J/kg if the combustion products are only H_2O and O_2 only (no H_2)?

b) Estimate the constant-pressure adiabatic flame temperature of hydrogen peroxide if the combustion products are only H_2O and O_2 only (no H_2) and the initial temperature is 298K.

c) If these combustion products are heated or cooled to a temperature of 2000 K at a total pressure of 0.1 atm, what is the mole fraction of H_2 **at equilibrium** in the products, now assuming that the products are H_2O, O_2 **and** H_2? You need to use the equilibrium constraint equations to determine the solution, but you can check your answer using GASEQ.

d) If 0.5 moles of H_2 is added to the reactant mixture, i.e.

$$H_2O_2 \text{ (liquid)} + 0.5 \ H_2 \text{ (gas)} \rightarrow ??? \ H_2 \text{ (gas)} + ??? \ O_2 \text{ (gas)} + ??? \ H_2O \text{ (gas)}$$

what is the heating value per unit total mass of reactants, again assuming the combustion products are only H_2O and O_2 only (no H_2)?

e) For the mixture of part (d), what is the mole fraction of H_2 at equilibrium in the products, again assuming a temperature of 2000K and pressure of 0.1 atm?