AME 436	Assigned: Wednesday 1/24/2018
Problem Set #1	• Due Wednesday 2/7/2018 at 4:30 pm in drop-off box in OHE 430N (back room of the OHE 430 suite of offices, where the Xerox machine is located) • Hard copies are preferred but you can email your assignment to the graders at ame436usc@gmail.com if you're off campus. **Emailed files must be a single .pdf file, not 20 .jpg images!** • DEN students submit through the usual channels.

Problem #1 (15 points)

a) For the following fuel/oxidant combinations and presumed products balance the following reactions and calculate the stoichiometric fuel to oxidant ratios on a molar basis and on a mass basis:

Fuel + oxidant	Presumed products
H_2 + air	H_2O and N_2
CH_4 + air	CO, H_2 and N_2
CO + N_2O	CO_2, H_2O and N_2
C_8H_{18} + NH_4NO_3 (ammonium nitrate)	CO_2, H_2O and N_2
Lithium (Li) + NO	Li_2O and N_2

Use the property data in the table below.

Species	Δh_f^o (kJ/mole)	Molecular mass (g/mole)	Species	Δh_f^o (kJ/mole)	Molecular mass (g/mole)
CH_4	-74.87	16	O_2	0.00	32
H_2O	-241.84	18	N_2O	81.55	44
H_2	0.00	2	CO_2	-393.51	44
CO	-110.54	28	C_8H_{18}	-250.29	114
NH_4NO_3	-365.56	80	N_2	0.00	28
NO	90.30		Li_2O	-595.8	30
Li	0	7			

b) For the stoichiometric fuel/oxidant/product combinations above, calculate the heating value in Joules per kg of fuel. **Watch units – kilojoules vs. Joules, kilograms vs. grams, moles vs. kilograms.**

Problem #2 (15 points) (from a previous year's midterm exam)

On Titan, one of Jupiter's moons, is an atmosphere of pure C_3H_8 at 0.2 MPa (2 earth atmospheres) pressure at a temperature of 240K. Deep underground are deposits of 40 mole percent O_2 and 60 mole percent N_2 that the Titans pump out of the ground. Unfortunately, most of the O_2/N_2 wells are located in politically unstable regions of Titan, so this O_2/N_2 mixture is a valuable resource which they call "fuel." The propane in the atmosphere, which they call "air," is "free" as far as Titans are concerned.

Thermodynamic data: average mixture properties $\gamma = 1.35$, $R = 290$ J/kgK, $C_P = 1120$ J/kgK

	C_3H_8	O_2	N_2	CO_2	H_2O	N
Δh_f^o (kJ/mole)	-104.7	0	0	-393.52	-241.83	+472.68
Molecular mass (g/mole)	44	32	28	44	18	14
K (equilibrium constant) at 2200K (dimensionless)	2.043×10^{-14}	1	1	2.037×10^{3}	1.644×10^{1}	1.238×10^{-8}

a) What is the stoichiometric "fuel" to "air" mass ratio (FAR) assuming the combustion products are CO_2, H_2O and N_2? **(Watch units – g vs. kg vs. moles, kJ vs J, etc.)**
b) What is the heating value (in J/kg) of the 40% O_2 / 60% N_2 "fuel" that Titans burn with C_3H_8?
c) What is the **constant-pressure** adiabatic flame temperature of "fuel' + "air" mixtures with equivalence ratio (ϕ) = 0.8 ?
d) The main product of stoichiometric fuel-air combustion (other than N_2, CO_2, H_2O) is N atoms, which are extremely toxic to Titans. Suppose that after combustion, the temperature of the products mixture were increased or decreased to 2200K (but still kept at 2 atm total pressure). Assuming that the mole fraction of N atoms (X_N) << 1, estimate the value of X_N at equilibrium.

<u>Problem #3 (15 points)</u> (from a previous year's midterm exam)

On Planet X (which is completely unrelated to Titan), the atmospheric pressure is exactly half that of earth's atmosphere. All other properties of the atmosphere, specifically the ambient air temperature (T_∞), composition (O_2 + 3.77 N_2), thermal conductivity (k), heat capacities (C_P, C_v) are exactly the same as on earth. How would each of the following properties be different on Planet X than on earth? In particular, state whether the property increase or decrease and by a factor of less than, more than, or exactly a factor of 2. In some cases there may be no change at all. **No credit without explanation.**

a) Stoichiometric fuel mass fraction (f) for methane burning in air
b) Heating value of methane burning in air
c) Constant-volume adiabatic flame temperature of methane burning in air

<u>Problem #4 (40 points) (definitely NOT from a previous exam…)</u>

For a carbon monoxide-oxygen (not air!) mixture with equivalence ratio 0.4, initial temperature 600K and initial pressure 10 atm:

a) Assuming constant specific heats and all CO burns to form CO_2, determine the constant <u>volume</u> adiabatic flame temperature for this mixture. The average of C_v of the CO / O_2 mixture at 600K is 735 J/kgK.
b) Determine the final pressure.
c) Repeat Problem 3a 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 0.4
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 0.4
6. In the box below the reactants box, enter the reactant temperature and pressure (600K, 10 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 (an example of which is shown in the Lecture 3 notes, page 9). You can get the thermodynamic data table from:

http://ronney.usc.edu/AME436/GasThermoData.xls).

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 10 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 "10" 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).

Problem #5 (15 points)

In a combustion experiment at 10 atm total pressure, the measured flame temperature was 3500K and the following combustion product mole fractions were measured:

H_2O: 0.52059 H_2: 0.29432

H and OH are also present in the products, but the mole fractions are unknown. No other chemical species are present in the products.

a) If it can be assumed that the products are in chemical equilibrium, determine the mole fraction of H in the products.
b) Determine the mole fraction of OH in the products.
c) Determine the H/O atom ratio {i.e. the total amount of H (in the form of H, H_2, H_2O or OH) to the total amount of O (in the form of H_2O or OH)}.
d) If the **reactants** (not **products**) were H_2 and O_2 only, what was the equivalence ratio of the reactants?

Use the equilibrium constant data from http://ronney.usc.edu/AME436/GasThermoData.xls or double click on one of the tables on Slide 8, Lecture 3.