

AME 436	Assigned: 2/1/08
Problem Set #1	Due: 2/8/08 at 4:30 pm in my office mailbox (OHE 430J) (email or fax to me at 213-740-8071 if you're off campus, DEN students can fax to the usual number)

Note: some of the special symbols on this page seem to show up properly only with Internet Explorer and not other web browsers in the html version, but everything looks fine in the pdf version.

Problem #1 (stoichiometry, heating values)

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
$C_3H_8 + \text{air}$	$CO_2, H_2O \text{ and } N_2$
$C_3H_8 + \text{air}$	$CO, H_2 \text{ and } N_2$
$C_3H_8 + N_2O$	$CO_2, H_2O \text{ and } N_2$
$C_8H_{18} + NH_4NO_3$ (ammonium nitrate)	$N_2, H_2O \text{ and } CO_2$
CH_3NO_2 (nitromethane) + air	$CO_2, H_2O \text{ and } N_2$

b) For the stoichiometric fuel/oxidant/product combinations above, calculate the heating value in Joules per kg of fuel. You'll need the enthalpies of formation and molecular weights for these species. **Watch units – kilojoules vs. Joules, kilograms vs. grams.**

Species	Δh_f° (kJ/mole)	Mole. Wt. (g/mole)	Species	Δh_f° (kJ/mole)	Mole. Wt. (g/mole)
C_3H_8	-104.68	44	O_2	0.00	32
H_2O	-241.84	18	N_2O	81.55	44
H_2	0.00	2	O_3	142.26	32

CO	-110.54	28	CO ₂	-393.51	44
NH ₄ NO ₃	-365.56	80	C ₈ H ₁₈	-250.29	114
CH ₃ NO ₂	-112.97	61	N ₂	0.00	28

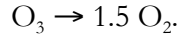
Problem #2 (flame temperatures, chemical equilibrium)

For a carbon monoxide-oxygen (not air!) mixture with equivalence ratio 0.25, initial temperature 400K and initial pressure 10 atm:

- a) Assuming constant specific heats and all CO burns to form CO₂, determine the constant volume adiabatic flame temperature for this mixture. The average of C_v for CO and O₂ at 300K is 700 J/kgK; assume that this C_v is the temperature-averaged and composition-averaged C_v for the mixture (though in part (e) you should discuss the problem with making this assumption.)
- b) Determine the final pressure.
- c) Repeat Problem 2a assuming the combustion products are CO, O, O₂, O₃ and CO₂ 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 0.25
 5. In the list of reactants click on "O2" then enter the number of moles of O2 needed to obtain an equivalence ratio of 0.25
 6. In the box below the reactants box, enter the reactant temperature and pressure (400K, 10 atm in this case)
 7. Under "Products" enter "CO" and hit return; repeat for O, O₂, O₃ and CO₂
 8. Click on the "calculate" button
- d) Show that the equilibrium concentrations of CO, O₂ and CO₂ predicted by GASEQ are consistent with a hand calculation (Lecture 3 notes, page 9). (You should find that the temperature is higher than 2500K, which is the maximum the tables on page 8 show, but if you double-click on the tables on page 7, you'll open up an excel spreadsheet which has the data up to 6000K. You can also get this table via a direct link from my website: <http://ronney.usc.edu/AME436S06/GasThermoData.xls>).
- e) 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).

Problem #3 (heating value, flame temperatures, chemical equilibrium) (from a previous year's midterm exam)

A new process has been invented to produce and store ozone (O₃) safely and economically (yeah right...) Ozone decomposes exothermically to form O₂ via the reaction



Thermodynamic data (*not all of this data is needed*):

	O ₃	O ₂	O
Δh_f° (J/mole)	1.427×10^5	0	2.492×10^5
Molecular weight (kg/mole)	0.048	0.032	0.016
C_p (J/mole K) (temperature-averaged)	57.18	36.49	20.84
K_i (equilibrium constant) at 2500 Kelvin (dimensionless)	3.01×10^{-7}	1	1.44×10^{-2}

- What is the heating value of ozone “fuel” in J/kg if the combustion product is O₂ only (no O₃, no O)?
- Estimate the constant-pressure adiabatic flame temperature of ozone if the combustion product is O₂ only (no O₃, no O) and the initial temperature is 300K.
- At a temperature of 2500 K and a pressure of 1 atm, what is the mole fraction of O atoms **at equilibrium** in the products? For this part assume the products contain O and O₂ but do not contain O₃.

Problem #4 (chemical equilibrium) (from a previous year's midterm)

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

- If it can be assumed that the products are in chemical equilibrium, determine the mole fraction of H in the products.
- Determine the mole fraction of OH in the products.
- Determine the H/O atom ratio {i.e. the total amount of H (in the form of H, H₂, H₂O or OH) to the total amount of O (in the form of H₂O or OH)}.
- If the **reactants** (not **products**) were H₂ and O₂ only, what was the equivalence ratio of the reactants?

Use the equilibrium constant data from the tables on page 8, lecture 3 or from

<http://ronney.usc.edu/AME436S08/GasThermoData.xls>).