ME382R

# Homework #1: Equilibrium

**1a. Download Cantera and run a sample problem.** Familiarize yourself with the code and how you edit it for different cases.

**1b. Use Canters to study equilibrium in fuel/air mixtures.**

*All students should do problems 5 and 6 and 6. 1-4 are assigned as indicated below.*

Goal: Learn to use Cantera for equilibrium problems and develop an understanding of the effect of various parameters on equilibrium characteristics.

For problems 1-4, present graphs that illustrate the main points. You will want to consider

(a) T adiabatic (if applicable)

(b) Equilibrium CO

(c) Equilibrium NO (NOx)

(d) Equilibrium unburnt HC

(e) CO2 “potential” –you may want to present as CO2/LHV to compare fuels

As a guide to your presentation, consider that concentrations of NO, CO, and unburnt HC in the range of <100 ppm (and perhaps <10 ppm) are significant from an environmental viewpoint. You may need to use a log graph in order to present your results adequately. For comparisons of different hydrocarbons, determine if members of a particular family (i.e. alkane, alkene, etc.) behave in a similar fashion. Also, try to correlate your results to temperature and pressure.

Grade: 80% Powerpoint presentation to class (50% calculations, 50% presentation)

20% solutions to 5 & 6

1. Determine the effect of equivalence ratio  on (a)-(e) for different hydrocarbons, coal, and hydrogen with air in a constant pressure (1 atm) adiabatic process.

2. Determine the importance of temperature (at 1 atm) on (b)-(e) for methane and one higher hydrocarbon. To do this, choose an equivalence ratio (e.g.  =1) and vary the temperature. Consider what is a reasonable range of temperatures.

3. Determine the effect of pressure on the quantities in (a)-(e). To do this, choose an equivalence ratio (e.g.  =1) and vary the pressure. Consider what is a reasonable range of pressures.

4. Determine the effect of using O2 as the oxidizer with methane but with trace amounts of N2 on (a)-(e).

5. Determine by hand the adiabatic flame temperature for a stoichiometric mixture of methane/air undergoing a constant pressure process assuming complete combustion. Compare this to the results obtained from Cantera assuming the same products as in your hand calculation and also assuming all possible products.

6. Determine by hand the adiabatic flame temperature and concentrations of product species for a mixture of methane/air with Assume that the products consist of H2O, CO2, CO, O2, and N2. Compare to results obtained from Cantera.

**Assignments for problems 1-4**

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| Isha, Tullie, Quinten, Aryton | 1 + presentation of solution to #5 |
| Ganesh, Gabriel, Robert | 2 |
| Ethan, Caelix, Ameya, | 3 |
| Junyuan, Joshua, Miles, Ty | 4 + presentation of solution to #6 |