ENAE 4930/5131: Combustion
Computer Project 1: Due Wednesday, December 8, 2021

Please turn in a typed report with the *plots embedded* into the document (MSword, LaTeX, etc.). In addition, email your python scripts, IPython notebooks, etc. that were used to complete this project. Do NOT use Excel for plotting. Instead, use Matplotlib if you are using Python.

Use of proper grammar, jargon, etc. is mandatory. Make sure that all of your plots look neat, are properly annotated, and the lines are distinguishable when printed in black and white.

Use the `gri30_highT.cti` to provide species and thermodynamic data for the gas and `graphite.cti` for graphite. On my MacBook these files can be found in the directory: `/anaconda3/pkgs/cantera-2.4.0-np115py37_2/lib/python3.7/site-packages/cantera/data`. These file can also be found at: `https://github.com/Cantera/cantera/tree/master/data/inputs`.

Problems

1. Add the species `HE` to the `gri30_highT.cti` file. Save the file with a different name in your own local working directory.

   Hint: Helium is a *atomic* noble gas, just like Argon.

2. Compute and plot the constant-pressure adiabatic flame temperature for CO, H_2, CH_4, C_2H_6, C_2H_4, C_2H_2, and C_3H_8 in air and as a function of equivalence ratio for $0.1 < \phi < 10$ *on the same figure* and *label each line*. Comment on any trends that you notice.

3. For mixtures of *propane and air*, 1): Plot the the constant-pressure adiabatic flame temperature and the mole fractions of the major species and 2): Plot the constant-pressure adiabatic flame temperature and mole fraction of pollutants (CO, NO, NO_2, and $C_{s,\text{graphite}}$ for mixtures of propane and air as a function of equivalence ratio. Comment on any trends you notice. In particular comment, on where NO and CO mole fractions peak. You MUST use at least 100 points in these plots.

4. Plot, on the same figure, the constant-pressure adiabatic flame temperature for *propane* with the following air surrogates as a function of ϕ

   a) $O_2 + 3.76\ N_2$,

b) O_2 + 3.76 He,
c) O_2 + 3.76 Ar,
d) O_2 + 3.76 CO_2,
e) O_2 + 3.76 H_2O,
f) 2 N_2O + 1.76 N_2.

Explain the reason that some air surrogates provide higher flame temperatures than others.

Hint: Cantera can be used to examine the specific heats, heats of reaction, and enthalpies of formation of the diluents and oxidizers in these air surrogates.

5. It is more accurate to thermodynamically treat soot (Carbon) as a condensed-phase species rather than a gas which is done in the `gri30.cti` file. However, condensed phase species are often in low concentrations for hydrocarbon combustion. As a result, it is common to approximate these low-concentration species as if they are a gas-phase species with enthalpy that is representative of the solid phase.

   In this problem you will be comparing the flame temperatures for C_2H_2 and air mixtures produced by assuming that carbon only exists in the gaseous form and by assuming that carbon can exist in the gas and solid phases.

   a) Modify your `cti` file to include `C(gr)` in the species list. Thermodynamic data for solid carbon can be found in `graphite.cti`. Save this modified file with a new name in your working directory. You should now have two different files.

      Note: If Cantera complains about the lack of transport data for `C(gr)` then copy and paste the transport information from H atom into graphite. (Transport data is irrelevant at this time, but could be necessary to get Cantera to initialize the gas.)

   b) Define a new gas phase using the modified Cantera input file. It is important to keep both gas mixtures. For example, you could name the two mixtures:

      ```
      gas_Cgas_only = ct.Solution('older_file.cti')
      gas_Cgr = ct.Solution('new_file.cti').
      ```

   c) Plot the adiabatic flame temperature for both cases (one including soot as a solid-phase species and the other excluding soot as a solid-phase species) as a function of equivalence ratio. Explain any differences in the flame temperature produced by the two different assumptions.

6. You may have noticed something strange with the flame temperature for acetylene at very fuel rich conditions. On the same figure, plot the constant-pressure adiabatic flame temperature and mole fractions of CO_2, CO, $C_{s,\text{graphite}}$), H_2, C_2H_2 for mixtures of acetylene and air for $0.1 < \phi < 10$. Use this figure, the chemical structure of acetylene, $\bar{h}^0_{f,\text{C2H2}}$, and T_{ad} when $\phi = \infty$ to explain this odd phenomena. Comment on whether storing large quantities of acetylene without any special precautions is a good idea.

   Hint: Matplotlib can make plots with dual y-axes.