AE/ME 6766/Seitzman
Spring 2021
Project #1
Due Mon., Feb 1

Equilibrium Combustion Product Properties

Learning Objects of this Project

1. Enable you to gain insight into the major products of combustion and adiabatic combustion temperatures as a function of various operating conditions.
2. Gain experience using a chemical equilibrium solver.
3. Give you practice presenting and describing results of your analysis in a clear and concise fashion.

Report Format

As indicated by Goal 3, you will prepare a short but complete report for this project. Please follow the report guidelines outlined on the class web page: (http://seitzman.gatech.edu/classes/ae6766/projectformat.html)
Remember that you are writing this as a **single**, comprehensive report – NOT a separate report on each of the required calculations included below.

When you present the results graphically, think carefully how to make graphs that clearly support your observations and conclusions – for example be careful of linearly scaled plots if you are trying to show a wide range of values and you want to be able to visualize what is happening at both small and large values – a log scaling may help. Also, there is no requirement (and it may not be helpful) to present your results in the same order, or grouped in the same way as the list of required calculations below. You may also find it useful to make comparisons by showing results from different calculations on the same graph – and even repeating the same results in multiple graphs if that helps.

Project Description

Overview

You will perform full chemical equilibrium calculations in this project. At a minimum, you are to determine the results listed in the following section. You may also wish to perform further analysis in order to better understand these concepts. You may present your results in any order you find logical and helpful in writing a coherent report – so not necessarily in the order presented below.

Required Calculations

1. Constant pressure, adiabatic product temperature (typical called *adiabatic flame temperature*) and product composition (in mole fractions) as a function of equivalence ratio for the range $0.4<\phi<2.5$. Reactants are ethene (also known as ethylene) and synthetic air (denoted below as "air") at a pressure of 1 atm and a reactant temperature of 288K. Include in your plots of composition all species that have mole fractions greater than 10^{-5} at an equivalence ratio of 1.0.

2. Constant volume, adiabatic product temperature (e.g., what might be achieved in a closed vessel), product pressure and product composition (in mole fractions) as a function of equivalence ratio ($0.4<\phi<2.5$) for combustion of ethene and "air", with an initial pressure of 1 atm and a reactant temperature of 288K. Show results for the same species as you did in item 1.

3. Adiabatic flame temperature and product mole fractions of ***six important/interesting*** species (major and/or minor species are okay) as a function of the initial (reactant) temperature and pressure for ethene-"air" mixtures at ϕ=0.7, 1.0 and 1.4. When you change the temperature and pressure, use some "practical" or "meaningful" ranges for your calculations – you must provide your motivation/reasoning for your choices. Similarly in your report, provide your reasoning for picking these ***important/interesting*** species.

4. Repeat item 1, this time for the reactants being **ethane** and "air".

5. Repeat item 1, this time for the reactants being ethene and **oxygen**.

Equilibrium Computer Tools

You may use any equilibrium solver tool at your disposal. You are NOT expected to write your own solver - use a widely available tool. Some options are:

1) **Gaseq** - available on the AE computer cluster, or the GT server (https://mycloud.gatech.edu/vpn/index.html, choose the AE-2019 desktop and look for the Gaseq icon on the desktop) or downloadable to your computer (PC version only) using the link on the class web page.
2) **EQUIL** in ANSYS **Chemkin** - also available on the GT server.
3) **NASA's Chemical Equilibrium** code, an online version is available at https://cearun.grc.nasa.gov. You can also request to get a copy from NASA's software catalog (https://software.nasa.gov/software/LEW-17687-1), but it is for U.S. release only.
4) **STANJAN** - an online interface is available at http://navier.engr.colostate.edu/code/code-4/index.html.