Problem #4: Pick a hydrocarbon fuel (post your fuel on the blog under Problem 4 topic so that no one else can pick the same fuel). You are to study how the flame temperature changes as this fuel is burned with air and pure oxygen. You are going to vary the equivalence ratio over a wide range (rich to lean) and see how the flame temperature changes for (a) PG model (two lines on one plot Tf vs phi), (b) IG model, and (c) equilibrium model. This will generate three plots each with two curves (for air vs. pure oxygen as the oxidizer).

Suppose that an equal ratio of C and CH4 will combust. We wish to see the effect of phi on the adiabatic flame temperature for combustion with air as well as pure oxygen. For this problem we will plot the adiabatic flame temperature vs phi for (a) PG model, (b) IG model, and (c) the flame temperature as the ratio of fuels changes.

First we must determine the chemical balance for theoretical air. This is done below:

 $aCH\_{4}+bC+d\left(O\_{2}+3.76N\_{2}\right)→eCO\_{2}+fH\_{2}O+gN\_{2}$ (1)

 $a=b=0.5$ (2)

 $e=1$ (3)

 $f=1$ (4)

 $d=1.5$ (5)

 $g=5.64$ (6)

It is necessary to note that for this equation to be usable, it is on a mole basis of one mole of fuel. This is why a and b are equal to 0.5, so that they will combine to make one kmol of fuel.

The above implies that the theoretical reaction is:

 $0.5CH\_{4}+0.5C+1.5\left(O\_{2}+3.76N\_{2}\right)→CO\_{2}+H\_{2}O+5.64N\_{2}$ (7)

The distinction has to be made that there is a difference between a phi less than on and a phi greater than one. For a phi less than one, there is excess oxygen produced:

 $0.5CH\_{4}+0.5C+α1.5\left(O\_{2}+3.76N\_{2}\right)→CO\_{2}+H\_{2}O+α5.64N\_{2}+zO\_{2}$ (8)

where α is the theoretical air percentage. z can be determined from another chemical balance:

 $2\*α\*1.5=3+2z$ (9)

 $z=1.5α-1.5$ (10)

For a phi less than one we get the following chemical balance:

 $0.5CH\_{4}+0.5C+α1.5\left(O\_{2}+3.76N\_{2}\right)→CO\_{2}+H\_{2}O+α5.64N\_{2}+(1.5α-1.5)O\_{2}$ (11)

It is worth noting that α is the inverse of phi.

For combustion with phi greater than one, we have incomplete combustion. This can be modeled several ways, but for the purpose of this study, it will be modeled as producing carbon monoxide in addition to carbon dioxide. This can be seen below:

 $0.5CH\_{4}+0.5C+α1.5\left(O\_{2}+3.76N\_{2}\right)→aCO\_{2}+bH\_{2}O+α5.64N\_{2}+cCO$ (12)

Once again, doing a chemical balance, *a*, *b*, and *c* can be determined:

 $b=1$ (13)

 $a=3α-2$ (14)

 $c=3-3α$ (15)

Now that we have a case for both a phi less than one, and greater than one, it is possible to determine the adiabatic flame temperature. This is the temperature of the exit when there is no heat transfer to the surroundings. This necessitates that:

 $\sum\_{}^{}γ\_{p}\*h\_{p}=\sum\_{}^{}γ\_{R}\*h\_{R}$ (16)

For the PG model, this simplifies to:

 $T\_{af}=T\_{i}+\frac{-∆h\_{c}^{o}}{c\_{p}[1+AF]}$ (17)

This can be said because the cp value is constant for PG gases. The numerator can be expressed as follows:

 $∆h\_{c}^{o}=\frac{\sum\_{}^{}γ\_{p}\*\overbar{h\_{p}^{o}}-\sum\_{}^{}γ\_{r}\*\overbar{h\_{R}^{o}}}{\overbar{M}\_{C+CH\_{4}}}$ (18)

With a phi less than one, this is constant as there is no enthalpy of formation changing in the products or reactants:

 $∆h\_{c}^{o}=-42708.2\frac{kJ}{kg}$ (19)

With a phi greater than one, this is not the case, and $∆h\_{c}^{o}$ must be calculated at each phi.

a.) Plot the adiabatic flame temperature for the fuel reacting with Air and pure oxygen over a range of phi’s

For air, this can be directly calculated using the above derivation. With oxygen, the only difference is the nitrogen term drops out of the chemical balance. The main effect this has is to drastically increase the temperature by decreasing the AF ratio. The graph can be seen below with the two temperature ranges super imposed:

Figure 1. Temperature vs. Equivalence Ratio for Air

b.) Do the same as in a, but us the IG model.

The reason the simplification is so simple for the PG model is that the Cp is assumed to be constant both across temperature ranges and species. For the IG model, this assumption cannot be made. Thus equation (16) must be solved.

Hence, and iterative method muse be employed as the exit temperature is not known, and what we are trying to solve for. Using TEST, we can determine the adiabatic flame temperature. For the IG model, it is plotted below:

Figure 2. Adiabatic Flame Temperature vs. Equivalence Ratio

We can see that the temperature is less than the PG model, which is to be expected. It also appears to be much less linear than the PG model, also to be expected. Note also, it is much more accurate as the lines are no longer linear, but rather nonlinear in nature.

c.) Plot the adiabatic flame temperature as the ratio of methane to carbon changes from zero methane to pure methane. Do this with the PG model with theoretical air.

This problem is a great way to determine the temperature of various mixtures of methane and carbon and what output temperature they could produce. This could be used for a variety of applications. If coupled with a cost of the fuel, it could easily be used to gauge what the optimal ratio of the fuels would be for max temperature output.

Once again, equation (17) is utilized.

However, this time the $∆h\_{c}^{o}$ is not constant. The chemical balance will have to be calculated at each iteration:

 $aCH\_{4}+bC+d\left(O\_{2}+3.76N\_{2}\right)→eCO\_{2}+fH\_{2}O+gN\_{2}$ (20)

Where a varies from 0 to 1, b varies from 1 to 0, and the remaining coefficients can be determined from below:

 $a+b=1=e$ (21)

 $2a=f$ (22)

 $d=1+a$ (23)

 $g=d\*3.76$ (24)

Looping over a and b, we can determine the adiabatic flame temperature. The results are plotted below:

Figure 3. The adiabatic flame temperature with various mixture percentages.

From Figure 3 it is clear to see that Methane has a higher adiabatic flame temperature than that of Carbon. It is interesting to note that the relationship between the two is not linear in nature. This graph could eventually be used to optimize the ratio of the two fuels to provide an ideal mixture.