

ME 524 – Combustion
Problem Set 2 – Due Tuesday, April 14, 4:30pm

Objective: The goal here is to understand how equilibrium codes find the compositions of mixtures containing large numbers of components. By the end of this problem set, you will be able to easily visualize how to write a code for full hydrocarbon combustion equilibrium containing of the order of 50 species.

In our system 1 kmole of ammonia (NH_3) is mixed with 1 kmole of O_2 and 0.5 kmoles of H_2S and allowed to come to equilibrium at 3000 K and 10 atm pressure. The equilibrium products are assumed to contain only NH_3 , NO , H_2S , SO_2 , H_2 , H , OH , O , O_2 , and H_2O .

1. Use the general Gibbs energy minimization approach outlined in the handout to find the kmoles of each species in the equilibrium mixture, and the mole fraction of each species. Present this in a clear table with three columns (species, kmoles, mole fraction). Put the species in the order given above. This involves working with equations 44 and 46 in the handout via some kind of programming. Also, to help debugging, use the following element order: N, S, O, H for $i=1-4$.

A couple of hints. In the past I've solved this kind of problem via Excel. The under-relaxation condition expressed by equation 49 is designed to prevent a minor species from getting too large too fast. I do not believe this will occur here, so this one under-relaxation condition can probably be omitted (the other definitely needs to be included). This will make the programming easier. Also, make sure your initial guesses for n_j do not add up exactly to n or you may get a zero division error on the first iteration. Note that this problem will require you to solve a 5x5 system of equations (Excel will do this, see the handout for how).

Properties. Our text includes all the data needed except for H_2S . The NIST Webbook is an excellent resource for these kinds of data when you cannot find a text resource.

On debugging. Convergence took me 13 iterations, so if you don't get there that fast, something is probably wrong. You can check your answers in a couple of ways. First, be sure your final composition gives you the correct original atom counts for N, S, O, and H. Even if you converge and get the correct atom counts, you can have the wrong final composition if you miscalculated a g^* . Incorrect final atom counts or failure to converge means an error elsewhere. Most errors, except for a miscalculated g^* , will lead to a rapidly diverging solution.

If you get stuck and want some help in debugging, please do the following. Start the calculation off with each $n_j=0.011$ kmoles and $n=0.1$ kmoles. Run the calculation for one iteration only, stop it, and then send us your spreadsheet. We'll have the same spreadsheet at hand, so any differences should immediately be apparent.

2. Use the Colorado State equilibrium code to check your answer:

<http://navier.engr.colostate.edu/~dandy/code/code-4/index.html>

This agreed very closely with my result.