Homework 7 Due 3/21/23

Syngas is a mixture of H_2 and CO, and it is a common fuel in many renewable and/or low-carbon combustion schemes. For this homework, you'll run the PREMIX 1-D flame code with a mechanism for syngas, then do some processing on the results to analyze the chemistry and transport.

Download the PREMIX package from the class website. It has all the executables and files you need. In addition, there is a manual for the code. To run the code, you modify the 'premix.inp' file using a text editor, and run the 'premix.exe' executable.

The gas phase mechanism that I'm using for syngas is from Quan-De Wang "An updated detailed reaction mechanism for syngas combustion" in RSC Advances Issue 9, 2014. The data are in the 'chem.inp' text file (units are mol, cm^3, and calories), and the transport parameters are in the 'tran.dat' text file.

A sample 'premix.inp' file is given, and it should run and converge. I recommend first running that case, and looking over the output in the text file 'premix.out.' A converged solution will end with:

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TWOPNT:  REFINE DID NOT PRODUCE A NEW MESH.

 TWOPNT:  SUCCESS.  BOUNDARY VALUE PROBLEM SOLVED.
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Which tells you that the final grid met the convergence criteria, and the problem is solved. The solution is given in text form in the output file, and you can cut and paste it into a spreadsheet.

Once you've verified that the code works, modify the input parameters so that you have a 1:1 H_2:CO mixture by volume, burning stoichiometrically (Φ=1) in air at 0.5 atm and 0.003 g/cm^2-s mass flow rate, with burner temperature of 400 K.

To make a converging input file, you should only need to modify:

1) The species and amounts denoted by the REAC, PROD, and INTM keywords. The REAC keyword denotes reactant mole fractions, and is critical. PROD and INTM values are guesses to get the code started on a convergent solution. You might start with equilibrium values for products, and something like 0.01 or 0.001 for intermediates. You'll have to add REAC, PROD, and INTM entries for your flame. One entry per line. Don't leave extra (blank) lines in the input file or you'll get an error.
2) FLRT which is the mass flow rate in g/cm^2-s.
3) PRES which is pressure in atm.

I'd leave everything else as-is. This simulation will be with mixture-averaged properties and no thermal diffusion. Run your input file, and verify that it converged. Temperatures should rise to the combustion level. An unburned solution will have temperatures fixed at around 400 K.

Getting the converged solution is step one, and should be really easy. Include your 'premix.out' file in your solution package. Most of the effort is in the processing, so see me asap if you can't get the code to converge.

For processing, you're going to make plots very similar to those we showed in class for the H_2/O_2 system. Specifically,

1) Plot species mole fractions versus distance over 0 to 1 cm with mole fraction on a log scale and distance on a linear scale.
2) Plot diffusion velocities for all species from 0 to 0.5 cm. You'll need to calculate binary diffusion coefficients at each point in the flow, then get mixture averaged diffusion coefficients and use those to get velocity. Automate with a spreadsheet or program. You did this on your last homework, and the same procedure applies here, just with more species.
3) Do a detailed analysis of H_2O_2:
    a. Plot the mass production rate of H_2O_2 from chemical reaction at every point in the flow by summing the chemical reaction rate terms in the mechanism for the 9 reactions involving H_2O_2. Use a spreadsheet or program for this, as it involves lots of repeat calculations. You'll need to get reverse reaction rates from equilibrium constants, and the data for these species are in the 'therm.dat' file. For the dissociation reaction of H_2O_2, instead of the complex reaction given in the Wang mechanism, you can use A = 1.2e17, n=0, and E_A = 45500 with no special third body efficiencies. That gives very nearly the same result as the expression used by Wang, and is much easier to calculate.
    b. Now calculate the mass production rate from the species continuity equation:

$$\frac{\dot{m}}{A}\frac{dY_i}{dx} + \frac{d(\rho Y_i V_i)}{dx} = \dot{\omega}_i \hat{M}_i$$

    where all the values are given in the solution (except the species diffusion velocities that you calculate in 2). You'll also have to calculate mass fractions from the given mole fractions. Compare the result in 3b) with that of 3a). Are they roughly similar quantitatively and qualitatively (Hint: they should be)?
    c. Plot on one page, three separate plots. H_2O_2 species velocity vs distance, H_2O_2 mass production rate vs distance, H_2O_2 mole fraction vs. distance. Plot these over the distance 0 to 0.5 cm. Discuss in a paragraph how the curves are related, and what causes the inflection points, minima, maxima, slope changes, etc.
    d. Plot reaction Rate of Progress (mol/cm^3-s) vs distance from 0 to 0.5 cm for every reaction involving H_2O_2. For the duplicate reactions, combine them into one curve. Discuss in a paragraph which reactions are primarily responsible for H_2O_2 production and which are responsible for H_2O_2 destruction.