Project 3: Premixed Laminar Flames (PR3_premix)

1. Hydrogen-Air Flame

In this exercise you use CHEMKIN IV to make calculations of premixed hydrogen-air flames. The emphasis is on the numerical accuracy of the solution, and the influence of transport properties and reaction mechanisms.

1. Read Section 7.4.2 in CHEMKIN_Input.pdf to understand all the relevant parameters for this project. Read the given example in Section 2.2.4 of CHEMKIN_Tutorials.pdf. Set up and run the 1-D premixed flame project with the given input files, `premixA.inp` and `chem_H2_RD37.inp` (which is the standard H_2 mechanism provided with Chemkin 3.7). What assumptions are being made about the molecular transport processes? Note the computed value of the laminar flame speed and the peak mole fraction of H.

2. The solution obtained in (1) is not numerically accurate for several reasons. Change and add parameters as needed to obtain numerically-accurate results. Report the accurately-computed values of the laminar flame speed and the peak mole fraction of H.

3. Investigate the four cases corresponding to mixture-averaged transport with and without thermal diffusion, and multicomponent transport with and without thermal diffusion. How does the transport model affect the laminar flame speed?

4. Plot the species profiles through the flame. Do so in a way that reveals the chemical behavior in the different regions of the flame. Comment on any similarities with the species evolution in the case of autoignition of a hydrogen-air mixture.

5. The attached figure shows experimental results of the laminar flame speed for hydrogen-air mixtures at atmospheric pressure and an unburnt temperature of 298K taken from Egolfopoulos & Law (Proc. Comb. Inst. **23**, 333-340, 1990). Compare the CHEMKIN IV computations (using multicomponent transport and thermal diffusion) with these experimental data.

6. Read the comments in the files `chem_Li.inp` and `tran_Li.inp`. These come from a leading chemical-kinetics research group. Use these data to calculate the laminar flame speed for a few values of the equivalence ratio, and comments on your findings.

2. Methane-Air Flame

The objective of this assignment is to use CHEMKIN IV to make calculations of a stoichiometric methane-air flame; and to study the structure of the flame, using the calculated properties.

1. Briefly examine the files `grimech30_dat.txt`, `thermo30_dat.txt`, `transport_dat.txt`, and `premixGC.txt`. The first three of these are the kinetic mechanism, thermodynamic data and transport data for the GRI 3.0 mechanism (see `http://www.me.berkeley.edu/gri_mech`). The fourth is a CHEMKIN IV input file. Read this file and report the problem that it is designed to solve.

2. Set up the project and run it using all of these files. (Make sure you correctly specify the thermodynamic and transport data files. It may take several minutes to run.) You may want to change some of the numerical parameters to investigate and improve the accuracy of the calculations, but this is not required.

   What is the calculated laminar flame speed? How does this compare to experimental data? Plot the major species against temperature.

3. Examine the Fortran program `prepost.f`. This program reads in (from file `mass.txt`) the profiles of species mass fractions obtained from the CHEMKIN IV calculation described in the previous question. As described in the comments in the program, `prepost.f` calls Chemkin routines to calculate various properties which are then output onto the files `mass.out`, `mole.out`, `create.out`, `destroy.out` and `props.out`. By studying `prepost.f` and the Chemkin routines called, identify and report the quantities output to each of these files. (Be precise, and give units.)

4. The Matlab script `CH4post.m` reads in the files generated by `prepost.f` and plots a simple figure. Answer the following questions by modifying and extending this script.

   (a) Plot the heat release rate and temperature against x and against the normalized coordinate
   $$x^* \equiv \dot{M} \int_{\hat{x}}^{x} \frac{c_p}{\lambda} dx, \tag{1}$$
   where $\hat{x}$ is the location of peak heat release.

   (b) Figures 5.5a-5.9 (attached) show computations for the same flame (but using a different mechanism). How do your calculations compare to those in the Figures? (You do not need to make careful quantitative comparisons, nor to present all the data: but comment on any significant observations.)

   (c) In the preheat zone, what is the temperature at the location where the heat release rate reaches 1% of its peak value?

   (d) Define $s \equiv x^* - x^*_{600}$, where x^*_{600} is the value of x^* where $T = 600K$ (in the preheat zone); and for the species H_2, O_2, H_2O, CH_4, CO and CO_2 define the normalized mass fractions by

$$\hat{Y}_j \equiv (Y_j - Y_j^o)/(Y_j^{600} - Y_j^o), \tag{2}$$

where Y_j^o and Y_j^{600} denote the mass fraction of species j in the reactants, and at the location where $T = 600$ (K), respectively. Plot $\hat{Y}_j$ vs s, for $s \leq 0$. What is the significance of these curves?

(e) Plot the "balance" of the species mass fraction conservation equation for CH_4, (vs. x^*) showing creation, destruction, net production (= creation - destruction), convection and diffusion. (Diffusion may be obtained as the remainder.) Identify the preheat zone and the fuel consumption zone. Is methane created in the flame?

(f) Plot the balance for CO and explain your observations.

(g) Plot the balance for H_2 and explain your observations.

(h) In flame theory, it is often assumed that in the reaction zone the dominant balance is between reaction and diffusion, with convection being small in comparison. Do your results support this assumption?

(i) Plot the creation and destruction rates, and the net production rates (creation minus destruction) of the species CH_4, CH_3, CH_2O, HCO, CO and CO_2. Comment on your observations.