Project 4: Non-Premixed Laminar Flames (PR4_oppdif)

1. Hydrogen-Air Flame

In this exercise you use CHEMKIN IV to make calculations of non-premixed hydrogen-air flames. The emphasis is on the numerical accuracy of the solution, and the influence of the timescale imposed by the flow.

1. Run `CHEMKIN IV` with the given input files, `oppdifA.inp` and `chem_H2_RD.inp`. Is the flow plane or axi-symmetric? What assumptions are being made about the molecular transport processes? Inspect the profiles of mixture fraction, temperature, species mole fractions, axial velocity, and normal strain rate. Record the peak temperature and the peak mole fractions of H_2O and H.

2. The solution obtained in (1) is not numerically accurate for several reasons. List the parameters affecting the numerical accuracy of the solution. Change and add parameters as needed to obtain numerically-accurate results. Record the number of grid points, the peak temperature, and the peak mole fractions of H_2O and H. Save the `XMLdata.zip` file as `XMLdata_B.zip`.

3. Perform as sequence of calculations for a decreasing sequence of values of `GFAC`, which can be interpreted as being proportional to the imposed flow timescale. For the smallest value of `GFAC` for which a flame exists, save the `XMLdata.zip` file as `XMLdata_C.zip`. For this case, how do T and X_{H_2O} vary with `GFAC`?

4. Make plots of temperature and major and minor species vs. mixture fraction, comparing the results from `XMLdata_B.zip` and `XMLdata_C.zip`. Choose the axes (log/lin/range) to show interesting features. Comment on differences between the results from the two cases. Comment on these plots compared to those obtained for complete combustion and for chemical equilibrium (from Project 1).

5. For a reasonably small value of `GFAC` (for which a flame exists) how sensitive are the calculations to the mechanism and to the transport model?

2. Methane-Air Flame

1. Set up and run `CHEMKIN IV` for an axisymmetric methane-air opposed jet non-premixed flame at atmospheric pressure and for both streams at 300K. Use the mechanism `RD_CH4.inp` and the standard Reaction Design thermodynamic and transport data. Use mixture-averaged transport properties and include thermal diffusion. Choose the jet separation and velocities to produce a stable flame in the center of the solution domain. Is this solution numerically accurate? Show the temperature profile.

2. By decreasing GFAC from 1.0, obtain solutions corresponding to progressively increasing strain rate. The nominal strain rate is defined by

$$a_{\text{nom}} \equiv (VFUE + VOXI)/(XEND * GFAC). \tag{1}$$

   Denote by a^* the highest value of a_{nom} for which you obtained a reactive solution. In addition to the case, $a_{\text{nom}} = a^*$, perform calculations for $a_{\text{nom}} = 0.1a^*, 0.01a^*$ and $0.001a^*$. Plot the peak temperature as a function of the effective nominal strain rate, a_{nom}.

3. For the four values of a_{nom}, plot T versus ξ. Make plots for selected species versus ξ. Discuss your observations. How do the major species and CO and H_2 compare to their equilibrium values?

4. Consider in this part the case $a_{nom} = 0.1a^*$. You can answer these questions by exporting the calculated profiles from `CHEMKIN IV`, and writing a Matlab script to post-process the results.

   (a) Different mixture fractions can be defined based on the different elements in the system. In an obvious notation, let these be ξ_C, ξ_O, ξ_N and ξ_{Ar}, and we define $\xi \equiv \xi_N$. For each of the mixture fractions (except for ξ_N), examine its deviation from ξ_N, especially for $\xi \leq 0.1$.

   (b) Under the conditions studied, the diffusivity of N_2 (and hence of ξ) is very well approximated by $D = AT^p$, with $A = 1.67 \times 10^{-5}$ (cm^2/sec) and $p = 5/3$, where T is the temperature in degrees Kelvin. Plot the scalar dissipation $\chi \equiv 2D(d\xi/dx)^2$ and the strain rate $-du/dx$ against ξ.

3. Methane/Air-Air Flame

One of the turbulent nonpremixed flames that we will study is the piloted jet flame D of Barlow & Frank (R.S. Barlow & J.H. Frank, *Proc. Combust. Inst.*, 27:1087–1095). The "fuel" used in this flame is 25% methane and 75% air (by volume). In spite of the oxygen in the fuel, the combustion is in the nonpremixed mode. An experimental and computational study of laminar nonpremixed flames using this fuel is described by Barlow et al. (R.S. Barlow, A.N. Karpetis, J.H. Frank and J.-Y. Chen, *Combust. Flame*, 127:2102-2118), henceforth BKFC.

1. Calculate the equivalence ratio of the "fuel". Calculate the stoichiometric mixture fraction for the nonpremixed combustion of this "fuel" with air.

2. Using `CHEMKIN IV`, make computations of the opposed jet laminar nonpremixed flame with the given "fuel" under the same nominal conditions studied by BKFC (see Table 2 of BKFC). Use multicomponent transport and thermal diffusion. Use the standard Reaction Design mechanism for methane, or, for extra credit, use GRI 3.0.

3. How do your computed peak values of the temperature and species mass fractions compare to those in Fig. 7 of BKFC?

4. Plot your computed mass fractions of CO and H_2 against mixture fraction, and comment on the comparison with Fig. 8 of BKFC.

5. List the differences between the configuration and models used in your computation compared to those used in BKFC.