Project 1: Thermochemistry (PR1_thermo)

1 Specific heats

In this exercise you will use Chemkin II to evaluate specific heats of various chemical species. You will use the Chemkin interpretor `ckinterp.exe` which takes `chem.inp` and `therm.dat` as input files and generates `chem.bin` and `chem.out` as output files. The Fortran code `cv` calls several Chemkin subroutines.

a) Examine the file `cv1.mech`; copy it to `chem.inp`; execute `ckinterp.exe` and examine the file `chem.out` which is produced.

b) Examine the file `cv.f90` to understand its operation. Execute the command `cv.exe`. Examine the file `cv.out` which is produced.

c) Examine the file `cvpost.m` and run it in Matlab. Comment on the plot produced.

The following questions can be addressed by modifying `chem.inp` and `cvpost.m`. (Remember to execute `ckinterp.exe` after changing `chem.inp`.)

d) Make a plot of c_v/R versus T for the species H_2, N_2, O_2, CO.

e) For diatomic molecules, a model for c_v is

$$\frac{c_v}{R} = \frac{5}{2} + \frac{\tau^2 e^{-\tau}}{(1 - e^{-\tau})^2},$$

where $\tau \equiv \Theta_v/T$ and Θ_v is the vibrational temperature. (See Vincenti & Kruger p. 135.) For H_2, N_2, O_2 and CO, take $\Theta_v = 6332K, 3374K, 2256K$ and $3103K$, respectively (values taken from McQuarrie & Simon). How does this model compare to the values of c_v/R obtained from Chemkin?

f) Make a plot of c_v/R versus T for the species $H_2O, HO_2, CH_2, CO_2, HCO$.

Your report should be about half a page of narrative, plus one figure for each of d), e) and f).

2 Chemical Equilibrium: Hydrogen-Air

In this exercise we examine *complete combustion* and *chemical equilibrium* of fuel-air mixtures. The Fortran code `h2eq` calculates the complete-combustion composition, calling the subroutine `temphy` to determine the adiabatic flame temperature. Chemical equilibrium is calculated by STANJAN which is called from the subroutine `cieqsj`.

- i) Examine the file `h2_1.mech`; copy it to `chem.inp`; execute `ckinterp.exe` and examine `chem.out`.

- ii) Examine the file `h2eq.f90`. Identify all calls to Chemkin subroutines and understand their function.

- iii) Execute the command `h2eq.exe` and verify that the output files `h2cc.out` and `h2eq.out` are produced.

- iv) Examine and execute the Matlab post-processing script `h2p1.m`.

Consider the composition of H_2-air mixtures as a function of mixture fraction according to the following models:

- a) complete combustion

- b) chemical equilibrium of H_2, O_2, N_2, H_2O

- c) chemical equilibrium of N_2 and all relevant $O - H$ species

- d) chemical equilibrium of all relevant $O - H$ and $N - O$ species

- e) chemical equilibrium of all relevant $O - H - N$ species, as contained in the file `h2.mech`.

Answer the following questions, using appropriate graphs (by modifying `chem.inp` and `h2p1.m`).

- 1. For model (c) identify the minor species with mass fractions greater than 10^{-6}.

- 2. For model (d) comment on the relative abundance of the oxides of nitrogen, NO, N_2O, NO_2.

- 3. Comment on model (e).

- 4. Discuss the variation of the peak temperature given by the different models.

3   Chemical Equilibrium: Methane-Air

Similar to the previous exercise, the Forton code `ch4eq` calculates the complete-combustion and chemical-equilibrium of methane-air mixtures. The output files can be post-processed using `ch4p.m`. The file `GRI.mech` contains the $C - H - O$ species used in the GRI mechanism for methane. (It does not include the N-species, except for N_2.) Notice that the species are grouped in lines as:

(a) major species (used in the complete combustion model)

(b) additional $O - H$ species

(c) additional C_1-species

(d) C_2-species

Run `ch4eq.exe` based on this mechanism. Answer the following questions using suitable graphs.

1. How well does the complete-combustion model describe the equilibrium composition of the major species for rich and lean mixtures?

2. How do the profiles of the minor $O - H$ species compare to those in the hydrogen flame?

3. Identify the 6 C_1-species that have the largest mass fractions.

4. Identify the 2 C_2-species that have the largest mass fractions.

4   Chemkin IV

1. Read Chapters 1, 2 and 3 of "Getting Started".

2. Read Section 2.1 of "Tutorials" to understand the Equilibrium model capabilities, input and output.

3. Using the Equilibrium model to make plots of the equilibrium temperature and minor species mole fractions for stoichiometric hydrogen air with an initial temperature of 300K over a range of pressures from 0.1 to 100 atmospheres.