Assignment 1

Instructions:

1. Make a report on the assignment.
2. The report should contain at least the following parts
   - Problem description
   - Assumptions
   - Procedure
   - Results & observations
   - Conclusions & outlook
3. The report should be handed in on /before 18th May 23:59 CET
4. You can do this assignment in a group of up to three or as an individual.
5. Please submit your assignment on Brightspace. If in a group, you still have to submit individually and indicate clearly name and student number of all authors at the beginning of your report.

6. Grading: Part 1: 30%; Part 2 40%; Part 3: 20%; Quality: 10%.

7. In case if we find elements of plagiarism in the assignments, students would be reported to the board of examiners.

Please refer to tutorial 1 slides on Brightspace for information on thermodynamics databases and use of the NASA CEA software. Partly-solved sample exercises are also available on Brightspace.

Part 1

- Calculate and plot the variation of C_p for H_2, O_2, N_2, CO_2, and H_2O from 600 to 2400K. Calculate the same also for the ethylene (C_2H_4).
- The C_p for the gas mixture can then be calculated by using the relation

$$c_{p,\text{mix}} = \sum_{k=1}^{N} Y_k c_{p,k}$$

Calculate and plot (in the same figure) the variation of $c_{p,\text{mix}}$ for reactants and combustion products from 600 to 2400K, assuming the reactants to be air and ethylene at equivalence ratios 0.4, 0.6, 0.8, 1.0, 1.2, 1.4, 1.6. Assume complete combustion. What are your observations in terms of Cp variation (max 200 words)?

- Compute and plot the flame adiabatic temperature for complete combustion of H2/air and reactant temperature of 1100K for the same equivalence ratios. Compare this with the adiabatic flame temperature in the case of ethylene/air combustion.

What are your key observations and conclusions? Where do differences come from? (max 200 words)

Part 2

<u>Chemical equilibrium</u> (Using NASA CEA code)

Note: **Bold** text indicates baseline conditions.

Note: Calculations have to be at constant pressure and enthalpy (sample input files for NASA CEA are available on Brightspace)

- Select hydrogen as fuel in the input file CEA
- Evaluate the variation in adiabatic flame temperature with Equivalence ratio. Say 0.4, 0.6, 0.8, **1.0**, 1.2, 1.4, 1.6, 1.8.
- Evaluate the variation in adiabatic flame temperature with Pressure, from **1**, 10, and 40 bar.
- Evaluate the variation in adiabatic flame temperature with air inlet temperature. 600K, **1100K**, 1600K, 2000K, 2400K.
- Now repeat the same using ethylene and compare results in relevant charts.
- Evaluate the NOx emissions (No and NO_2) for ethylene and H_2 fuel for the same equivalence ratios for an inlet temp of 600K and 1 bar.
- Draw relevant conclusions from the exercise.

CEA instructions: After downloading and unpacking the software, double-click on CEA executable (cea-exec). A subfolder will be created. Copy and past the input files on Brightspace within this folder. Edit the file as required by your exercise and save. Then run FCEA2m. A prompt will open: insert the exact name of your input file and press Return. An output file and an excel file will be created, containing the results of the computation.

For further information refer to software's instructions (links provided on Brightspace and the tutorial's slides).

Part 3

Estimating NOx

- From CEA, find equilibrium temperature and NO mass fraction for ethylene/air combustion at $\phi = 0.4,\ 0.6,\ 0.8$ and 0.99, for $\mathrm{T_{reactants}} = 600\mathrm{K}$ and $p = 1$ bar. Then, consider the following reaction, assuming the reaction at equilibrium has the adiabatic flame temperature found from CEA:

$$\mathrm{N_2 + O_2 \rightleftharpoons 2NO}$$

Evaluate the amount of NO using equilibrium. Plot the NO mass fraction as function of equivalence ratio and compare it with the results from CEA. What are your observations? What changes as compared to the CEA results and why?

Note: you have to consider that the equilibrium reaction occurs as second step after the complete reaction of ethylene with air.

- Now compute the amount of NO at 10 bar. Compare the results with CEA and comment on the differences.