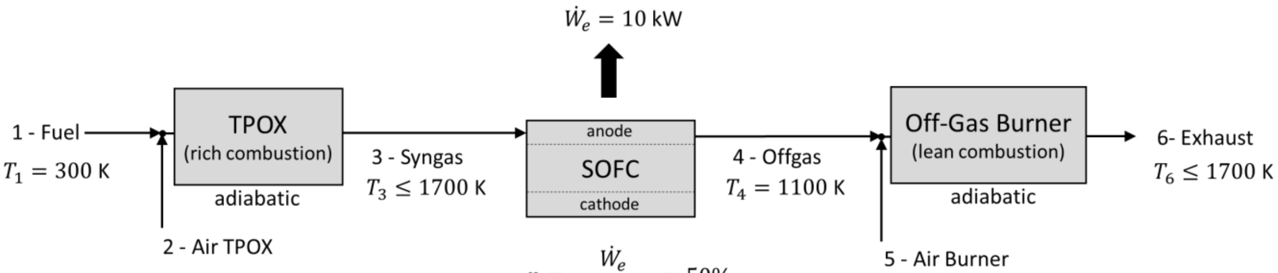
Computational Assignment (CA) of Combustion

(Due date: 10th May)

Problem description:
Consider the electricity production system sketched in the figure. The system generates an electric power $\dot{W}_e$ of 10 kW using a Solid Oxide Fuel-Cell (SOFC) that has an efficiency η of 50% and a fuel utilization U_f of 0,65 for both H_2 and CO. The SOFC is coupled with a fuel pre-processing reactor based on Thermal Partial Oxidation (TPOX) in order to produce synthetic-gas (syngas) rich in H_2 and CO. Downstream of the SOFC, an Off-Gas Burner is used to combust the off-gas under lean conditions before it leaves the system. Note that, the low-energy-content off-gas contains residual H_2 and CO, which have not been converted into H_2O and CO_2 inside the SOFC since the fuel utilization is not complete, i.e. $U_f < 1$.



$$\eta = \frac{\dot{W}_e}{\dot{m}_3 \, LHV_3} = 50\%$$

$$U_f = 1 - \frac{x_{i,4}}{x_{i,3}} = 0{,}65 \qquad i = H_2\,, CO$$

According to the sketch, the following conditions are known:

- Consider both TPOX and Off-Gas Burner to be adiabatic and operating at 1 atm.
- The fuel stream (1) enters at a temperature of 300K and is composed of 30% vol. methanol and 70% vol. methane (**for even group numbers**) or 70% vol. propane (**for odd group numbers**).
- Due to material constrains, the syngas stream (3) should exit the TPOX at a maximum temperature of 1700K. Note that, for this purpose, the temperature T_2 of the air TPOX stream (2) must be adjusted.
- Due to material constrains, the exhaust stream (6) should exit the Off-Gas Burner at a maximum temperature of 1700K. Note that, for this purpose, the temperature T_5 of the air Burner stream (5) must be adjusted.

Objectives and Procedures:
For the TPOX, the main objective is to maximize the LHV of syngas, while avoiding production of solid carbon, which could damage the SOFC.
Carry out the basic design using the following procedure:

1) Develop an "in-house" model for simplified calculations, i.e. mass and energy balances considering dissociation under equilibrium (H_2O, CO_2, H_2, CO and N_2 in the products). NOTE: use water-gas shift reaction for equilibrium calculations and, verify the critical equivalence ratio ϕ_{cr} for initial solid carbon formation using the Boudouard reaction (without considering carbon in the products).
2) Compare the simplified model calculations (as function of ϕ and reactants temperature) with the equilibrium results from Cantera (*equilibrium_calc_template.py*) and comment.

3) Based on the Cantera results and SOFC operation data, suggest a reasonable range of operating conditions for the TPOX and select a design point of operation (i.e. mass flow rate, temperature and composition of streams (1), (2) and (3) providing the TPOX conversion efficiency: $\eta_{TPOX} = \dot{m}_1 LHV_1 / \dot{m}_3 LHV_3$

4) Use the Well-Stirred Reactor (WSR) model from Cantera (*WSR_calc_template.py*) to estimate the suitable range of residence times for TPOX operation and, comment about deviations from equilibrium.

For the Off-Gas Burner, the main objective is to efficiently burn the off-gas mixture while minimizing NO_x emissions (NO and NO_2 in the products).

5) Based on the SOFC operation data and TPOX design point of operation selected in task 3), estimate the off-gas composition and compare its LHV with the one of the original fuel stream (1). Develop an "in-house" model for simplified calculations, i.e. mass and energy balances for main species (without dissociation).

6) Compare the simplified model calculations (as function of λ and reactants temperature) with the equilibrium results from Cantera (*equilibrium_calc_template.py*) and comment.

7) Based on the SOFC operation data and Cantera results, suggest a reasonable range of operating conditions for the Off-Gas Burner and select a design point of operation (i.e. mass flow rate, temperature and composition of streams (4), (5) and (6).

8) Develop an "in-house" model for simplified post-processing of NO formation as function of residence time, based on the Zeldovic mechanism and assuming O concentration in equilibrium (see examples 4.3 and 4.4 from Turns; available in fenix). Compare the simplified model NO predictions with results from Cantera's WSR model (*WSR_calc_template.py*) as function of residence time and comment. Additionally, estimate the suitable range of residence times for Off-Gas Burner operation.

Note: the calculations using the "in-house" models can be done in python, octave (a free version of Matlab) or excel.

Report Structure:
The report of the work should have a maximum of 16 pages (additional pages will not be considered). The font should be *times new roman* (or similar) with a minimum size of 10 pt. The report should include the following sections:

Identification: Group number and name/number of group elements

Method, Results and Discussion: Provide the required method/results/discussion for each task following the procedure order. **Note**: regarding the method, provide a description of the "inhouse" model equations and simplifying assumptions (i.e. Cantera model do not need to be described in detail); for the results requested in the tasks, try to resume them into figures and tables and, limit their discussion short but relevant comments.

Report delivery:
The report and associated files (used to solve all tasks) should be delivered by email (**miguel.mendes@tecnico.ulisboa.pt**) till **10th May (end of the day)**. Only one element of the group should send the email (with CC to all other elements) writing in the subject: **CA – Group GXX** (where XX is the group number)