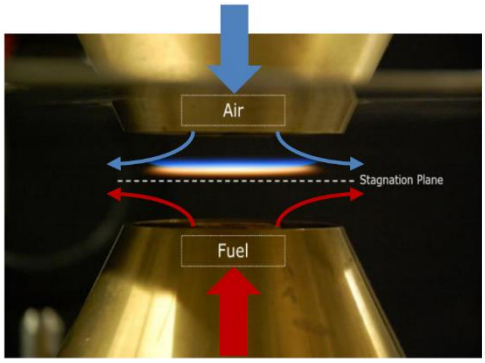
PROJECT ASSIGNMENT #3: FLAMES

General Information:

- Due date: Thursday, November 2, 2023 11:59PM
- Submission on MyCourses
- Write your answer in the word processor of your choice, and upload it as a pdf file in MyCourses. **Don't forget to include your name and your McGill ID number.**
  - Name your file as follow: ProjectNumber_FullName_McGillNumber.pdf
  - For example: P3_JohnSmith_0123456789.pdf
- To perform Cantera calculation, don't hesitate to explore Cantera's documentation examples: https://cantera.org/examples/index.html for several applications such as JN, Python, or Matlab, that you can adapt to your software. Make sure to understand what you are using.
- When presenting graphs, do your best to make them readable. Labels for y- and x-axis are required, legend if more than 1 curve, title if needed, consider using log-scale if needed …

Part I – Non-premixed flame

In most practical combustion systems, fuel and oxidizer are separated, and combustion occurs only when they meet, leading to a non-premixed flame, also called diffusion flame. In this exercise, we will investigate its characteristics by using a counterflow object in Cantera.



Diffusion flame in Alternative Fuels Laboratory

A counterflow is composed of two independent channels facing each other. The oxidizer is sent through the top burner while the fuel is sent through the bottom one. The resulting flame stabilises at the location where the flux of fuel and air are equal to the stoichiometric condition.

At P = 1 atm and Tin = 300 K, we will consider a fuel inlet composed of pure iso-octane and an air inlet with the usual composition, as stream 1 and 2, respectively. For your setup, the nozzles spacing will be 2 cm and an air inlet velocity of 1.5 m/s. To stabilize the flame approximately halfway between the nozzles, the total pressure of both streams is equalized such that:

$$\rho_{\text{fuel}} \cdot u^2_{\text{fuel,nozzle}} = \rho_{\text{air}} \cdot u^2_{\text{air,nozzle}}$$

Use the counter flow diffusion reactor in Cantera. As usual, use Jerzembeck mechanism to perform your calculation. To get started you can use the following Cantera example:

https://cantera.org/examples/python/onedim/diffusion_flame.py.html

1) Calculate the fuel inlet velocity
2) Compute the diffusion flame, and plot the temperature, mass fraction of oxygen and iso-octane (Y_{O2} and Y_{C8H18}), as a function of the spacing between the nozzles. Plot the results on one single graph using double y axis. Comment your results.
   - **Disclaimer:** the computing might take a long time (~10min). It's normal, we are using a heavy hydrocarbon as a fuel and the more complex is the simulation, the more time is needed. You can try out your code on a lighter fuel first, with the default mechanism 'gri30.yaml' to check it is working properly.
3) Implement the Bilger's mixture fraction Z, and plot T, Y_{O2}, and Y_{C8H18} as a function of the mixture fraction Z, one a single graph. Describe your results.
4) What is the value of the stoichiometric mixture fraction ?

5) Calculate the equilibrium temperature of a stoichiometric mixture of iso-octane and air, at the same conditions. How does this temperature compare to the peak temperature of the diffusion flame? Explain.
6) Using the same setup of diffusion flame, obtain the solution for three different air nozzle velocity of 0.1, 2.0, and 3.3 m/s. On a single graph, plot the results of the three flames: T, Y_{O2}, and Y_{C8H18} as a function of the mixture fraction Z. Explain your results.
    - This part can take ~30min to compute. Prepare it first on a lighter fuel, lighter mechanism, and once you know it's working, launch it properly.

Bonus) Let's consider the same setup, but the fuel is diluted with some nitrogen. For the three following fuel composition:

- Fuel 1: $X_{C8H18} = 1.00$, $X_{N2} = 0.00$
- Fuel 2: $X_{C8H18} = 0.90$, $X_{N2} = 0.10$
- Fuel 3: $X_{C8H18} = 0.80$, $X_{N2} = 0.20$

Plot T as a function of the mixture fraction Z on a single graph. Plot Y_{C8H18} as a function of the mixture fraction Z on a single graph. Plot Y_{O2} as a function of the mixture fraction Z on a single graph. Explain your results. *The difference between the results of Fuel 1 and Fuel 2 is very small but please try to extract a conclusion out of it using Zst.*

In this part, I expect comments on the structure of a diffusion flame, its extinction limits, the strain rate…

Part II – Premixed flame

Premixed flames take slightly less time to compute than simulations of non-premixed flames

In the initial stage of the design of a new combustion system, a few key parameters are evaluated with simple correlations or calculations. In previous projects we have used 0D reactors whereas in this project we will use a 1D reactor, namely, the laminar freely propagating flame.

In this part of the project, we will investigate different aspects of a laminar premixed flame and how they can be used to make basic calculation related to combustion systems. For example, pollutant emissions (NO_x and CO), can be evaluated as function of combustor residence time. Effect of richness and pressure can also be estimated with this approach.

A mixture of iso-octane and air is studied in this exercise, with φ=0.75, P = 1atm, and Tin = 300K. Use Cantera lamina freely propagating flame, to obtain a solution, following this example :

https://cantera.org/examples/jupyter/flames/flame_speed_with_sensitivity_analysis.ipynb.html

1) Compute the free flame following the given conditions. On the same graph, plot the temperature profile, and the mass fraction of C_8H_{18}, O_2, CO, NO, CO_2 and H_2O versus the grid.
2) To better relate this problem to a practical system, it is better to look at the results temporally instead of spatially. Convert the spatial coordinates to temporal coordinates, using the flame grid and velocity field.
    - **Hint:** Write a function that takes the flame grid and velocity field and returns the corresponding time scale: $t_i = \sum_{j=1}^{i} \Delta t_j = \sum_{j=1}^{i} \frac{\Delta x_j}{u_j}, \quad i = 1,2,3 \dots, n$ where Δx_j is the grid spacing at position j, u_j is the velocity of the flow at position j, and n is the number of grid points.
        - First, the function will use the velocity field and grid spacing to convert to time coordinate using the above formulas. (Use numpy vector function rather than looping through each element.)
        - Then, use the maximum heat release position in the flame solution to define the zero of the time scale instead of the boundary of domain. Adjust the time scale so that t = 0 is aligned with the maximum heat release.
3) Plot the same graph than II.1 but using the calculated time scale instead of the grid points.
4) Plot the velocity function of time, as well as the heat release of the flame on a secondary axis.

5) Plot the temperature function of time, as well as the heat release of the flame on a secondary axis.
6) Plot the specie net production rates of the same species than II.1 versus time.
7) Using the four graphs, describe the time evolution of the species. Describe the flame structure, the specie consumption and production, the temperature profile, etc.
    - **Hint:** you will need to zoom on the graph close to the peak of heat release to better see the flame structure and specie profiles, to do so, specify a limit on the display of the x axis: "pl.xlim"
8) Repeat the simulation for φ = 0.60, 0.65, and 0.70, and extract the mass fraction of NO and CO, and T. Plot NO, CO and T vs time on three separate graphs for the three equivalence ratios. Explain the results.
9) Varying equivalence ratio from φ = 0.5 to φ = 1.5 in steps of 0.1, plot the laminar flame speed (S_l (m/s)) versus the equivalence ratio. Explain the trend.
10) Changing T_{in} to 600K, and φ to 0.6, vary the initial pressure with the following values: 1, 2, 4, 8, and 16atm.
    - Plot the laminar flame speed versus initial pressure. Explain the results.
    - Compute and plot the flame thickness δ_D versus pressure, where $\delta_D=\lambda/f°Cp$, λ: heat conductivity, $f°$: laminar burning flux, Cp: heat capacity. State your assumptions and explain your results.

Part III – For graduate students (undergrads – bonus points) - Sensitivity analysis

Using the second part of the Cantera example supplied for part II, you will analyse the sensitivity of the laminar flame speed at different richness for the chemical kinetic mechanism. The logarithmic sensitivity is defined as:

$$\text{Sensitivity: } \frac{\partial \ln S_u}{\partial \ln k}$$

where S_u is the laminar flame speed, and k is the reaction rate constant. As shown in the example, each reaction is individually perturbed by 0.01 and then the impact on S_u is calculated.

1) Using the same perturbation, identify the 10 most sensitive reactions for φ =0.5, 1.0, 1.5, lean, stoichiometric, and rich respectively, of an iso-octane mixture. Plot the logarithmic sensitivity for these 10 reactions using the graph template.
2) Comment on the impact of the different reaction types for these 3 conditions.
3) Explain the difference of ranking between the lean, stoichiometric, and rich cases.