MECH 652: Dynamics of Combustion

PROJECT ASSIGNMENT #3: FLAMES

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Part I – Non-premixed flame

Problem 1: Calculate the fuel inlet velocity

Velocity of fuel = 0.759 m/s

Problem 2: Compute the diffusion flame, and plot the temperature, mass fraction of oxygen and iso-octane (YO2 and YC8H18), as a function of the spacing between the nozzles. Plot the results on one single graph using double y axis. Comment your results.
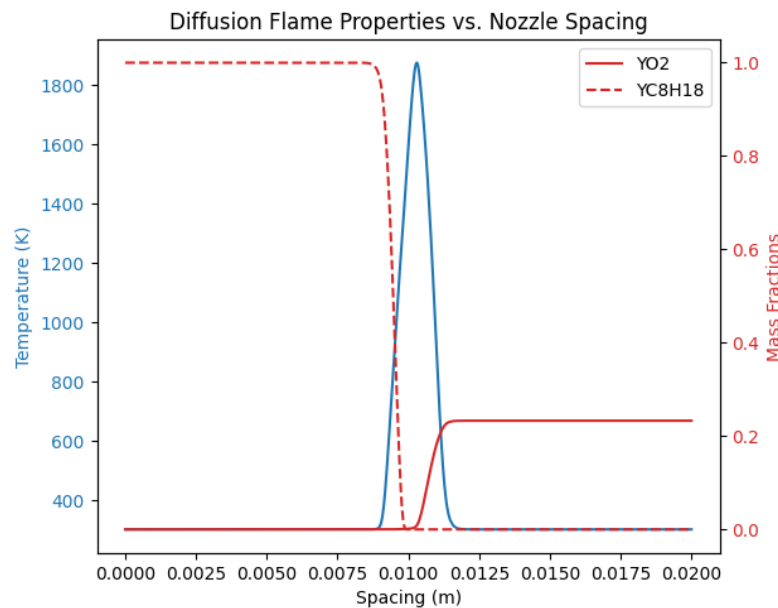

Fig 1 – Diffusion flame properties vs Spacing between nozzles

The above fig. 1 shows the diffusion flame properties vs nozzle spacing. The plot shows the reaction zone marked by a rise in the temperature.

- In the reaction zone, there is a gradual rise in the temperature which is a characteristic of diffusion flame. The temperature curve is symmetric with a steep increase and decrease in the values. The peak temperature is close to 1876 K.
- The above plot also shows the mass fraction of O2 and C8H18 varying in spacing. YO2 (O2) and YC8H18 (C8H18) curves show no variation in the outside of the flame region. In the flame region, there is a gradual decrease in the value of YO2 and YC8H18, as the reactants are consumed in the reaction. The rate of decrease of the fuel is higher as compared to the rate of decrease of O2. This

can be explained by the fact that at the onset of the reaction, the fuel gets consumed faster and gets converted into radicals.

Problem 3: Implement the Bilger's mixture fraction Z, and plot T, YO2, and YC8H18 as a function of the mixture fraction Z, one a single graph. Describe your results.
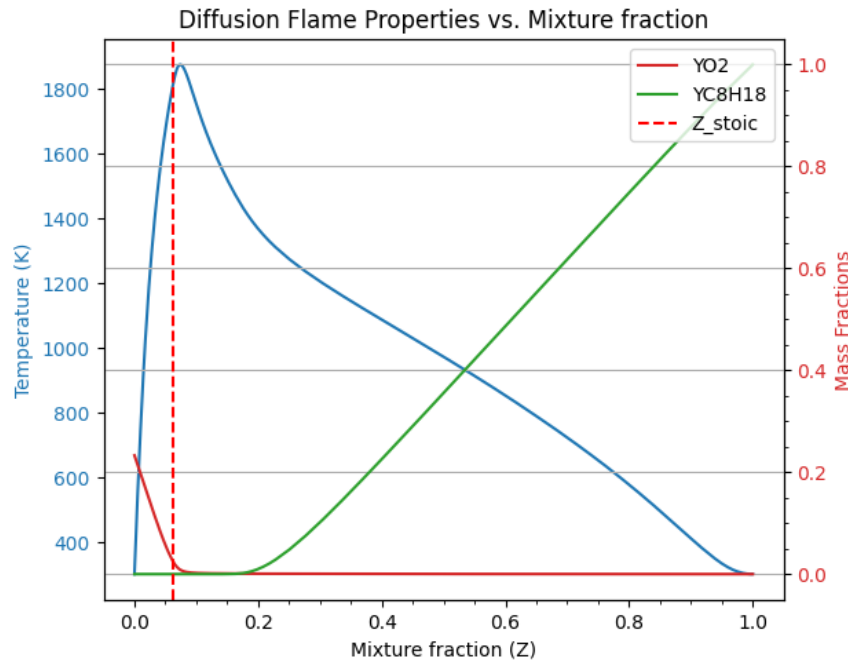

Fig 2 – Diffusion flame properties vs Mixture Fraction

Fig. 2 shows the Diffusion Flame properties vs Mixture fraction (Z) plot. The mixture fraction Z is Bilger's mixture fraction. The following points can be inferred from the above plot:

- In the above plot, Y_C8H18 = 1 represents the mass fraction of fuel at the fuel inlet boundary and Y_O2 = 0.23 represents the mass fraction of O2 at the oxidizer inlet boundary.
- At the fuel inlet, the temp value is close to fuel inlet temp, i.e., 300 K. As it move towards the flame front, the temperature continues to increase and it is highest close to Z = Z_st. In this case the peak temperature is close to 1876 K.
- Z = Z_st represents the flame boundary, beyond which the fuel mass fraction is zero. The flame propagates and stabilizes itself at Z = Z_st. At the flame boundary, the Y_O2 is close to zero as well, which can be seen from the plot.

Problem 4: What is the value of the stoichiometric mixture fraction ?

- The stoichiometric mixture fraction is 0.0621.

Problem 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

The equilibrium temperature is 2273.56 K.

The significant difference between the equilibrium temperature and the temperature of non-premixed counter flow diffusion flame can be explained by various points:

- The equilibrium temperature is calculated under the assumption that all the chemical reactions are in thermodynamic equilibrium and all the reactants are allowed to convert into product, releasing all available chemical energy in a way such that the minimum Gibbs free energy of the system is reached. However, this assumption is not correct as most chemical reactions are not at thermodynamic equilibrium and reactions continue to occur at the flame front. Thus not all available energy is released and hence the less temperature in later case.
- In a non-premixed counterflow diffusion flame, fuel and oxidizer streams mix at the flame front and chemical reaction takes place only at the flame front with finite rates. This mixing process involves the transport and diffusion of species and heat. Whereas, in the calculation of equilibrium temperature the time taken for chemical reactions to occur is not considered. All the chemical energy stored are released all at once and hence the higher temperature of the flame.

Problem 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, YO2, and YC8H18 as a function of the mixture fraction Z. Explain your results
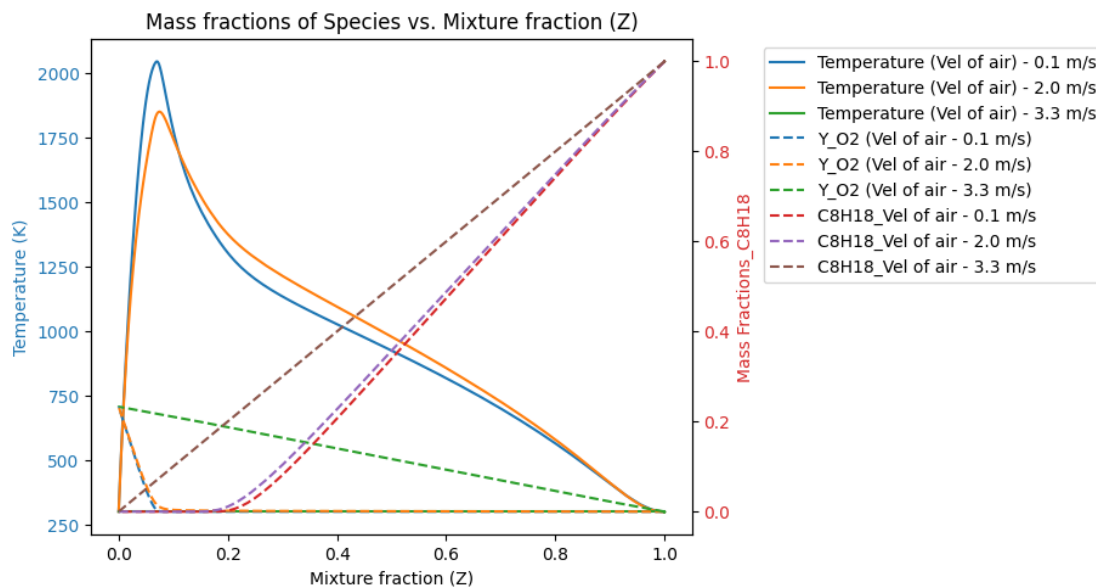

Fig 3 – Diffusion flame properties vs Mixture Fraction for different velocities

The above Fig 3, shows the combined plot of the Temperature and Mass fraction of O2 and C8H18 vs Mixture fraction for all the velocities of air. The following observations can be made from it:

- For the first two velocities, i.e., 0.1 m/s and 2.0 m/s, combustion takes place whereas as the third case, i.e., 3.3 m/s there is no combustion due to the very high speed of air which first leads to flame stretching and later flame gets extinguished.

- For the two velocity cases in which the combustion takes place, the temperature is higher for air velocity 0.1 m/s than for air velocity 2.0 m/s. This is because of a decrease in the residence time as the air velocity increases, and there is relatively less time available for combustion.
- Higher velocity of air means higher flame stretching, and hence for the velocity of air – 2.0 m/s, the temperature is higher in the region away from the flame boundary towards the fuel inlet side.
- There is very little effect of the velocity change on the mass fraction of C8H18 and the mass fraction of O2. The mass fraction of C8H18 is a little higher for an air velocity of 2.0 m/s than that for an air velocity of 0.1 m/s. This might be the effect of the higher velocity air stream restricting the flow of fuel stream and hence the higher mass fraction of C8H18.

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

• Fuel 1: XC8H18 = 1.00, XN2 = 0.00

• Fuel 2: XC8H18 = 0.90, XN2 = 0.10

• Fuel 3: XC8H18 = 0.80, XN2 = 0.20

Plot T as a function of the mixture fraction Z on a single graph. Plot YC8H18 as a function of the mixture fraction Z on a single graph. Plot YO2 as a function of the mixture fraction Z on a single graph. Explain your results.

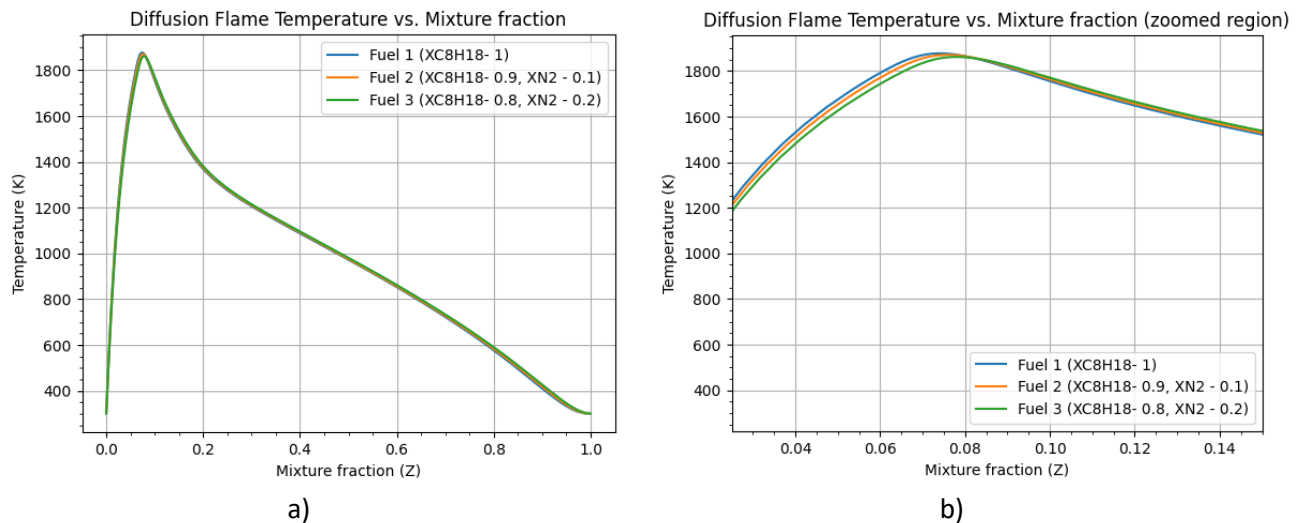a)   b)

Fig - 4a) Diffusion flame temperature vs Mixture Fraction for different fuels, 4b) Zoomed region in the same plot showing the difference in the values for different values

The above plot shows the flame temperatures for different fuels with varying levels of nitrogen gas blending. Adding the nitrogen gas to the fuel is the case of fuel dilution. Nitrogen gas being inert does not take part in the reaction mechanism. The following inferences can be made from the above plot:

- There is very little effect in the temperature values of nitrogen blending as the temperature plot for all the cases overlap each other. However, the zoomed plot shows the decrease in the flame temperature with the increase in the blending percentage of nitrogen

- This can simply be explained by the fact that there is less fuel available for the burning and hence less heat release and thus bringing down the flame temperature.
- With the fuel dilution, the mass fraction of fuel at the inlet decreases, and hence Z_st increases. This can also be seen in Fig 4b. However, this change is not so significant.
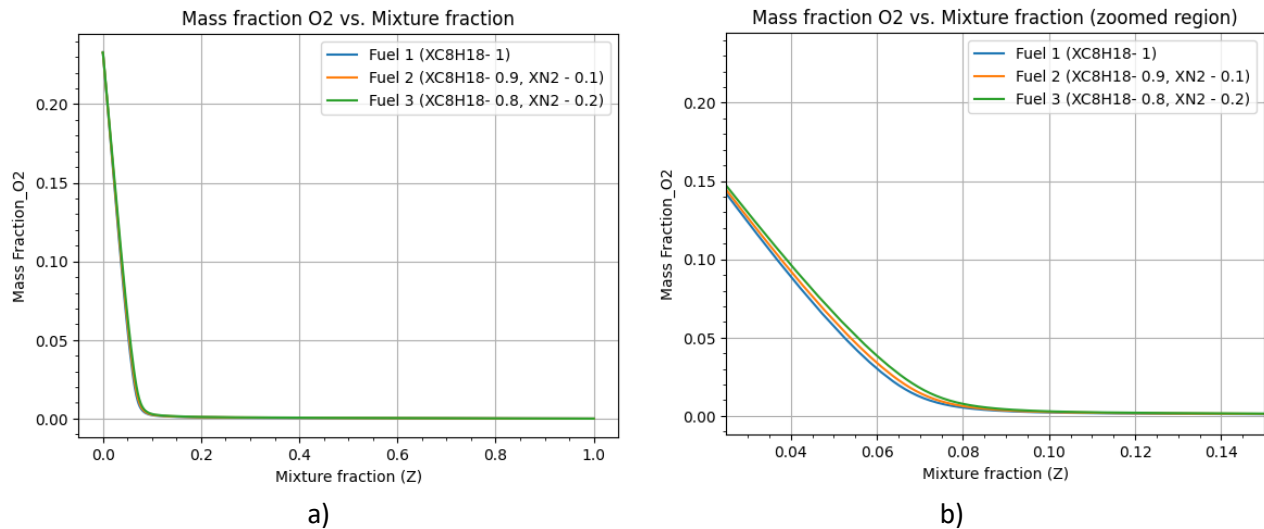

Fig - 5a) O2 Mass fraction vs Mixture Fraction for different fuels, 5b) Zoomed region in the same plot showing the difference in the values for different values

The above plot shows the O2 mass fraction values for different fuels with varying levels of nitrogen gas blending. The following inferences can be made from the above plot:

- The effect of nitrogen gas blending is not so significant as it can be seen from the above Fig 5. However as seen in the Fig 5b., the mass fraction of O2 is very little higher in the case of fuel 3 as compared to other fuel concentrations.
- This might be because with the increase in the blending percentage, the amount of fuel coming in the reaction zone is less and hence there is less consumption of oxygen, and hence higher mass fraction the air-stream close to the reaction zone.
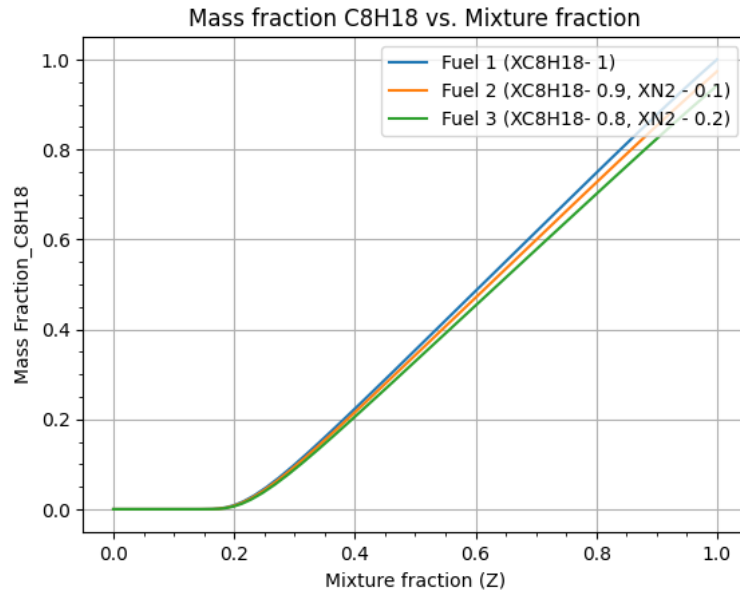
Fig 6 – C8H18 mass fraction vs Mixture Fraction for different fuels

The above plot shows the C8H18 mass fraction values for different fuels with varying levels of nitrogen gas blending. The following inferences can be made from the above plot:

- In the plot it is clearly seen that mass fraction of C8H18 is the lowest for the fuel 3 case which has the highest blending percentage of nitrogen.
- However, as the fuel stream moves closer to the the flame boundary region, this difference gets reduced owing to high consumption rate of the fuel. In all the three cases, the fuel is getting consumed in the reaction with at approximately same rate and hence the same mass fraction.

Part II – Premixed flame

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.

<u>Problem 1: Compute the free flame following the given conditions. On the same graph, plot the temperature profile, and the mass fraction of C8H18, O2, CO, NO, CO2 and H2O versus the grid.</u>
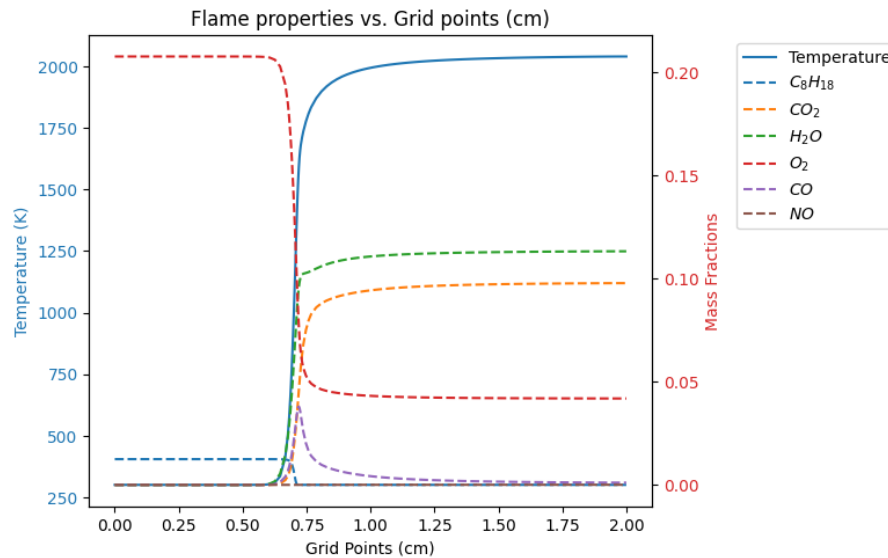

Fig 7 –Flame properties vs Grid points

<u>Problem 2 & 3: 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. Plot the same graph than II.1 but using the calculated time scale instead of the grid points.</u>
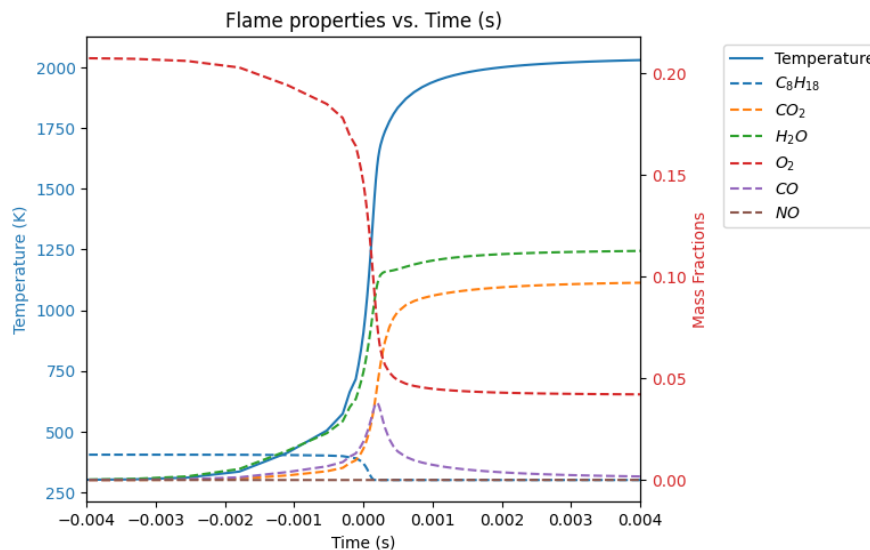

Fig 8 –Flame properties vs Time (s)

Problem 4: Plot the velocity function of time, as well as the heat release of the flame on a secondary axis.
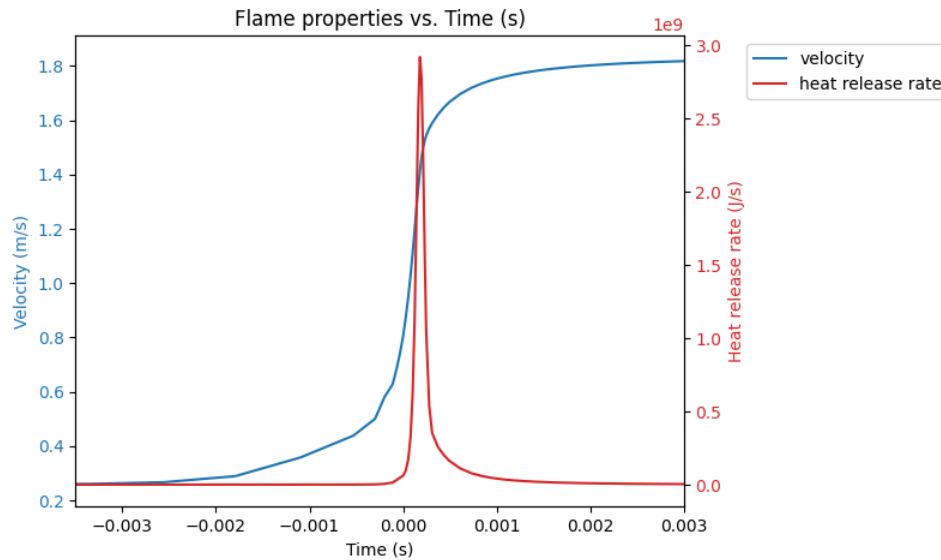

Fig 9 –Velocity and heat release rate vs Time (s)

Problem 5: Plot the temperature function of time, as well as the heat release of the flame on a secondary axis.
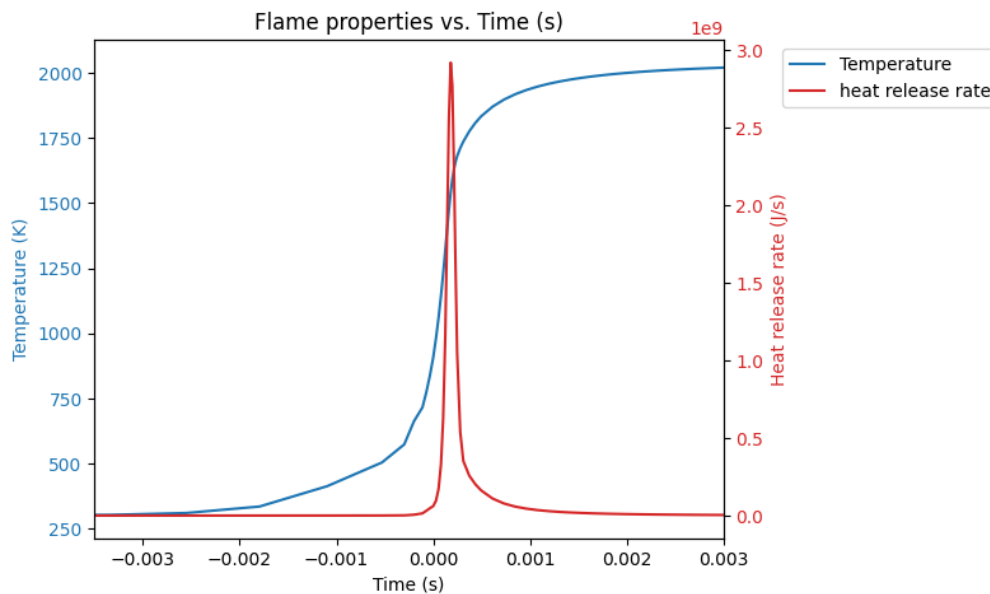

Fig 10 –Temperature and heat release rate vs Time (s)

Problem 6: Plot the specie net production rates of the same species than II.1 versus time.
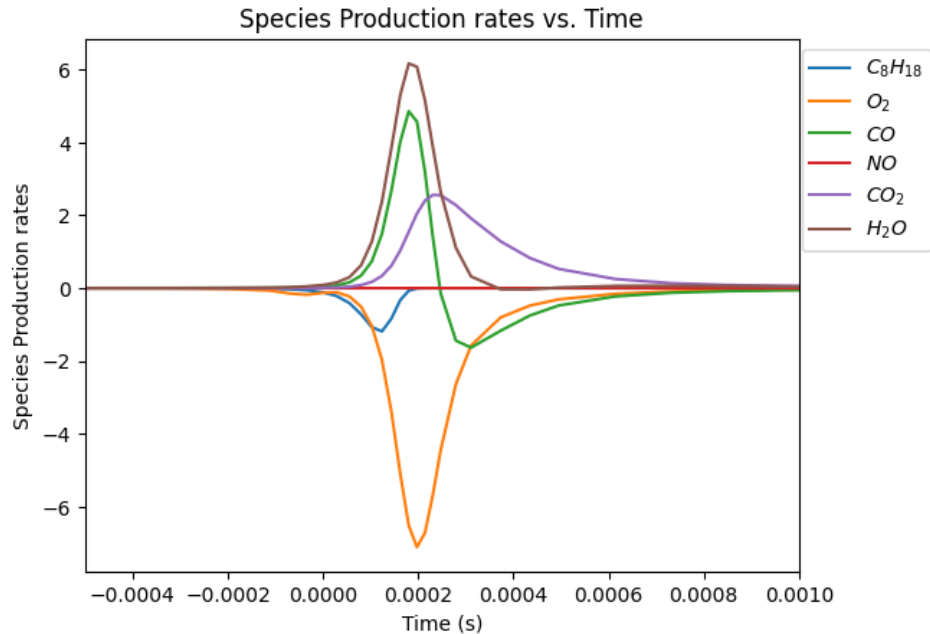
Fig 11 –Species production rate vs Time (s)

Problem 7: Using the four graphs, describe the time evolution of the species. Describe the flame structure, the species consumption and production, the temperature profile, etc.

Temperature profile –

- Considering the width as 2 cm, a steep rise in the temperature is seen around 0.7 cm location, marking the start of the ignition. This can be seen in Fig 7, temperature vs width plot. The peak temperature is around 1980 K.
- In Fig 7, the length of the preheat zone is relatively short, which signifies the sudden rise in the temperature, and it is indicative of premixed flame. The same can be seen from Fig 8, which shows the temperature rising from 300 K to 1986 K in the span of 6 milliseconds.

Flame Structure –

- The flame is planar and premixed. Fig 12 on the next page, shows the heat release rate vs width plot. As seen from this fig, the flame zone is marked by the steep increase and steep decrease in the heat release signifying a thin flame. The same can be seen from Figs 9 & 10.
- Also, a well-defined and symmetric peak is indicative of controlled and stable combustion.

Time Evolution, and Species Consumption and Production –

C8H18 –

- Fig. 8 shows the time evolution of C8H18, which is close to its initial value before the start of the combustion. In the flame region, the mass fraction of C8H18 goes to zero gradually which means complete consumption of the fuel in the flame region.

- As seen in the species production rate plot, the production rate for C8H18 is close to 0 before t = 0. Afterward, the production rate becomes -ve., which means C8H18 is getting consumed in the reaction. The consumption rate is high and in a relatively short period of time, there is complete consumption of fuel. This is because fuel is lean, and hence enough oxidizer is available for the complete combustion.
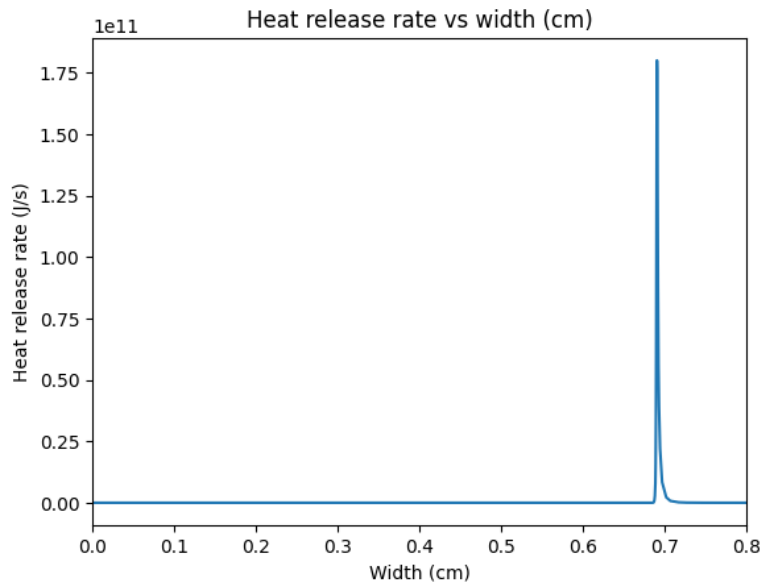

Fig 12 –Heat release rate vs Width (cm)

O2 –

- Fig. 8 shows the time evolution of O2, which is close to its initial value before the start of the combustion. In the flame region, the mass fraction of O2 decreases gradually to a fixed value and remains constant later. This means there is incomplete consumption of O2 during the combustion which makes sense as the phi – 0.75, i.e., it is a fuel-lean case.
- As seen in the species production rate plot, the production rate for O2 is close to 0 before t = 0. Afterward, the production rate becomes -ve., which means O2 is getting consumed in the reaction. The consumption rate is very high for O2 at the beginning of the reaction but as the reaction progresses it decreases, and O2 stays in the reaction domain for a longer period.

CO –

- Fig. 8 shows the time evolution of CO, which is zero before the start of the combustion. During the combustion process, CO gets formed as an intermediate species, which later acts as a reactant in the formation of CO2. This is seen from the fact that, the mass fraction of CO gradually goes to zero afterwards.
- CO is initially produced in the reaction domain, this can be seen from the above species production rate plot. This is because as the fuel C8H18 is getting consumed and CO is initially

formed. However, in the later part of the reaction, CO is consumed in the production reaction of CO2. This is seen from the production rate of CO going to negative in the later part of the reaction. The consumption of CO in the production of CO2 continues for a longer time.

NO –

- Fig. 8 shows the time evolution of NO, which is zero during the period of the combustion process. A similar trend is seen in Fig. 11, the species production rate plot.
- NO has a very low level of production during the complete reaction time. NO being the temperature-dependent species, gets only formed when the temperature is relatively higher.

CO2 –

- Fig. 8 shows the time evolution of CO2, which is zero during the initial period of the combustion process, but its mass fraction increases as the reaction progresses and later reaches the constant value as the fuel gets completely consumed.
- CO2 is not produced during the initial part of the reaction as one of the reactants to form CO2 is CO, which is produced in the initial reaction. However, as the reaction progresses, the production rate of CO2 increases, and the production continues for a long time as long as CO and oxygen radicals are present in the reaction domain. This can be seen from Fig. 11.

H2O –

- Fig. 8 shows the time evolution of H2O, which is zero during the initial period of the combustion process, but its mass fraction increases as the reaction progresses and later reaches the constant value as the fuel gets completely consumed.
- As seen in Fig 11, the production rate of H2O is very high during the initial phases of the reaction due to the abundance of H radical and O2 which leads to the formation of H2O. However, as the O2 concentration reduces the production rate of H2O decreases.

Problem 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.
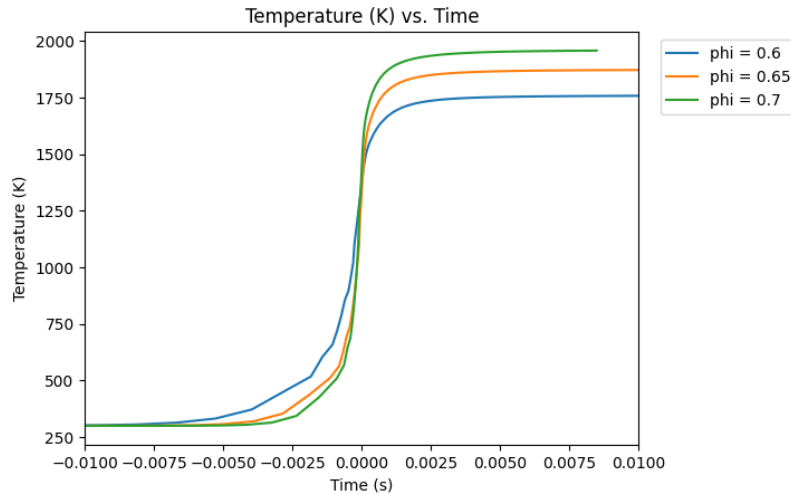
Fig 13 –Temperature vs Time plot for different equivalence ratios

- As can be seen from Fig 13, the flame temperature increases with an increase in the equivalence ratio from 0.6 to 0.7. This is simply because increasing the equivalence ratio means increasing the amount of amount of fuel in the reactant mixture, and hence more heat is released.
- As stated above, as a result of an increase in the amount of fuel, more heat is released and hence the temperature rises very steeply. This can be seen from Fig. 13, where the time taken for the flame to reach its peak temperature is the lowest for phi = 0.7 indicating faster reactions in this case.
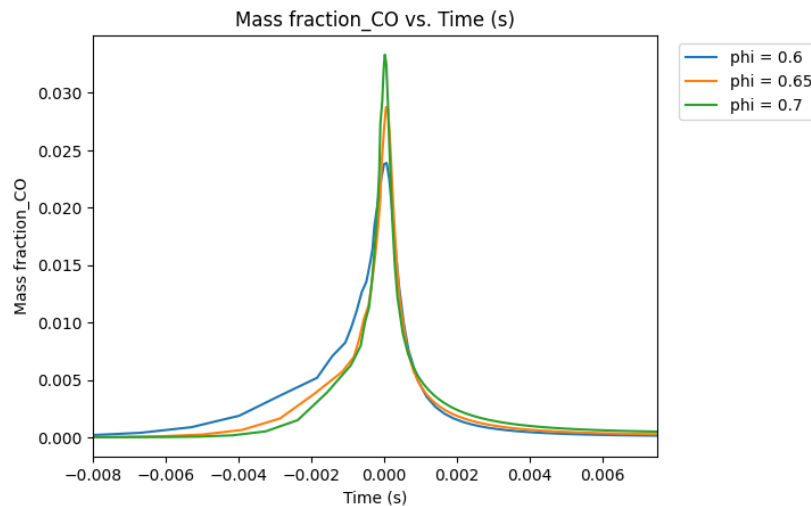

Fig 14 – CO Mass fraction vs Time plot for different equivalence ratios

- The above plot Fig. 14 shows the mass fraction of CO variation over time in the complete combustion domain. CO is generally an intermediate species during combustion of Hydrocarbon and it later leads to the production of CO2.
- As shown in the plot, similar to the explanation above, CO concentration increases during starting time of reaction and decreases to 0 in the later part of the reaction.

However the rate of CO increase is highest for phi – 0.7 case, simply because the more amount of fuel leading to high number of radicals, faster reactions and thus faster production of CO. For the same reasons, the mass fraction of CO is again the highest for phi – 0.7 case.
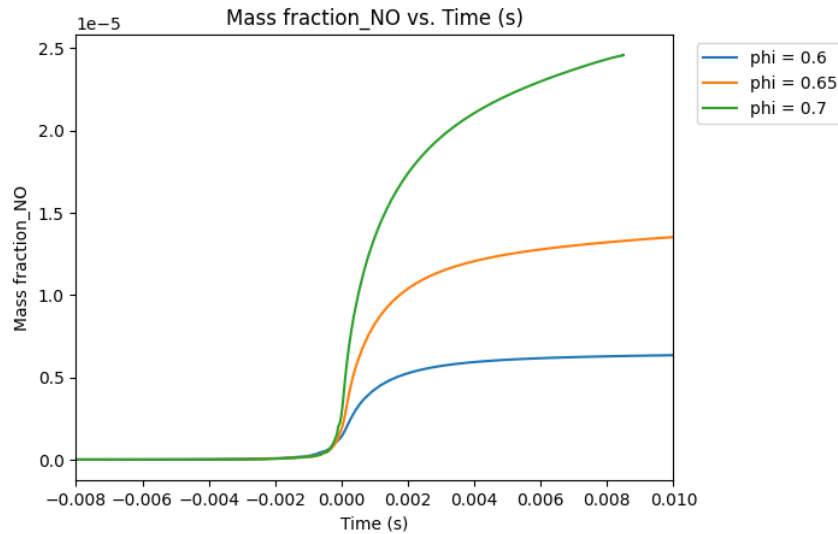

Fig 15 – NO Mass fraction vs Time plot for different equivalence ratios

- The above plot Fig. 14 shows the mass fraction of CO variation over time in the complete combustion domain. NO is a temperature-dependent species during the combustion of Hydrocarbon with oxidizer as air.
- It simply means that the higher the flame temperature, more is the concentration of NO. The same can be seen in the Fig. 15. The mass fraction of NO is highest for the phi – 0.7 case simply because of higher flame temperature.
- As NO is mostly a final product in the combustion, hence its concentration does not decrease to 0 as seen with CO case, instead it increases to a value for that particular temperature and then remains constant as a combustion product.

Problem 9: Varying equivalence ratio from ɸ = 0.5 to ɸ = 1.5 in steps of 0.1, plot the laminar flame speed (Sl (m/s)) versus the equivalence ratio. Explain the trend.

Fig 16 on the next page shows the plot for laminar flame speed for different equivalence ratios. As the equivalence ratio increase from phi – 0.5 till phi – 1.1 and then decreases till phi – 1.5.

This increase and decrease in the laminar flame speed can be explained by following reasons:

- As the phi increases from 0.5 to 1.0, the excess air provides more oxygen and hence promotes faster combustion. The flame front propagates more quickly because there is a higher concentration of oxygen available for the combustion reaction.
- The laminar flame speed reduces in the fuel-rich mixtures because the excess fuel limits the availability of oxygen for combustion, resulting in a slower flame front propagation.
- In the above situation, Ideally the laminar flame speed should be decreasing after phi – 1.0, but a change in phi from 1.0 to 1.1 might not be so significant to bring changes in the flame speed because of the faster reaction rates of iso-octane.

- Moreover, there is a strong correlation between the laminar flame speed and adiabatic flame temperature, which also shows similar behavior. i.e., its peak is observed on the fuel-rich side close to the stoichiometric equivalence ratio.
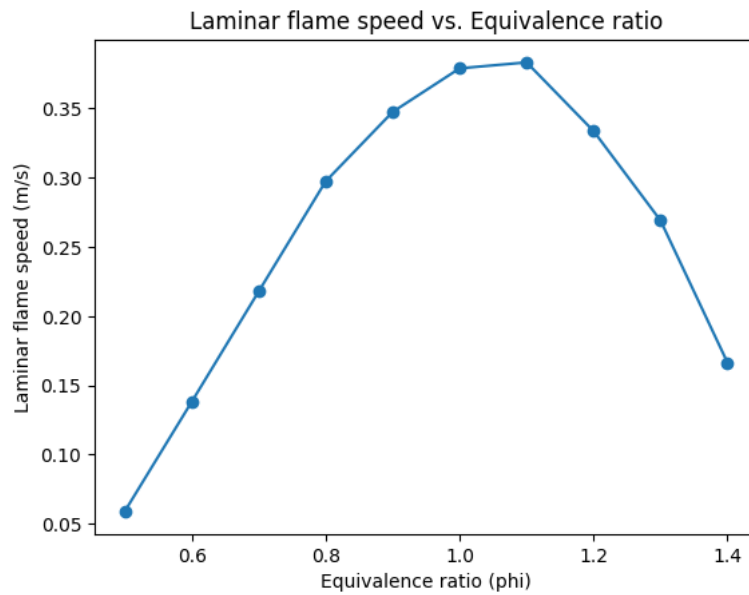

Fig 16 – Laminar Flame Speed vs Equivalence ratio

Problem 10: Changing Tin to 600K, and φ to 0.6, vary the initial pressure with the following values: 1, 2, 4, 8, and 16atm.
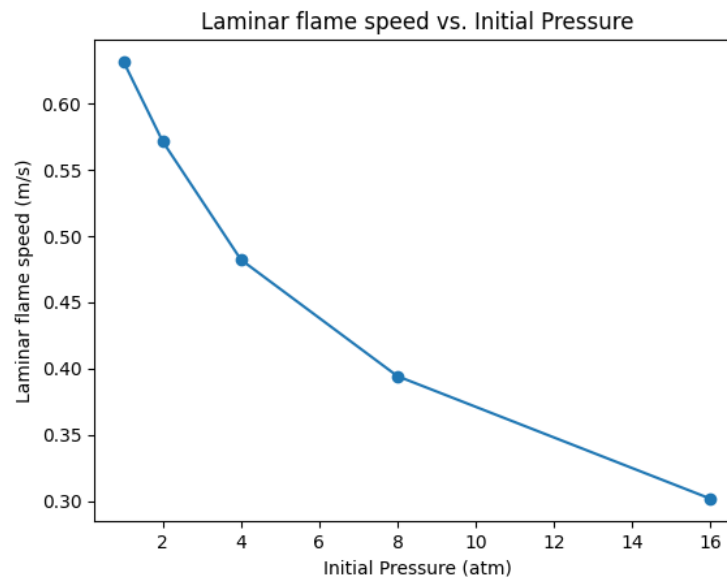

Fig 17 – Laminar Flame Speed vs Initial pressure ratio

Fig 17 shows the plot for laminar flame speed vs initial pressure ratio. As the initial pressure increases from 1 atm to 16 atm, the laminar flame speed continues to decrease.

- This is primarily due to the increased density of the reactants at higher pressures, thus making the gas denser for the flame to pass through.
- One other reason, which might play a role in reducing the flame speed is the reaction mechanism. As the pressure increases, the chain-termination reactions become more active than compared to chain-branching reactions, and hence a retarding effect is applied to the overall progress of the reaction.
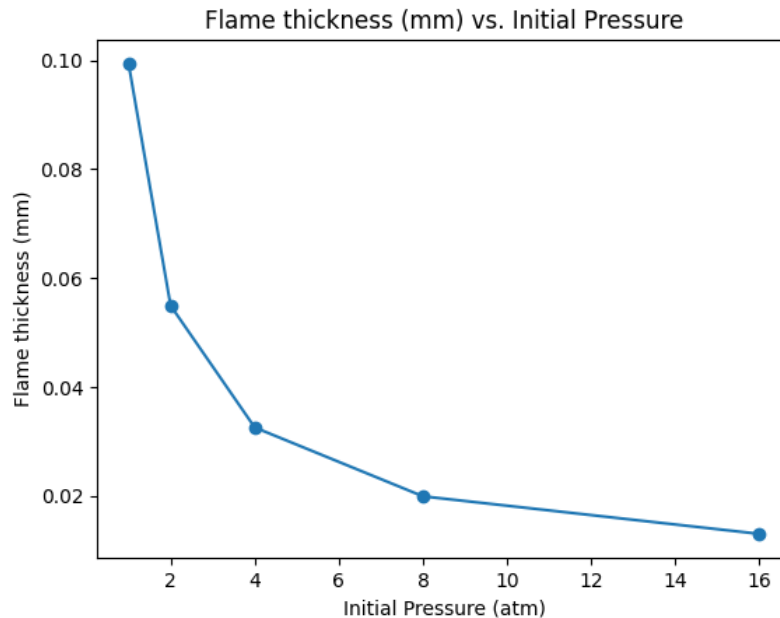

Fig 18 – Flame thickness (mm) vs Initial pressure ratio

The following assumptions are made to derive the relation of flame thickness –

- The first assumption which is made in the derivation of the relation, is the mixture being sufficiently off-stoichiometric, such that the reaction is governed by the concentration Y of the deficient reactant and the complete combustion can be described by one reactant reaction.
- The combustion process is assumed to be isobaric as the flame speed is much smaller than the speed of sound.
- In the narrow flame region due to rapid depletion of the reactant, it is assumed that diffusive transport which is described by second-order differential has a greater influence than the convective transport, described by first-order differential.

Fig 18 shows the plot for flame thickness vs initial pressure ratio. As the initial pressure increases from 1 atm to 16 atm, the flame thickness continues to decrease. However the decrease is relatively small at higher pressures.

The reason being the flame thickness becomes insensitive to pressure at higher pressures. This is because the increase in pressure tend to increase in the rates of molecular collisions and hence resulting in faster completion of the reaction, and hence thin reaction zone.

Part III –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: Sensitivity: $\partial \ln Su \ \partial \ln k$ where Su 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 Su is calculated.

Problem 1: Using the same perturbation, identify the 10 most sensitive reactions for ф =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.
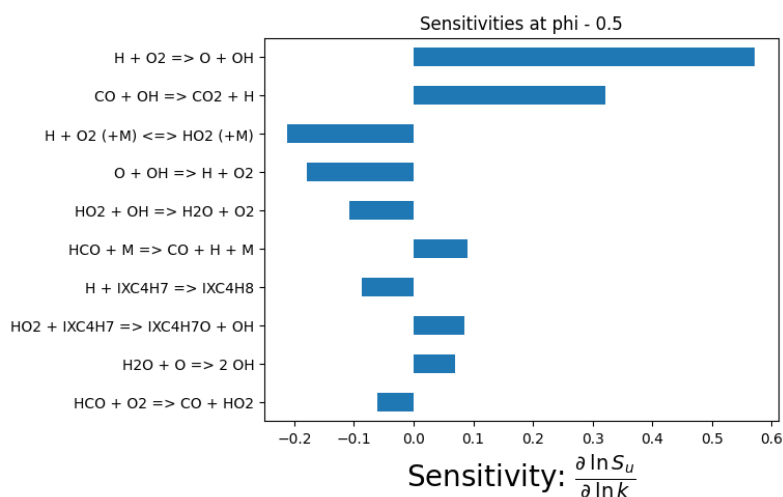

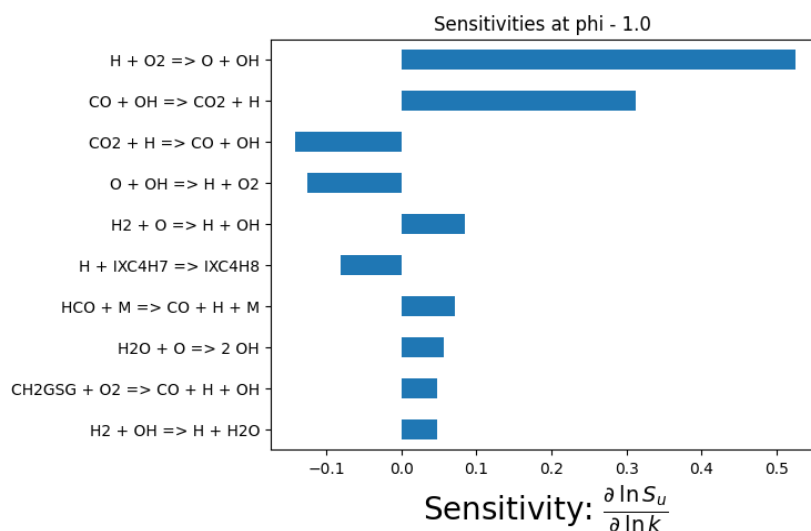Fig 19 –Laminar flame speed Sensitivity for different reactions at phi – 0.5

Fig 20 –Laminar flame speed Sensitivity for different reactions at phi – 1.0
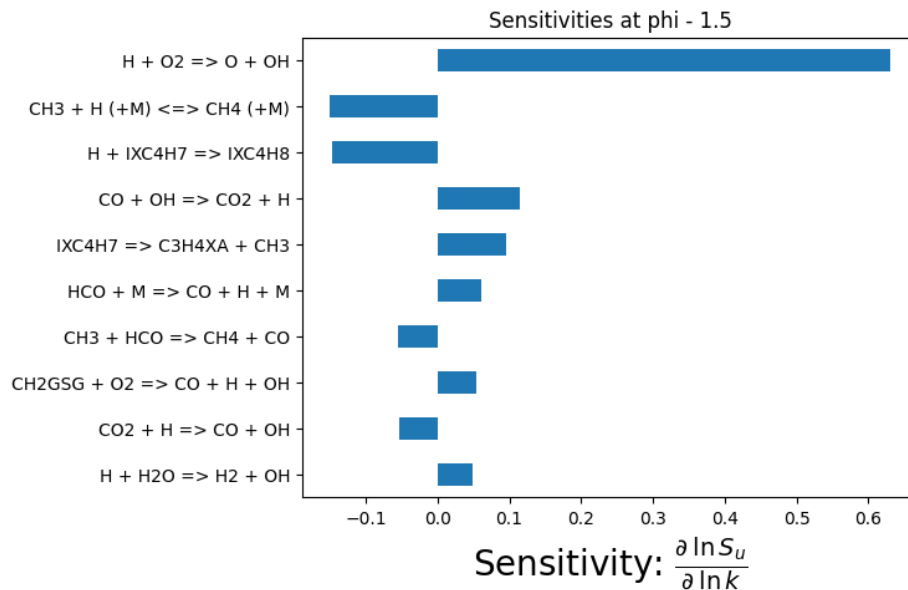
Fig 20 –Laminar flame speed Sensitivity value for different reactions at phi – 1.5

Fig 18, 19 & 20 shows the dependency of laminar flame speed on the different reaction in various cases of phi.

Problem 2: Comment on the impact of the different reaction types for these 3 conditions.

- For all the cases presented above, If the sensitivity is positive, it means that an increase in the reaction rate leads to an increase in the laminar flame speed. This suggests that the reaction is promoting the combustion process. On the other hand, if the sensitivity is negative, it indicates that an increase in the reaction rate results in a decrease in the laminar flame speed.
- In all three cases above, almost all the reactions are bimolecular. The prevalence of bimolecular reactions is a result of their favorable collision dynamics and higher likelihood of successful reactions under a typical condition.
- Along with this, Chain initiation reactions have the highest positive sensitivity, because it leads to the generation of more free radicals leading to an increase in the combustion rate and hence higher laminar flame speed.
- Chain propagation reactions also have positive sensitivity, however the magnitude of such reactions are not as high as the chain initiation because of the higher consumption than generation of radicals, however it contributes in the progression of combustion.
- All chain termination reactions shown in the above plots has negative sensitivity. These reactions lead to the loss of radicals and bring the chain reaction to an end. If termination reactions are highly negative sensitive, small changes in their rates can impact the lifetime of radicals and, consequently, the overall decrease the combustion and the laminar flame speed.

Problem 3: Explain the difference of ranking between the lean, stoichiometric, and rich cases.

The sensitivity ranking of reactions in lean, stoichiometric, and rich conditions affecting the laminar flame speed can vary due to differences in reaction pathways, concentrations of reactants and intermediates, and temperature profiles.

Fuel Lean condition (phi – 0.5)

- In lean conditions, there is an excess of oxidizer relative to the fuel. Hence all the reactions involving the consumption of oxidizer (O_2) will have higher sensitivity in lean conditions. This is demonstrated by the first five reactions shown in the Fig. 19 which has either the OH radical or O_2 present in the reactant side.
- The first reaction promotes radical generation, whereas the second reaction enhances the consumption of oxidizer. So these two reactions enhance the combustion process. The third reaction in the list, which leads to the production of HO_2 from H & O_2, and hence has a chain termination effect has the highest negative sensitivity. This is the result of a higher concentration of oxidizer which results in the recombination of H radical and O_2 gas to form HO_2.

Stoichiometric condition (phi – 1)

- At stoichiometric conditions, the fuel and oxidizer are present in the ideal ratio for complete combustion. Sensitivity analysis therefore highlights reactions involved in maintaining the balance between fuel and oxidizer.
- The first two reactions are the same as the lean condition. But the third reaction, which is a bi-molecular dissociation reaction of CO_2 into CO and OH, shows the increased concentration of CO_2 in the reactant due to complete combustion. This reaction has the highest negative sensitivity. The increased rank of the combination reaction (H and $IXC4H7$ to form $IXC4H8$) which has a negative sensitivity also shows the increased concentration of the fuel.

Fuel Rich condition (phi – 1.5)

- In rich conditions, there is an excess of fuel relative to the oxidizer. Sensitivity analysis indicates that reactions involving fuel consumption become more influential. In this condition, termination reactions that lead to radical loss play a significant role in controlling the flame speed in rich conditions.
- This is seen from the second and third reactions, which are chain termination reaction leading to the consumption of H radical and the formation of CH_4 and C_4H_8, respectively. More heavy hydrocarbon reaction leading to the production of radicals that enhance the combustion of fuel in a rich environment have higher sensitivity. This is seen from the fifth reaction which is the dissociation reaction of C_4H_7 leading to the formation of CH_3 radical.