MECH 652 Dynamics of Combustion

Department of Mechanical Engineering- McGill University

Project: 3 Flames

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1.

1)

→ The total pressure of both streams is equalised such that

$$\therefore \int_{fuel} u^2_{fuel} = \int_{air} . u^2_{air}.$$

$$\therefore \int_{fuel} = 4.6 \ kg/m^3$$

$$\therefore \int_{air} = 1.205 \ kg/m^3$$

$$\therefore u_{air} = 1.5 \ m/sec$$

$$\therefore 4.6 \times (u^2)_{fuel} = 1.205 \times 1.5$$

$$\therefore (u^2_{fuel}) = 0.590$$

$$\boxed{\therefore u_{fuel} = 0.77 \ m/sec}$$

- Calculated flame velocity based on equal pressure on the both sides of flame and flame velocity can be found as 0.77 m/sec.
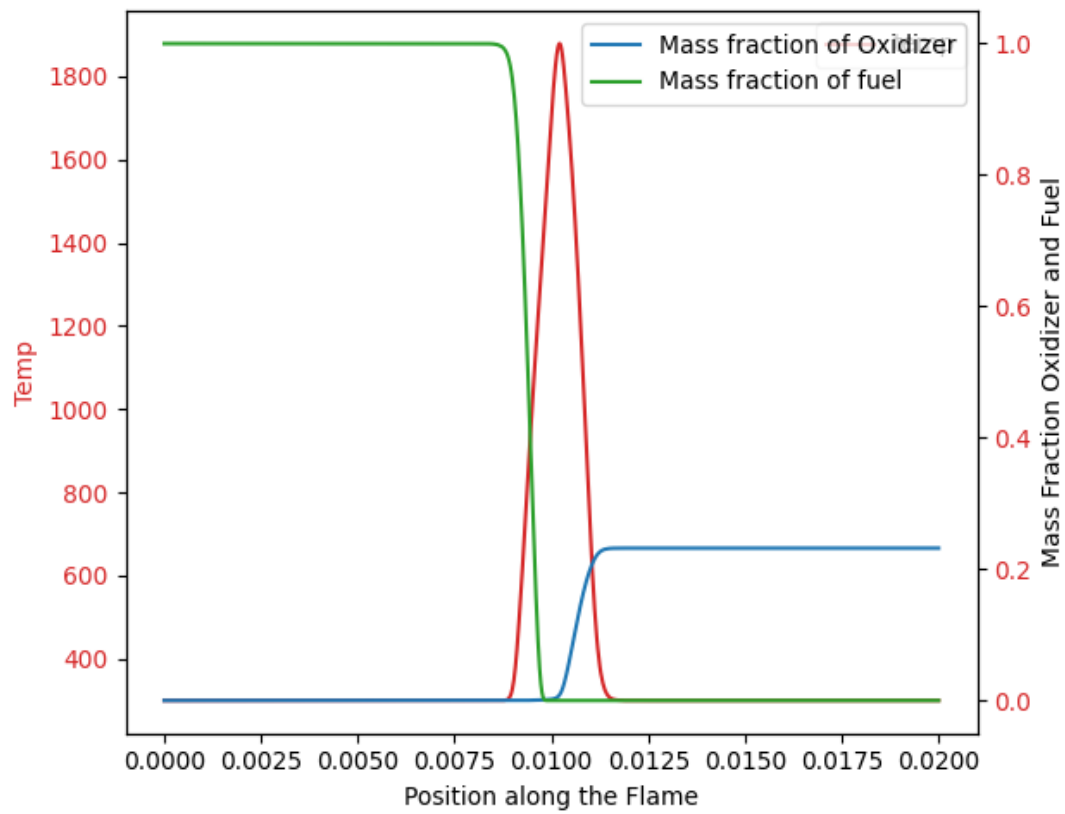
2.

Fig 1. Temp vs Position of Flame Position and Mass Fractions Vs Flame Position
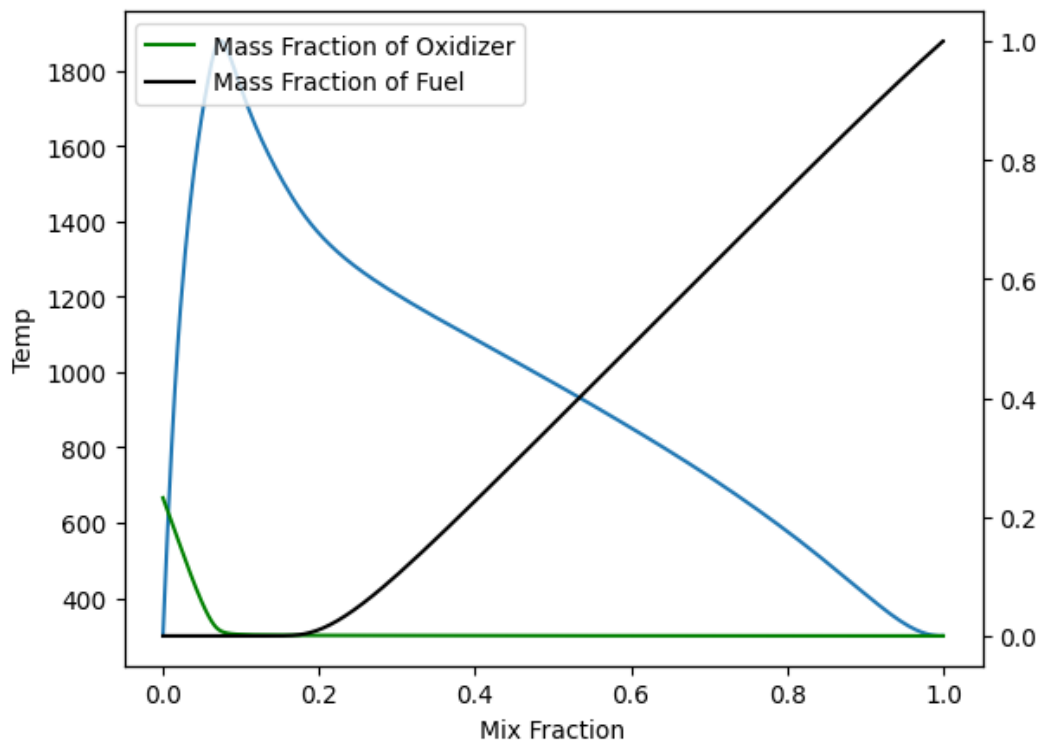
3.

Fig 2.Temp vs Bilger Mixture fractions and Mass Fractions vs Bilger Mixture Fraction

4. 0.07342 as per calculation.
5. Equilibrium Temperature of stoichiometric mixture of iso octane and air is 2273.56 K while the maximum temperature of counter-flow diffusion flame is 1879.154K. Equilibrium temperature

can be achieved under the condition of no heat losses to the surroundings while Counter flow diffusion flame which is coming from opposite nozzles of fuel and oxidizer is subjected to heat loss to surroundings. Also, counterflow diffusion flame is subjected to strain rates which lower down the temperature of flame.

Hence actual flame temperature of diffusion flame will always less than adiabatic or equilibrium temperature.
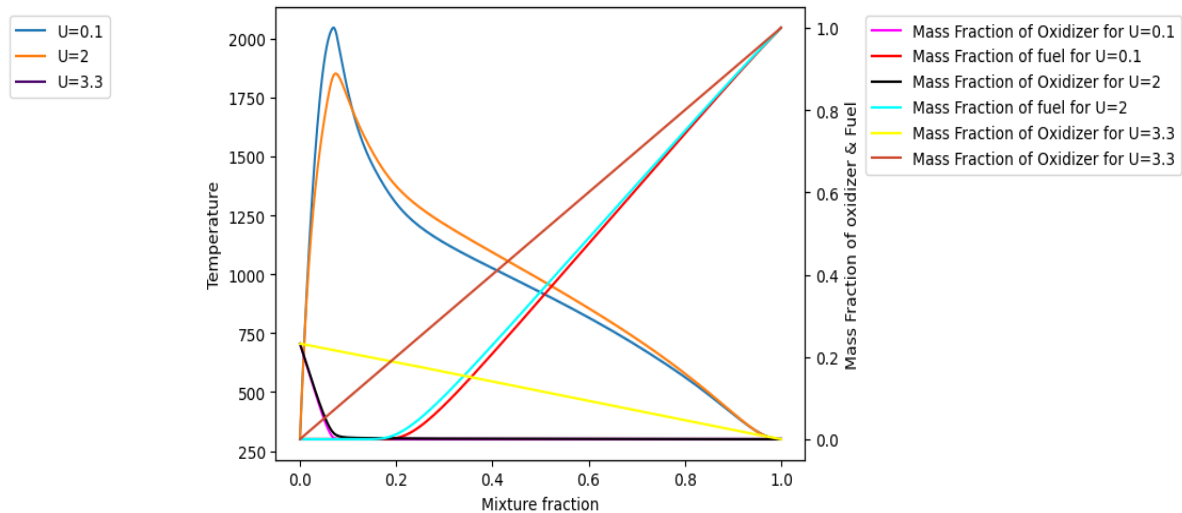
6.

Fig 3. Temp vs Mixture Fraction and Mass fraction of oxidizer and fuel for different air inlet velocity

- From graph, increase in inlet velocity of air lead to decrease in Flame temperature. As strain under the flame will increase which leads to lower flame temperature. While for U = 3m/sec no flame will be ignited as we can not see any temperature profile on graph.
- Mass fractions of fuel and oxidizer behaves in following manner:
- For U= 0.1 m/sec and U = 2 m/sec curve of mass fractions behaves in the similar way as mass fraction of oxidizer and fuel both gone a decrease till the flame condition is achieved.
- However, for U=3 m/sec no flame will be ignited as strain rate of flame is very high which leads to extinction of the flame.
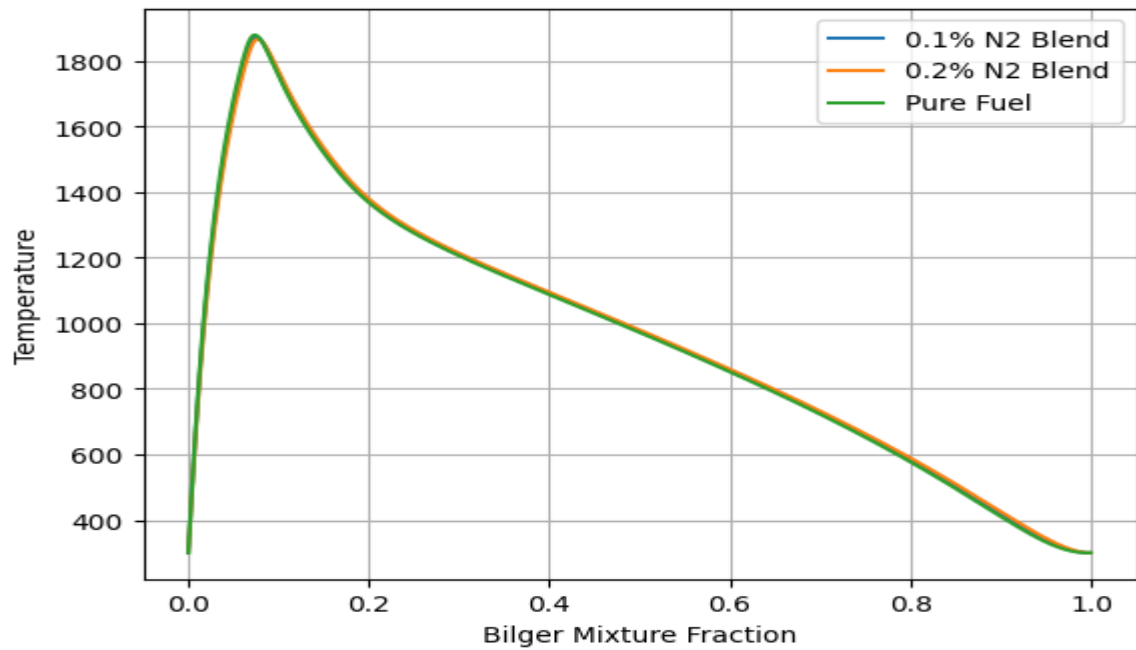
7. Bonus question:

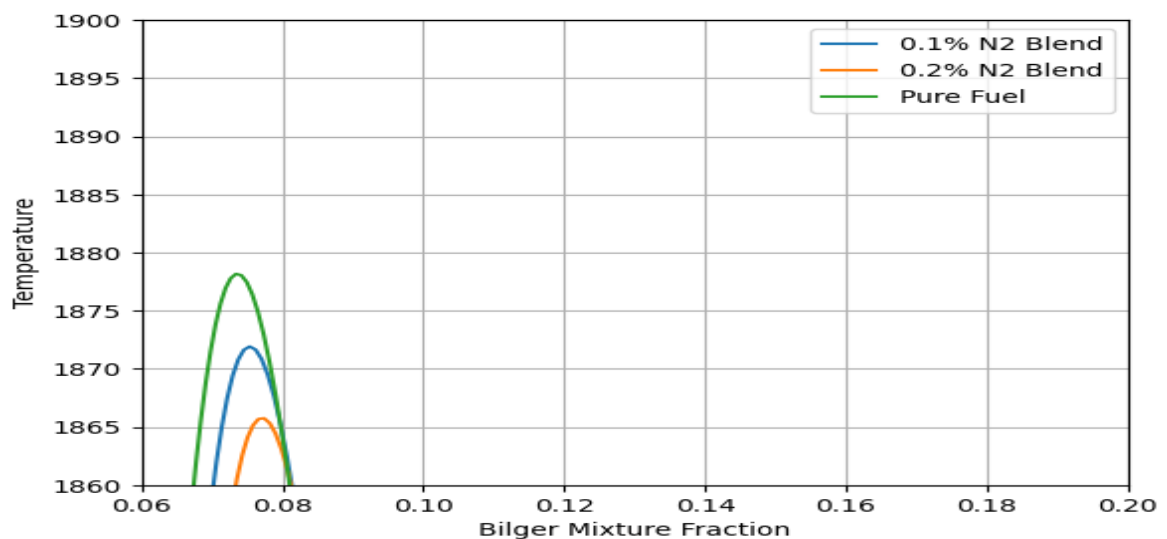Fig 4. Temperature vs Mixture Fraction for three different fuels

Fig 5. Enlarged plot of Temperature vs Mixture Fraction for three different fuels

- From Enlarged graph we can see that temperature of the flame goes little bit down as we increase the concentration of N2 as additional nitrogen in the fuel soak up the flame temperature which makes little difference in temperature of the flame.
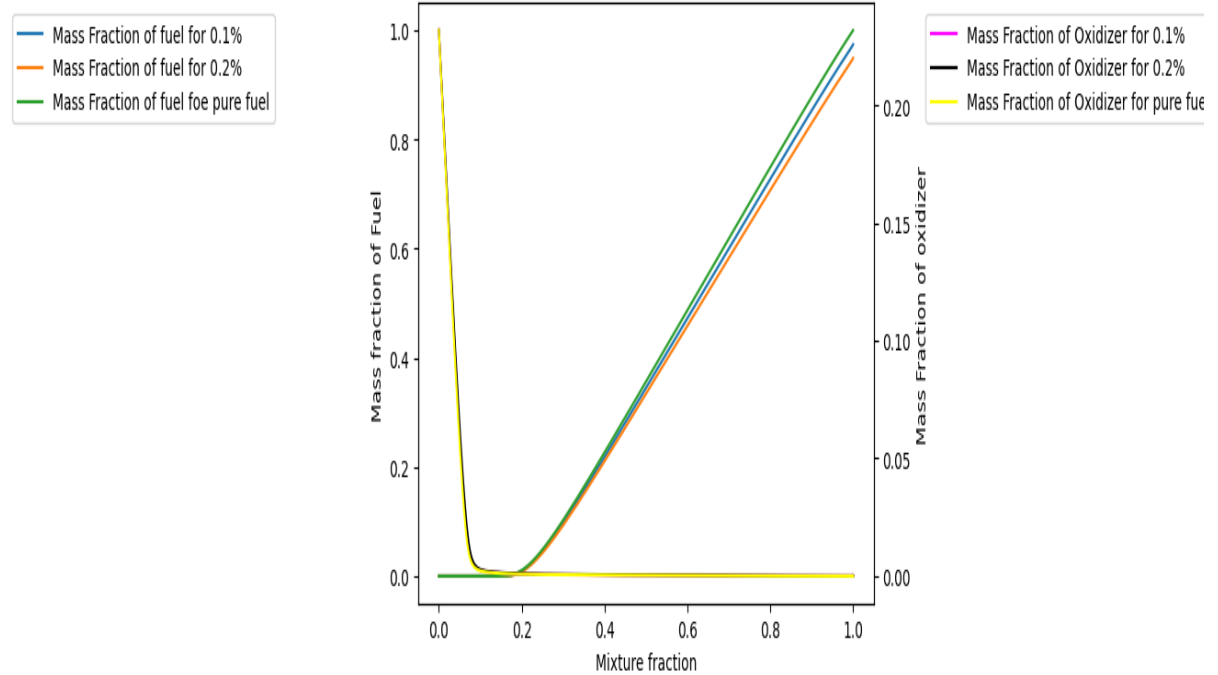
Fig 6. Mass Fraction of Fuel vs Mixture Fraction and Mass fraction of oxidizer vs Mixture Fraction for three different fuels

- As seen from graph mass fraction of the fuel and oxidizer very little difference can be found for three different fuels. It can be concluded that interception of mass fraction of fuel with oxidizer get decreased with increase in N2 in fuel.
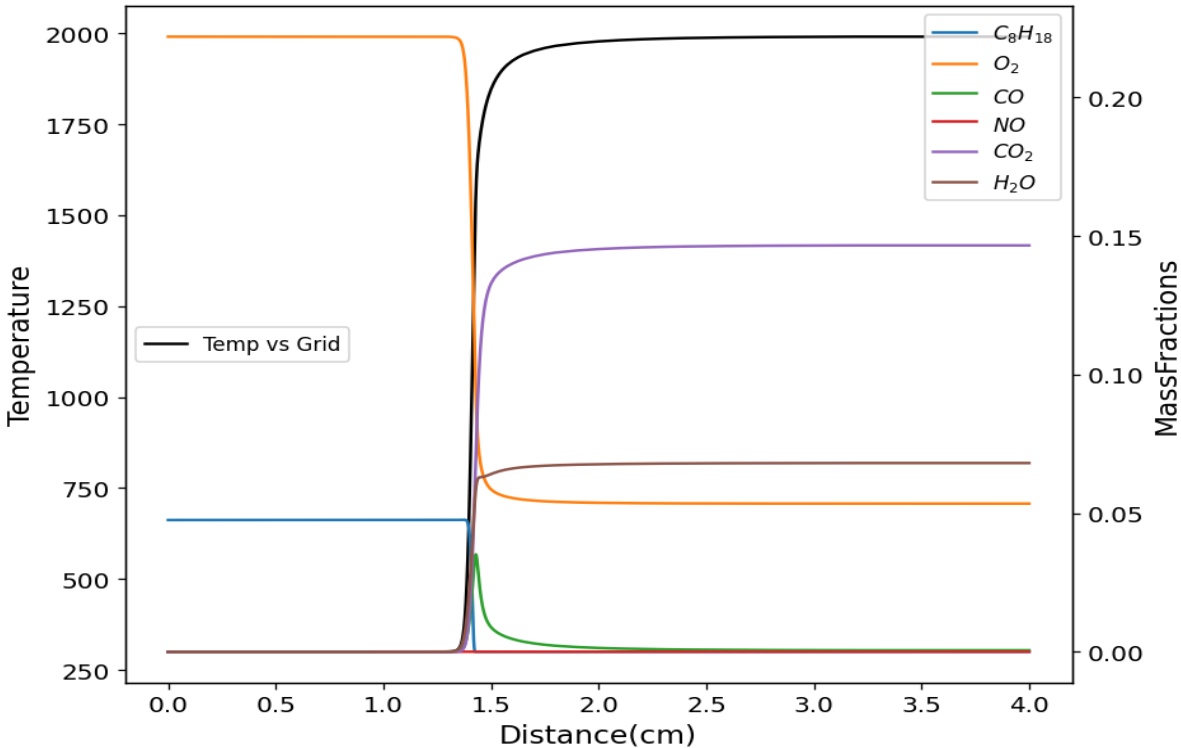
Part 2: Premixed Flames

1.

Fig 7. Temperature vs Flame grid and Mass Fractions of different species vs Flame Grid

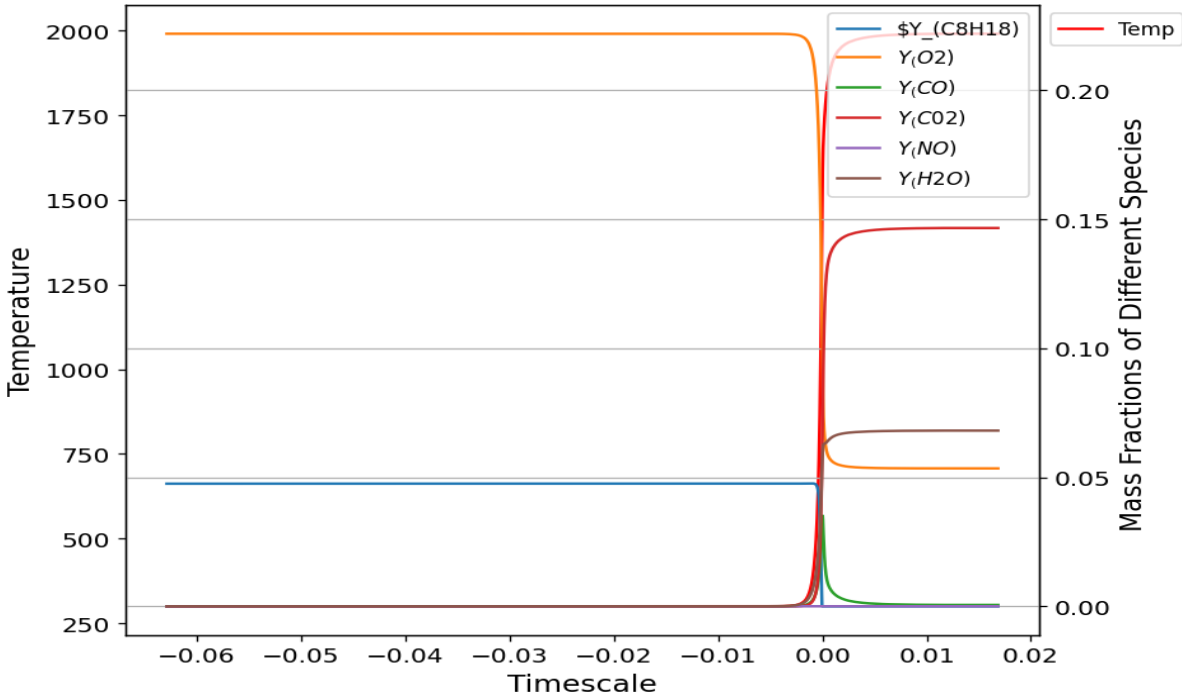2. Conversion of Grid Points to time scale coordinates.
3.

Fig 8. Temperature vs Time Scale and Mass Fractions of different species vs Time Scale
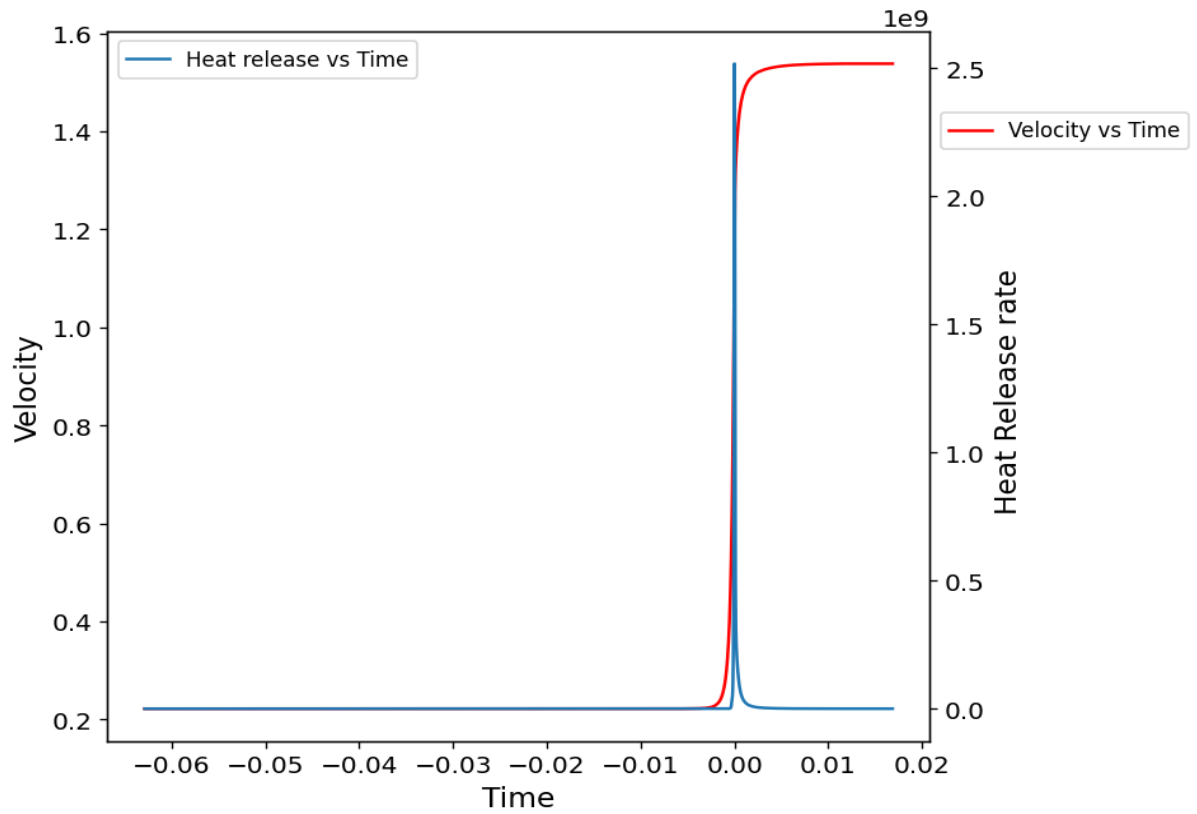
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Fig 9. Flame Velocity(m/sec) vs Time Scale and Heat Release rate vs Time Scale
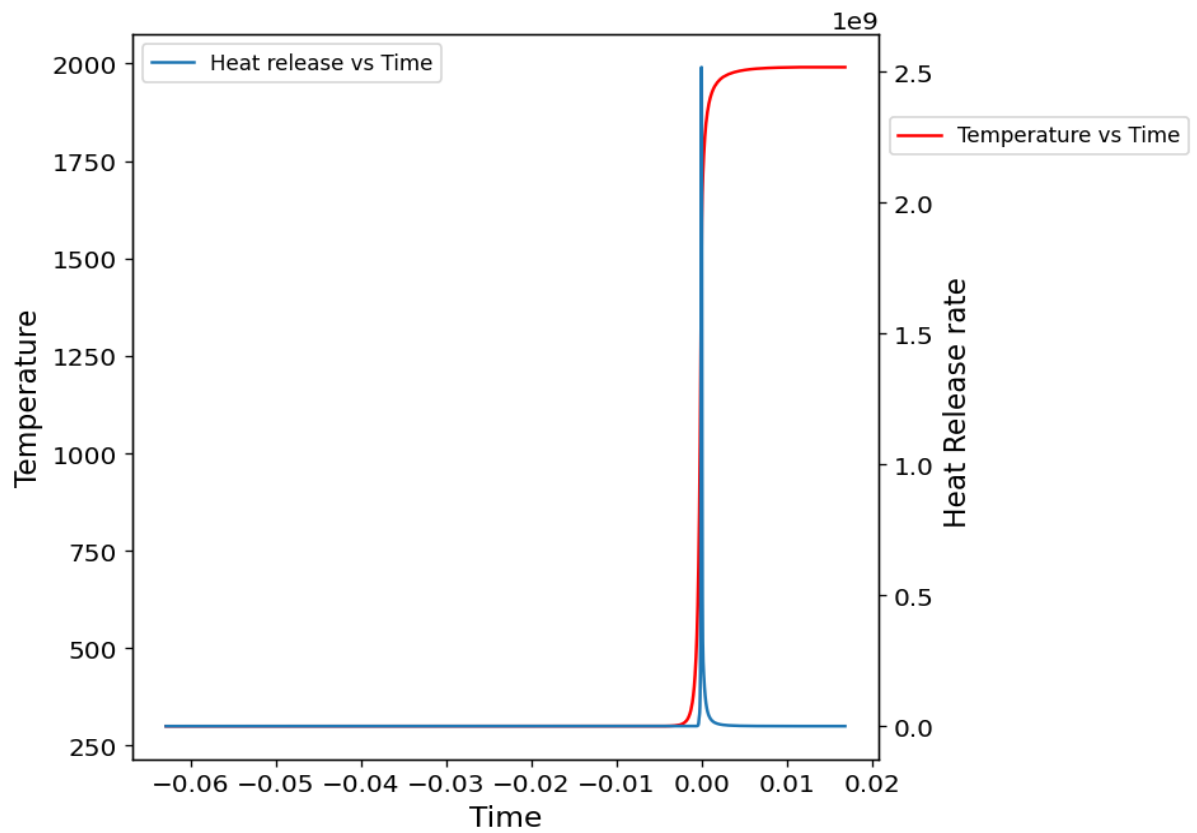
5.

Fig 10. Temperature(K) vs Time Scale and Heat Release rate vs Time Scale
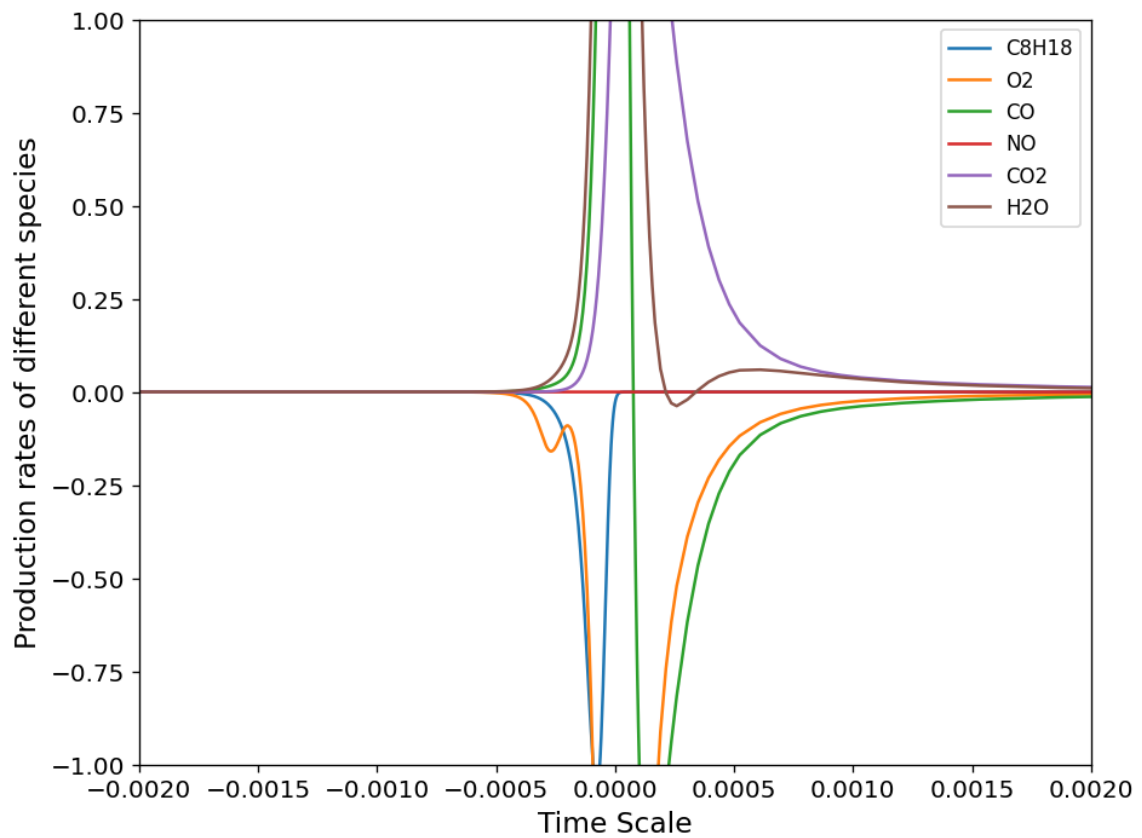
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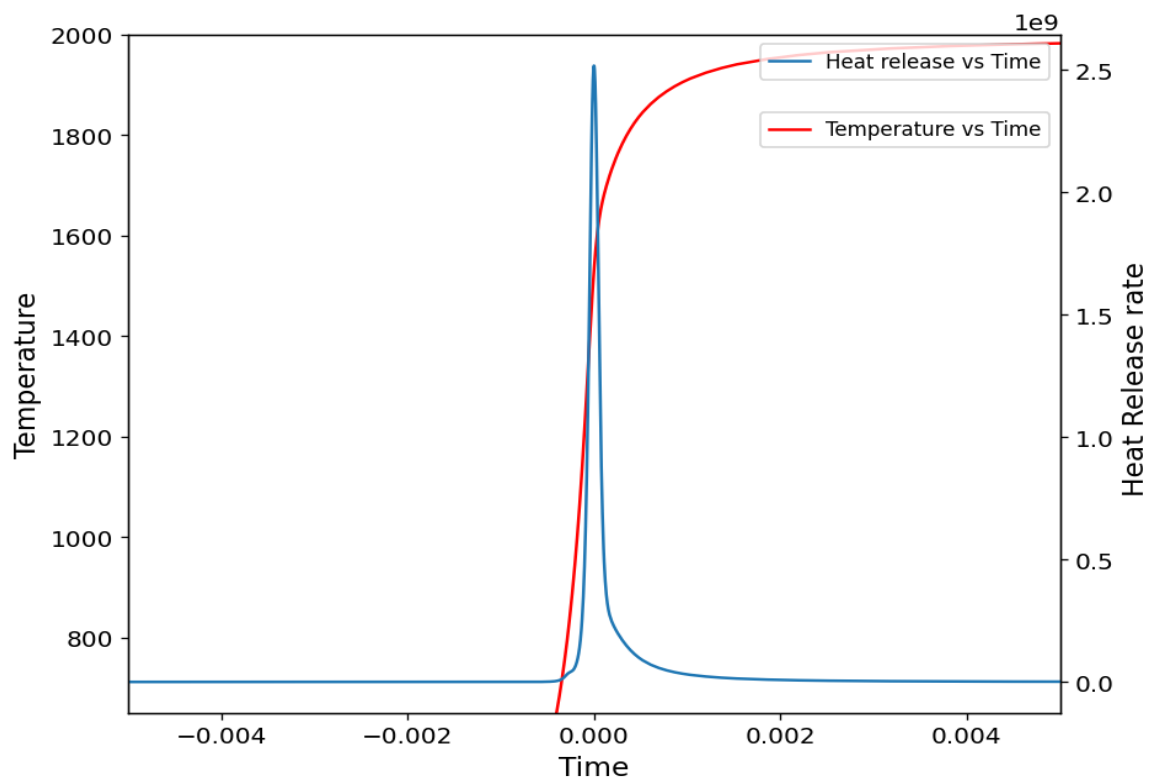Fig 11. Enlarged View of Net Production rates of different species vs Time scale

7.

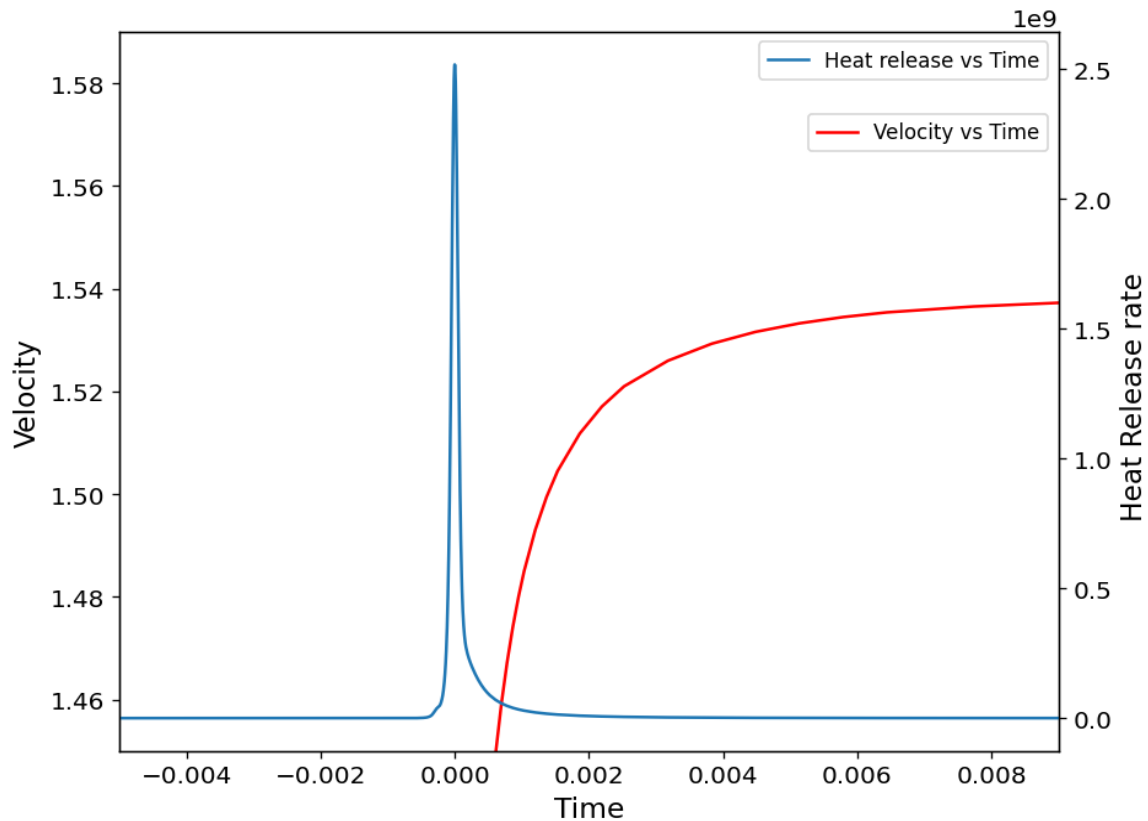Fig 12. Enlarged view of Temp(K) vs time and heat release rate vs time

Fig 13. Enlarged view of Velocity(m/sec) vs time and heat release rate vs time

Premixed laminar flame:

- For graph of temperature vs time scale and mass fractions vs time scale mass fractions of reactants i.e., fuel and oxidizer decreased as they are consumed during reaction and goes to zero at time scale 0 which is set to be at a point where we get maximum heat release. Also for products (CO, CO2,NO,H2O) mass fractions values raised after 0 time scale that means products get formed after this time scale. Also flame get thin as reaction progresses.

- For graph of velocity vs time scale and heat release vs time scale. As reaction proceeds towards 0-time scale i.e. point of maximum heat release rate goes up, while heat release get maximum at time scale 0 and gets decreased as time scale progress which indicates heat loss. At the same time velocity become maximum after time scale and it goes to a constant as flame propagates in forward direction.

- For a graph of temperature vs time scale and heat release vs time scale. As reaction proceeds towards 0-time scale temperature goes maximum. While heat release rate would behave same as explained above.

- For a graph of net production rate of species, production rates of reactants goes down as we approach to time scale while production of products (CO, CO2, NO,H2O) increases as flame propagates.
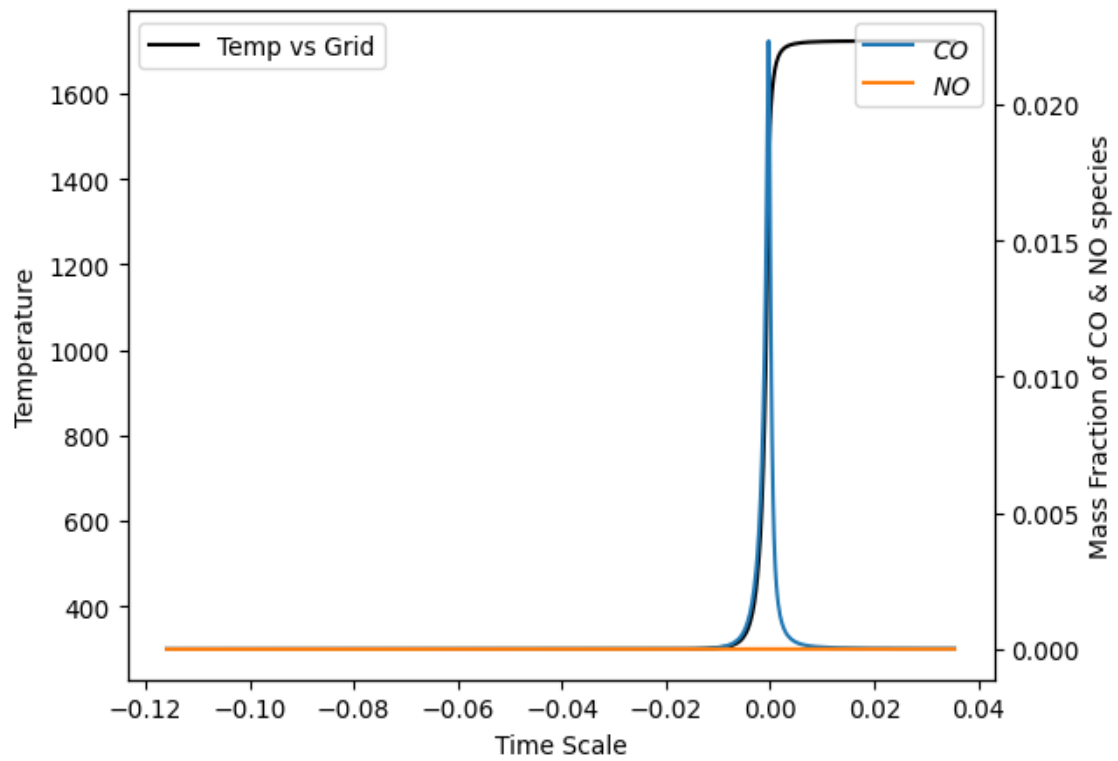
8.

For Equivalence ratio of 0.60:

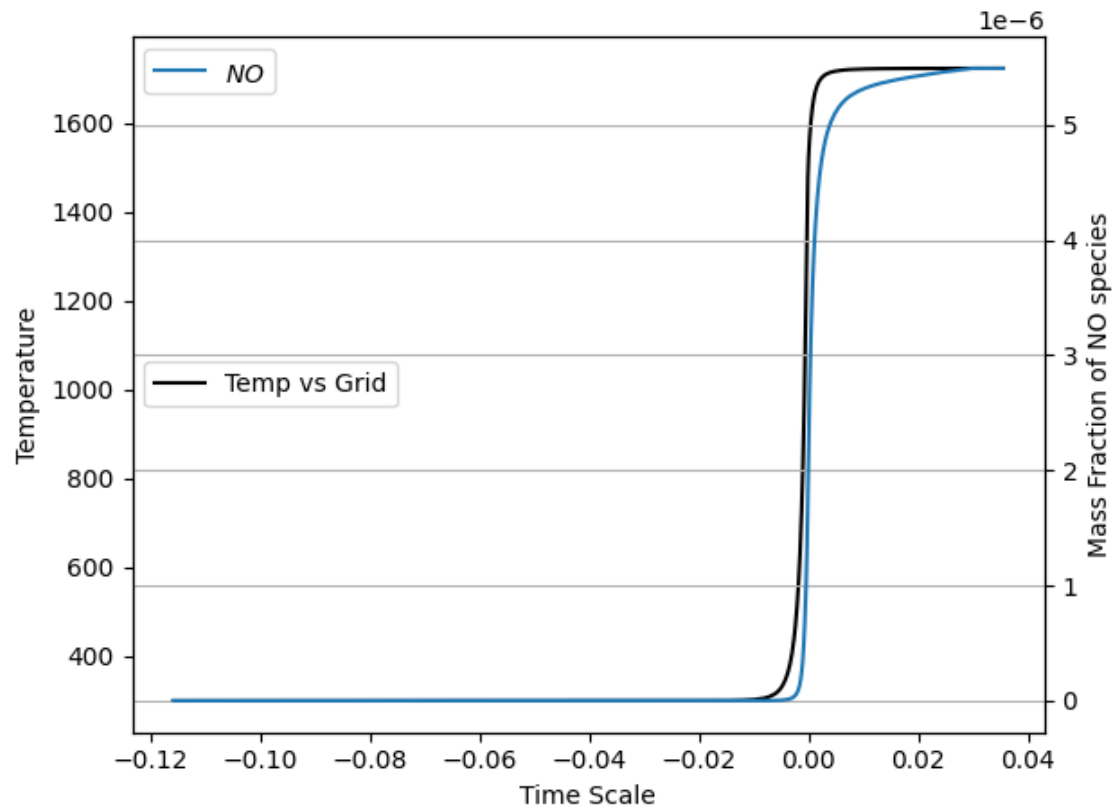Fig 14. Temperature vs Time Scale and Mass Fractions of CO, NO vs Time scale for phi = 0.6

Fig 15. Temperature vs Time Scale and Mass Fractions NO vs Time scale for phi = 0.6

For equivalence ratio : 0.65

Fig 16. Temperature vs Time Scale and Mass Fractions CO,NO vs Time scale for phi = 0.65

Fig 17. Temperature vs Time Scale and Mass Fractions NO vs Time scale for phi = 0.65
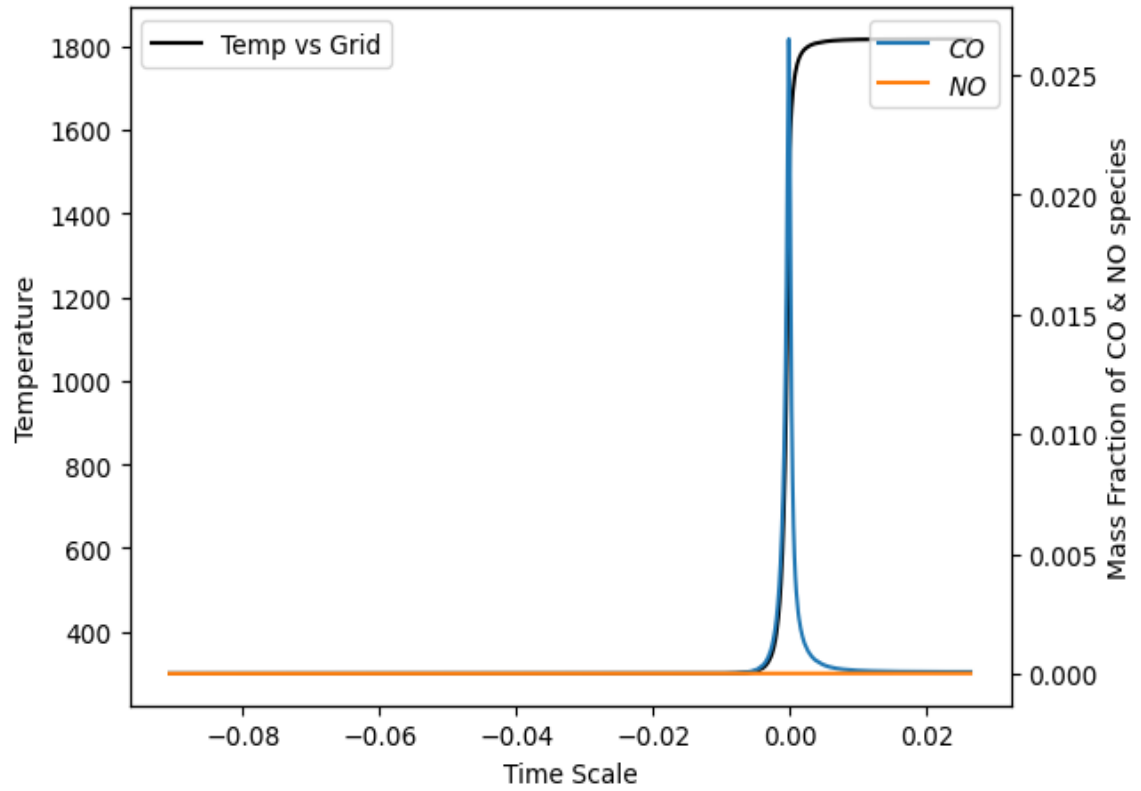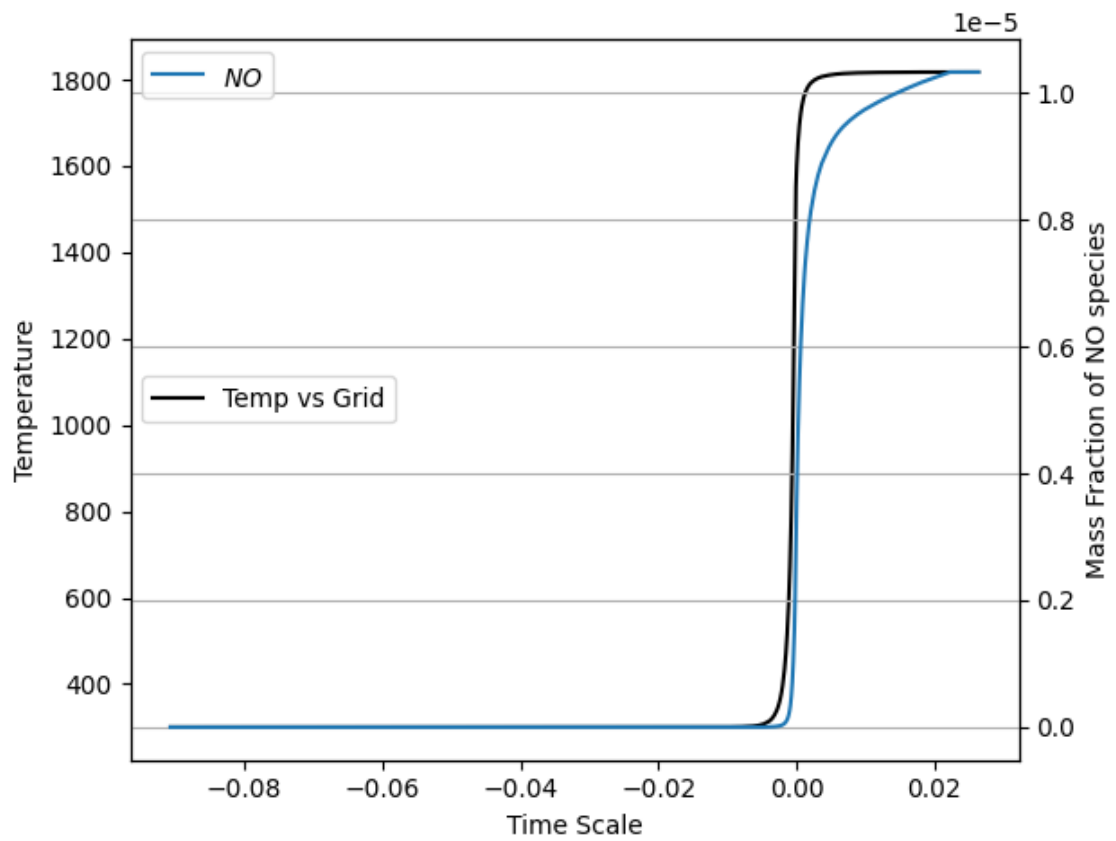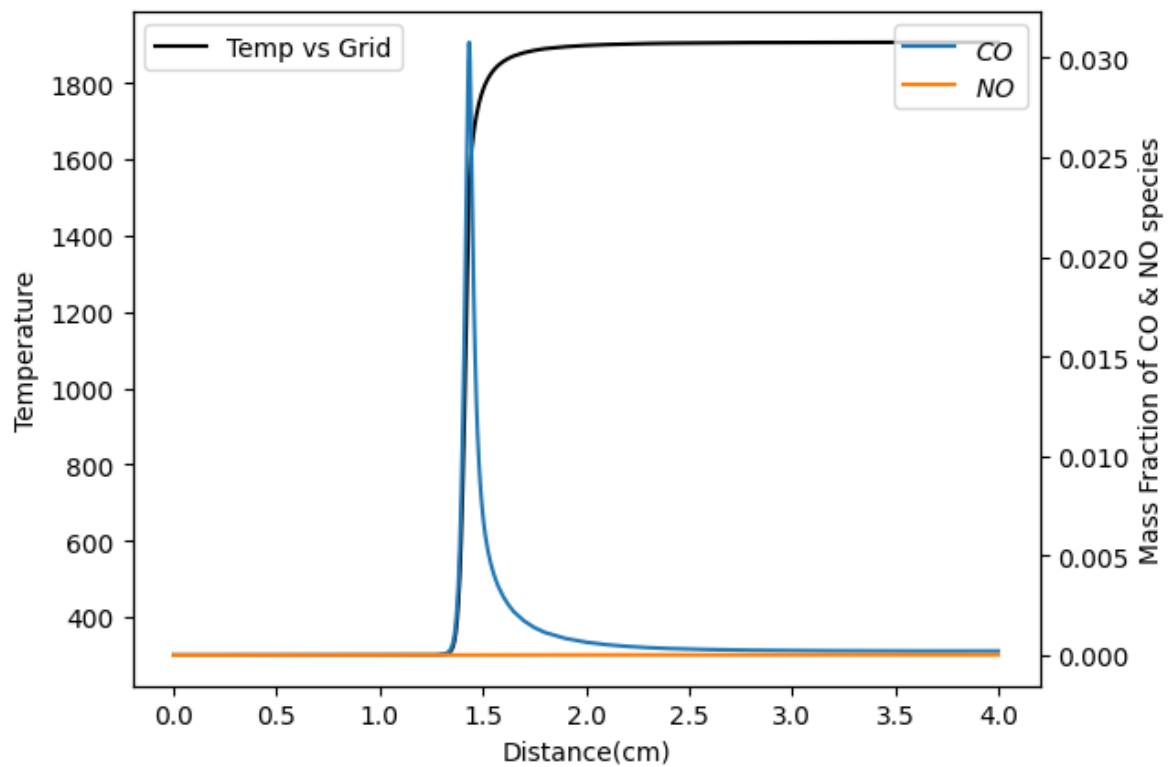
For Equivalence ratio = 0.7

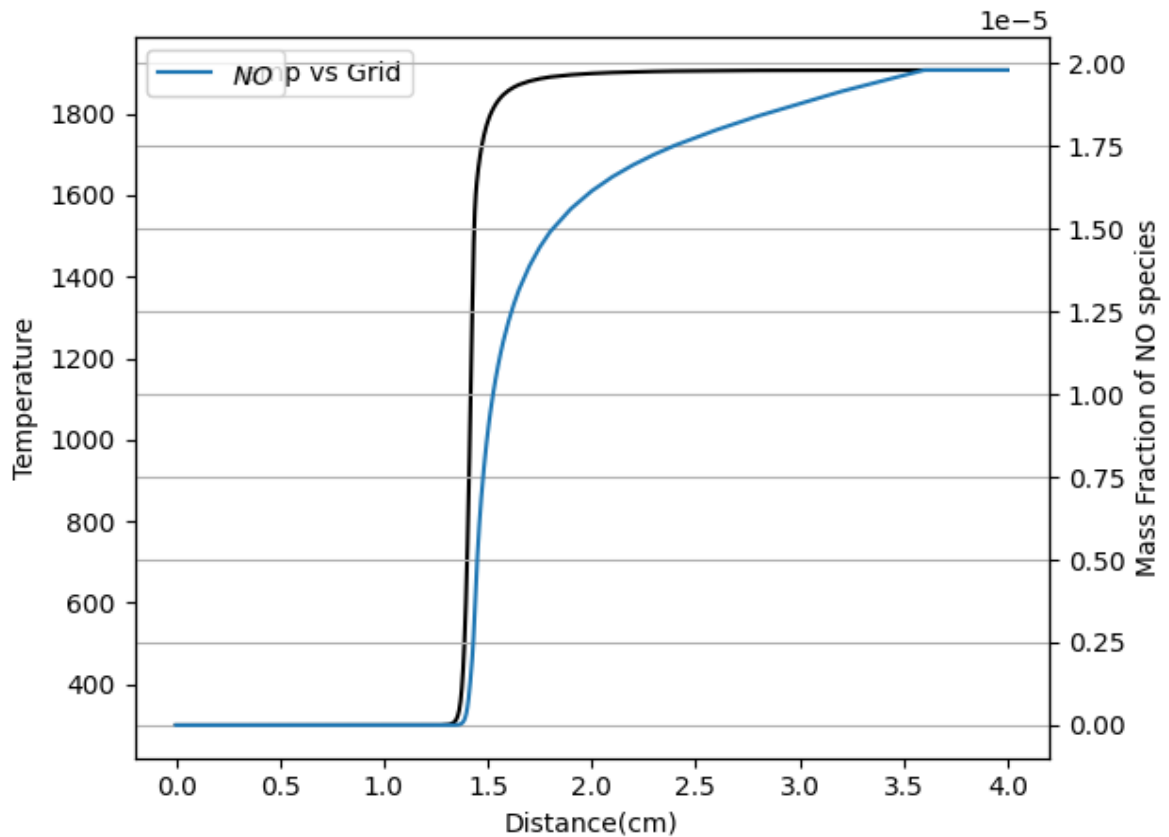Fig 18. Temperature vs Time Scale and Mass Fractions CO,NO vs Time scale for phi = 0.7

Fig 19. Temperature vs Time Scale and Mass Fractions NO vs Time scale for phi = 0.7

- For three different flames of having equivalence ratio of 0.6, 0.65, 0,7, Flame temperature get increased as we increase equivalence ratio. Increase in equivalence ratio higher fuel concentration which leads to higher heat release results in high temperature of the flame.
- Concentration of CO and NO increased as we increase equivalence ratio. Increase in equivalence ratio leads to decrease in amount of oxygen as well as increase in fuel concentration available for burning fuel which leads to formation of intermediate species like CO and NO as there are insufficient oxygen available to form the complete species (CO2). Also increase in fuel concentrations generates more CO as C atom increase while at high equivalence ratio Temp of flame increase which leads to higher formation of NO by zeldowich mechanism.
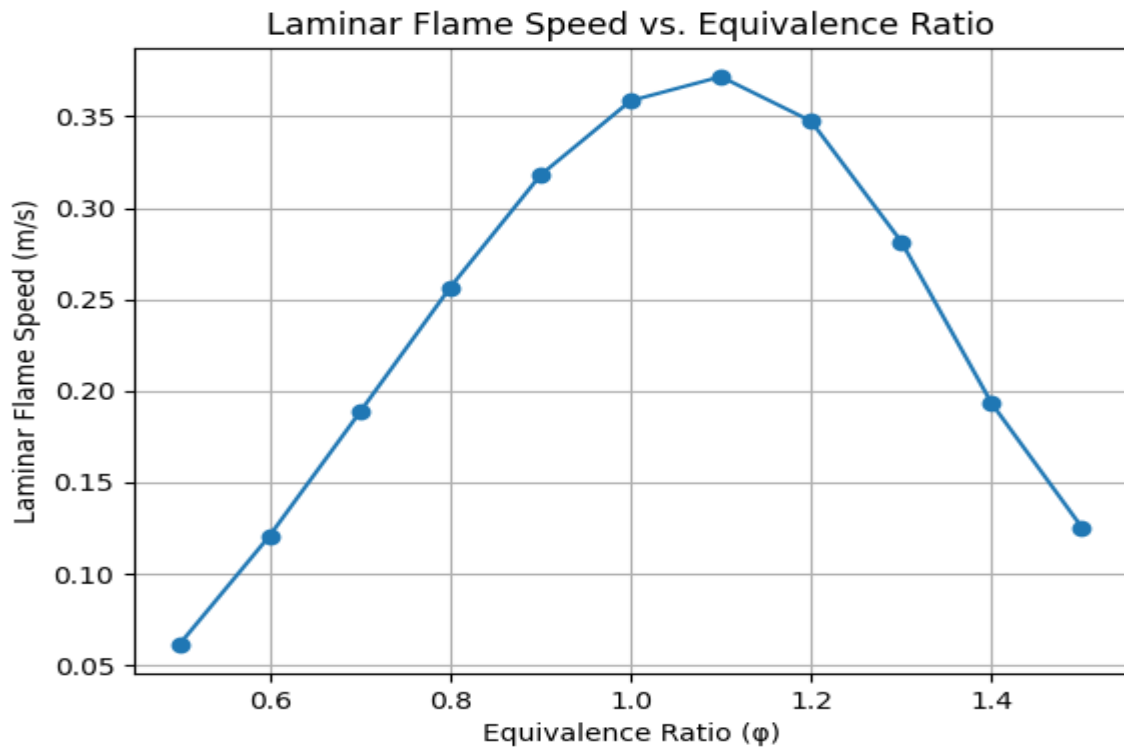
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Fig 20. Laminar Flame Speed(m/sec) vs Equivalence Ratio

As we increase equivalence ratio reaction goes to complete combustion which leads to higher flame temperature results in higher flame propagation rates and flame progresses with distance. Maximum flame speed can be found at an equivalence ratio of 1.13 at the same temperature of the flame is also maximum.
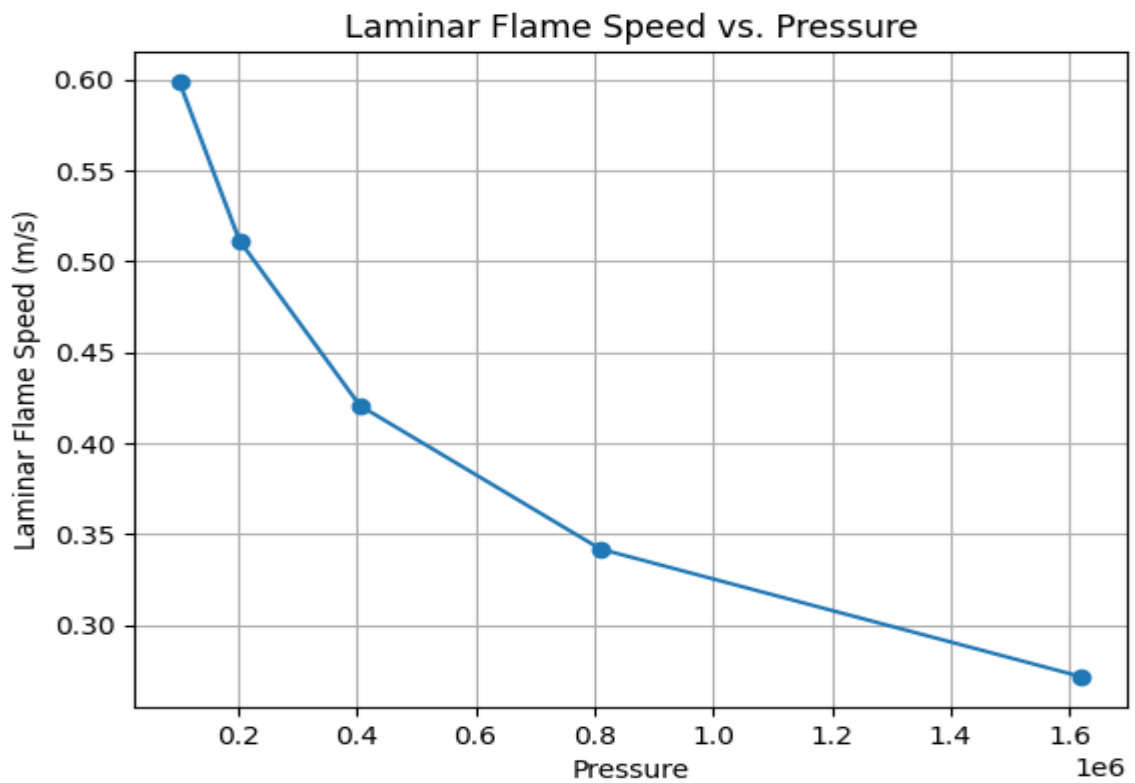
10.

Fig 21. Laminar Flame Speed(m/sec) vs Pressure

- From the equation of flame speed $S_L \approx ((P_0)^{(n/2)-1)}) * (\alpha*w)^{(1/2)}$ by flame thicken model. Where n is the order of the reaction, α is thermal diffusivity and w is the reaction rates. As we increase pressure of the reaction flame speed decreases. Also some of the reactions are pressure dependents which limits the reaction leads to reduce in flame velocity.
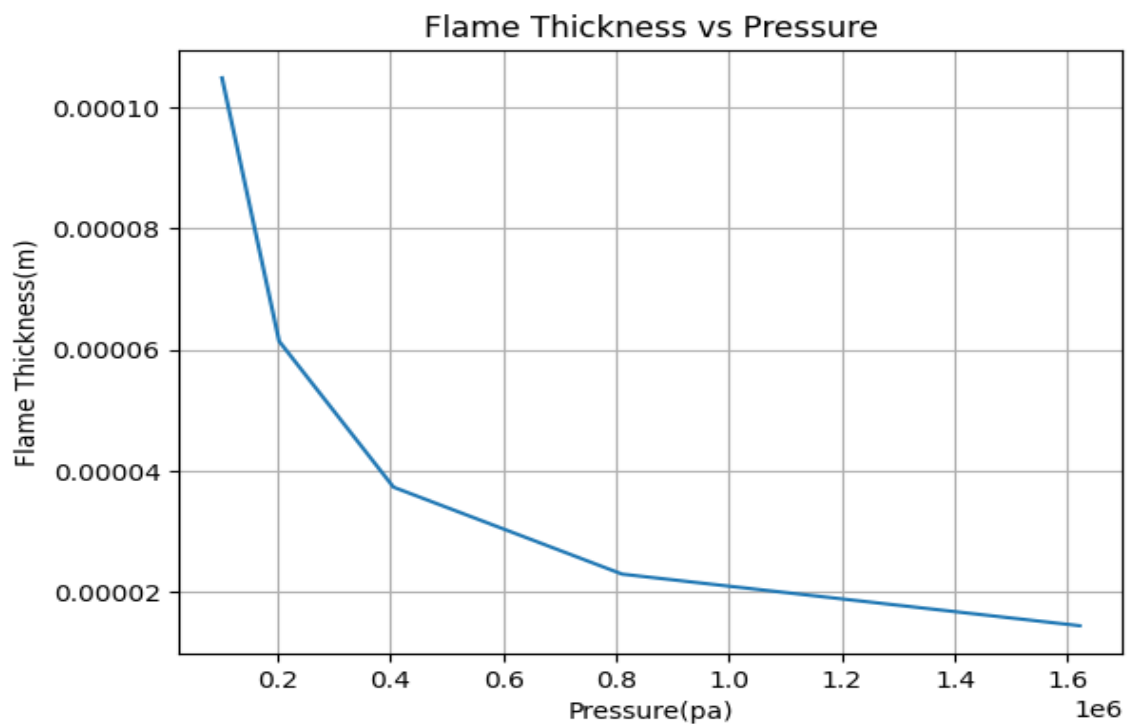

Fig 22. Laminar Flame Thickness(m) vs Pressure(pa)

- From graph flame thickness decreases as flame front gets decreases which leads to thin flame. Also, it can be concluded that some elementary reactions which are pressure dependent affects the flame thickness.

Part 3: Sensitivity Analysis

1.

- Sensitivity Analysis for equivalence ratio of 0.5:
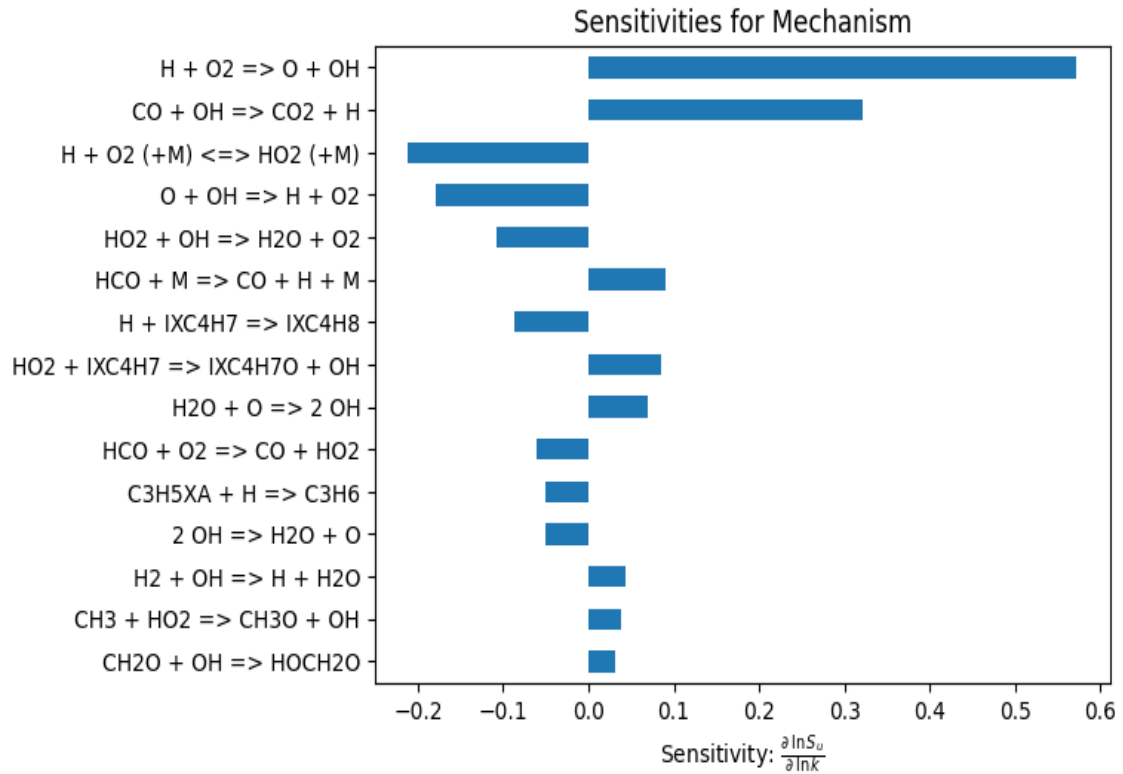

Fig 23. Sensitivity Analysis of Reactions for Equivalence Ratio of 0.5

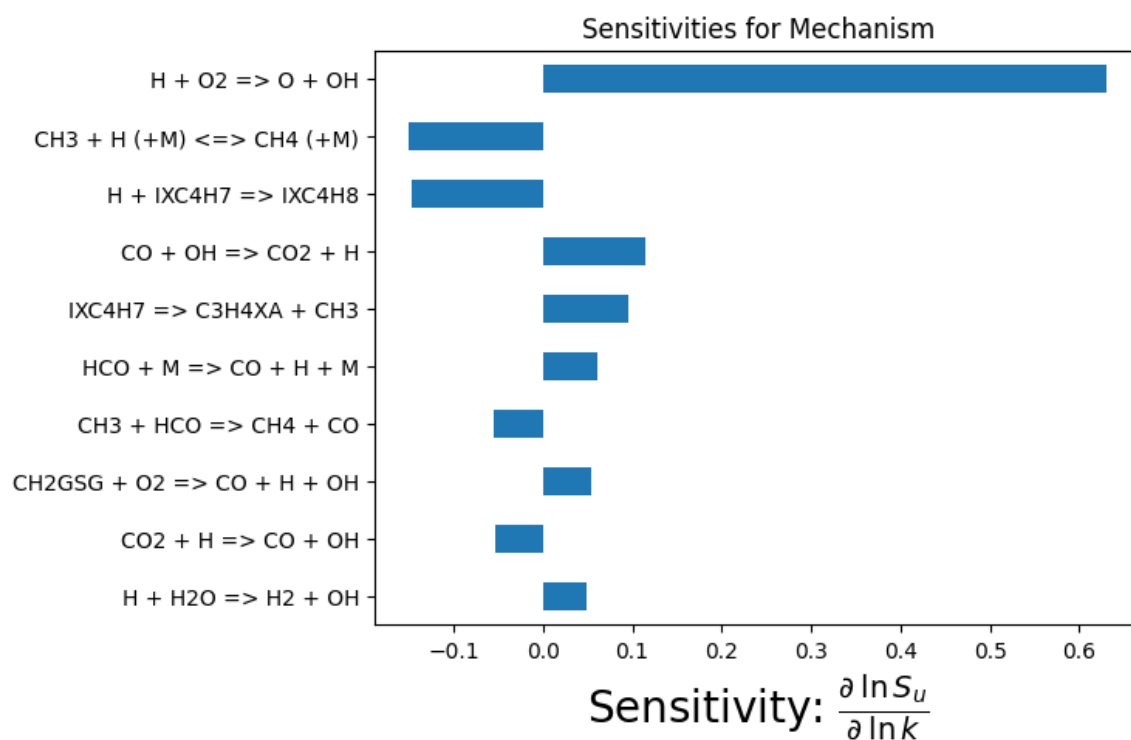- Sensitivity Analysis for equivalence ratio of 1.0:

Fig 24. Sensitivity Analysis of Reactions for Equivalence Ratio of 1.0
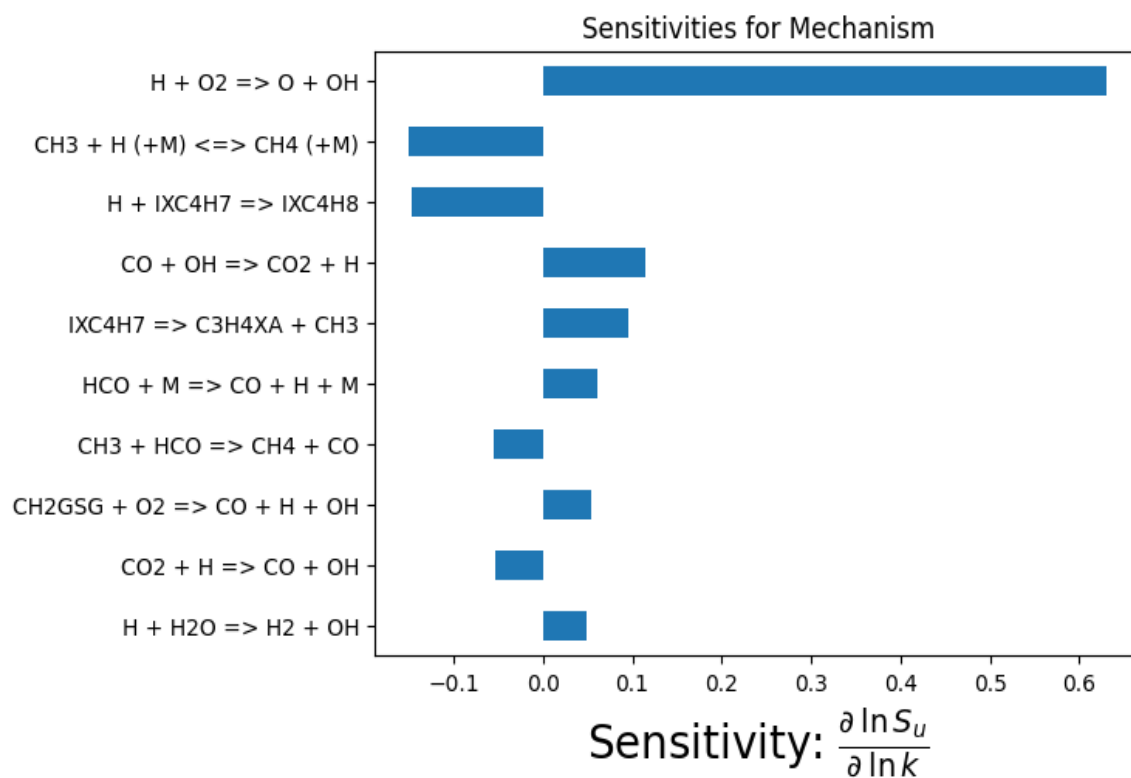
- Sensitivity Analysis for equivalence ratio of 1.5:

Fig 25. Sensitivity Analysis of Reactions for Equivalence Ratio of 1.5

Sensitivity Analysis shows the dependence of elementary reaction on entire chemical reaction process. We have found sensitivity analysis of Iso octane react with air using Jerzembeck mechanism.

2.
- The reaction which is most sensitive to chemical reaction is reaction of OH. This reaction is chain branching step which has positive sensitivity to the overall reaction.
- We also have some of reaction which has negative sensitivity to the overall reaction like reactions in which third body collider M is present. In case of lean mixture that reaction is H + O2 + M = HO2 + M. While for fuel rich and stoichiometric condition that reaction is CH3+H+M = CH4 + M.
- CO + OH = CO2 + H governs a large part of heat release and thus rate-limiting to chemical reactions.
- We do have some similar reactions which are sensitive to overall chemical reaction in fuel rich and stoichiometric conditions like split of H atom from IXC4H8 and gives to IXC4H7.

3.
- Increase in equivalence ratio as changing condition from fuel lean to fuel rich will increase sensitivity of elementary reactions.
- Small difference can be found in in increase in sensitivity of the elementary reactions.
- Reactions which have negative sensitivity in case of fuel rich and stoichiometric condition shows no effect in sensitivity by increasing equivalence ratio.
- Increase in equivalence ratio leads to increase in concentration of fuel which creates dependence on elementary reactions.
- From the reference of Combustion by J.Warnatz and U.mass sensitivity for methane air reactions, in which increase in equivalence ratio leads to decrease in sensitivity of primary equation like formation of OH.

References :

1. Combustion Physical and Chemical fundamentals, modelling and simulation, experiments, pollutant formation by J. warnatz , U.Mass, R.W. Dibble
2. Combustion Physics by C.K. Law

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

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