

MECH 652 Dynamics of Combustion
Department of Mechanical Engineering- McGill University

Project: 2 Reactors

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Question: 2

1. Molecularity:

Reaction	Molecularity
R1	Bimolecular
R2	Bimolecular
R3	Trimolecular
R4	Bimolecular
R5	Bimolecular
R6	Bimolecular

2. Reaction Type:

Reaction	Type of Reaction
R1	Global
R2	Initiation
R3	Termination
R4	Propagation
R5	Propagation
R6	Propagation

3. Pressure Dependency:

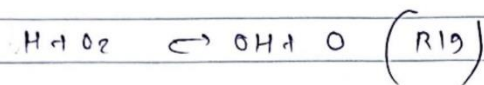
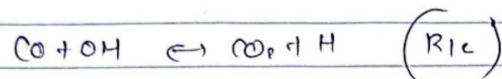
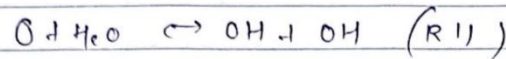
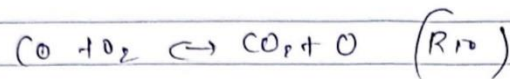
Reaction	Dependency
R1	Pressure Independent
R2	Pressure Dependent
R3	Pressure Dependent
R4	Pressure Independent
R5	Pressure Independent
R6	Pressure Independent

4.

5. Rate of Equation:

Rate of Equation for OH and O is given by following.

→ following elementary reaction system.



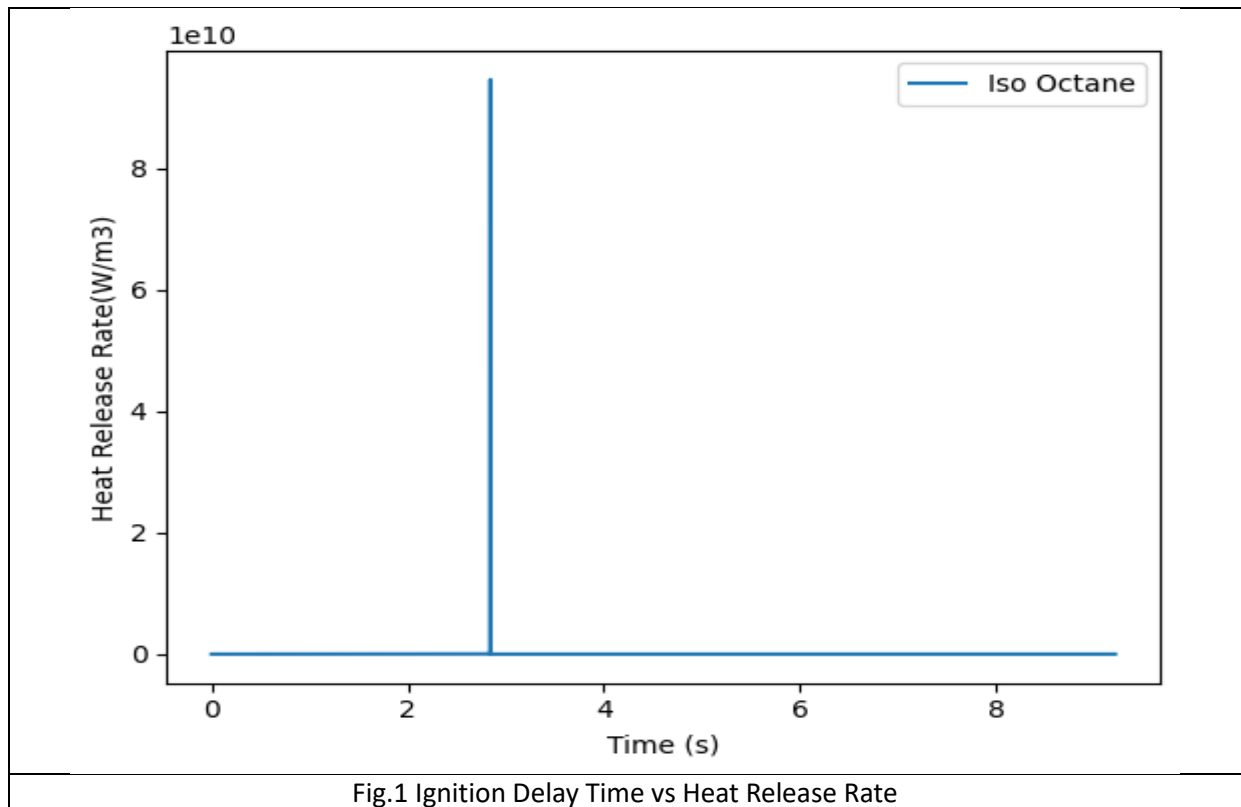
∴ From law of mass action ∴

$$\begin{aligned} \frac{d[\text{OH}]}{dt} = & k_{11f} [\text{O}] [\text{H}_2\text{O}] - k_{11b} [\text{OH}]^2 \\ & - k_{12f} [\text{CO}] [\text{OH}] + k_{12b} [\text{CO}_2] [\text{H}] \\ & + k_{13f} [\text{H}] [\text{O}_2] - k_{13b} [\text{OH}] [\text{O}] \end{aligned}$$

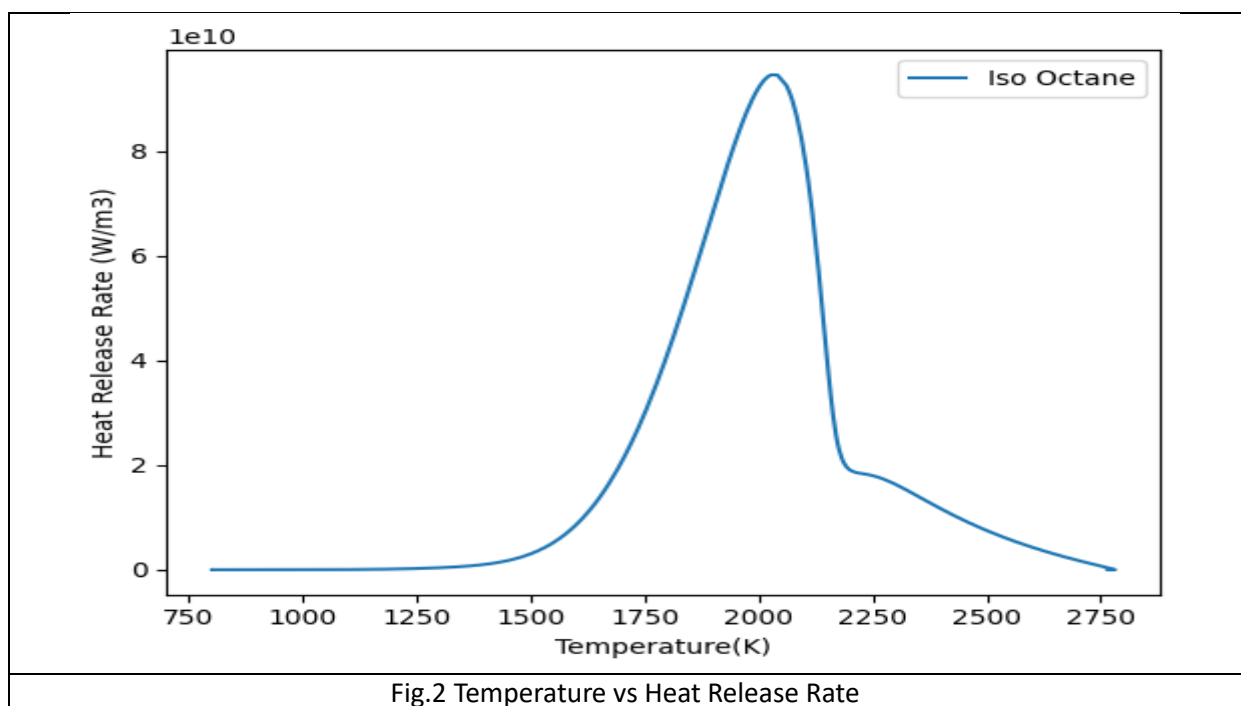
$$\begin{aligned} \frac{d[\text{O}]}{dt} = & k_{10f} [\text{CO}] [\text{O}_2] - k_{10b} [\text{CO}_2] [\text{O}] \\ & - k_{11f} [\text{O}] [\text{H}_2\text{O}] + k_{11b} [\text{OH}]^2 \\ & k_{13f} [\text{H}] [\text{O}_2] - k_{13b} [\text{OH}] [\text{O}] \end{aligned}$$

Question – 3

1. Volume and Surface Calculation:
2. Heat Release :



3. Yes, mixtures ignite and time requires to ignite mixture is 2.84 seconds for Iso-Octane at given condition of Inlet Temperature 800K and Pressure of 1atm.
4. Heat Release vs Temperature:



5. Comparison with lighter fuel methane:

Mixture of Methane and Air will ignite at 143 seconds at 800 Temperature and 1 atm Pressure. Which is quite slow compared to Iso octane as Methane have higher resistance to reactivity which leads to greater ignition delay.

CH₄ is a lighter fuel compared to iso octane which contains less amount of chemical bond energy which can release at time of ignition.

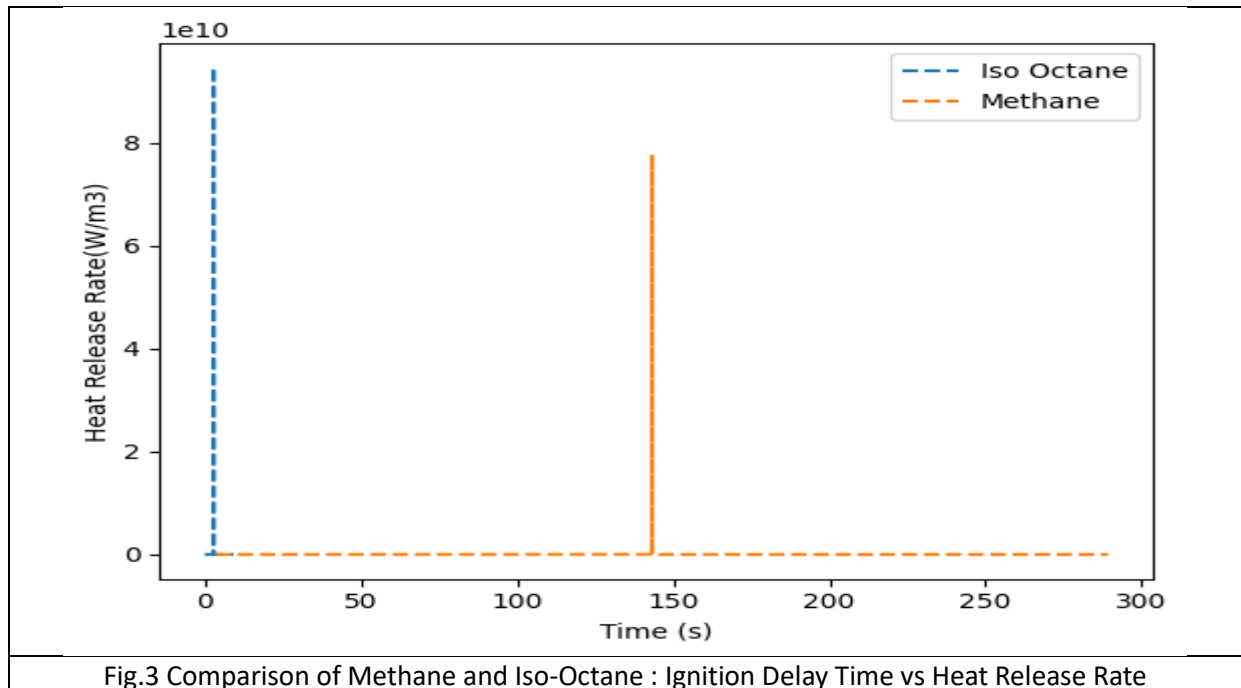


Fig.3 Comparison of Methane and Iso-Octane : Ignition Delay Time vs Heat Release Rate

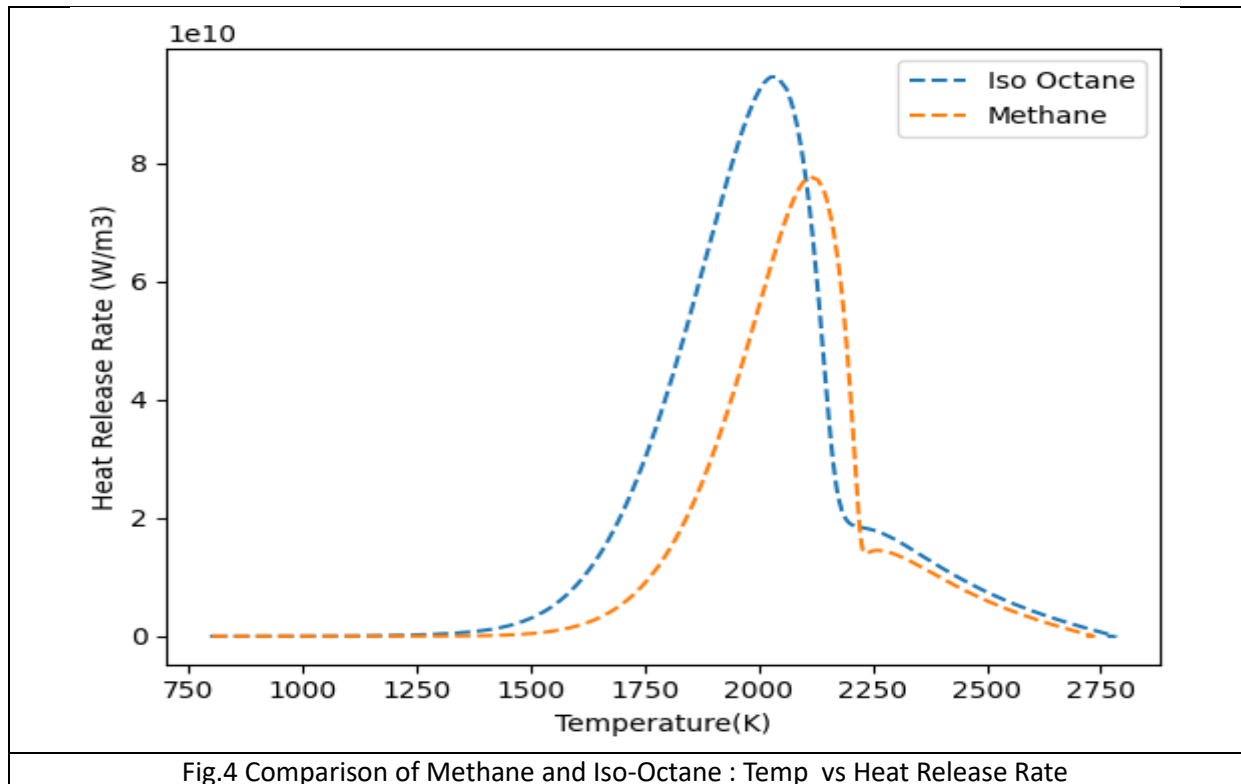
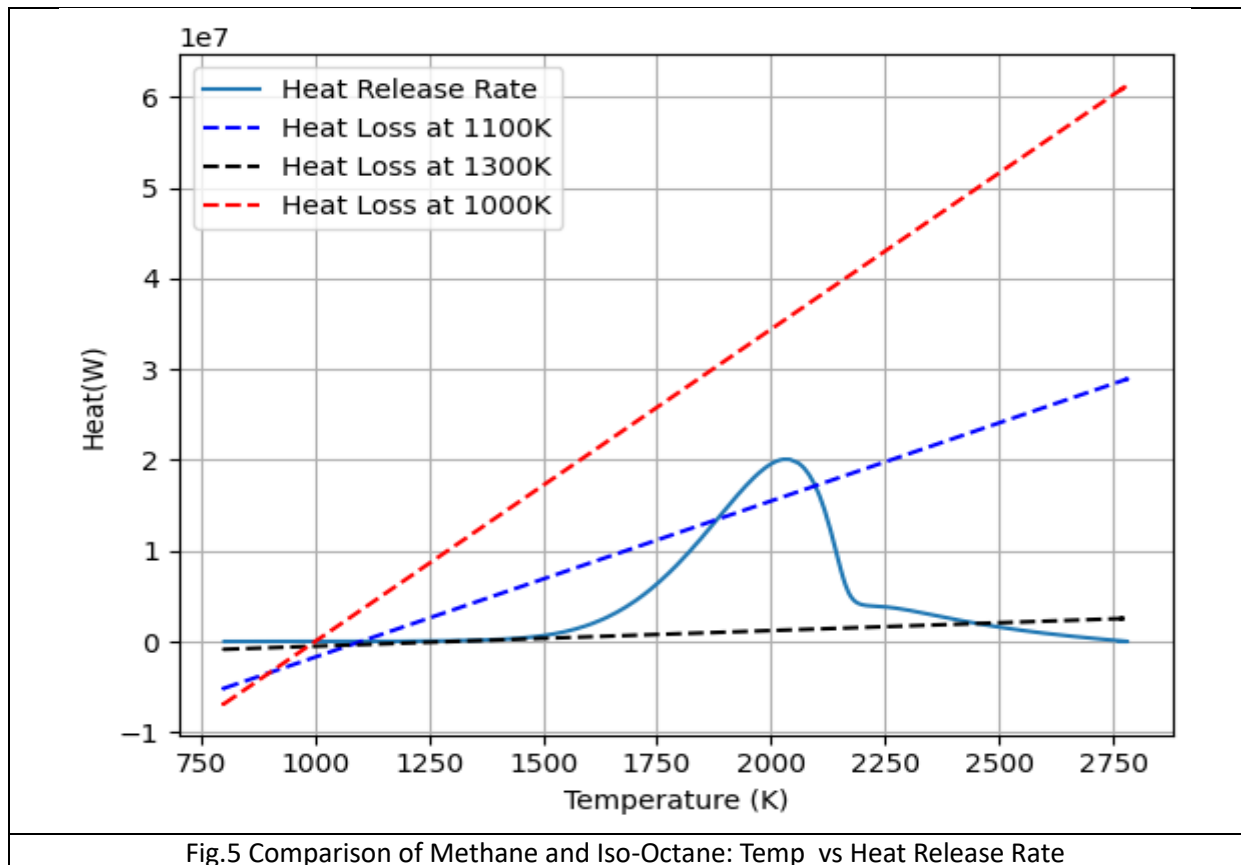


Fig.4 Comparison of Methane and Iso-Octane : Temp vs Heat Release Rate

Semenov Theory

- 6.
7. Plot of Heat release and Heat loss for 3 different conditions:



8. Mixture ignition at different environmental condition:

For $T_{\text{environment}} = 1300 \text{ K}$: Mixture will ignite as heat loss curve is tangent to heat release curve within ignition condition ($T_{\text{en}} - 500$). At this point mixture will ignite as heat release value is greater than heat loss value above critical point. Which leads to possible ignition.

For $T_{\text{environment}} = 1100 \text{ K}$: Mixture will not ignite as heat loss value is higher than heat release value which leads to no ignition.

For $T_{\text{environment}} = 1000 \text{ K}$: Mixture will not ignite as heat loss value is higher than heat release value which leads to no ignition. Also, it will never intersect with heat release curve.

9. As per Semenov theory at 1300 K surrounding temperature ignition will take place as temperature difference is greater than 500K and will continue to ignite. But by defining wall with Cantera with the same surrounding condition doesn't ignite.

10.

S- Curve

11. Increase in pressure and temperature will decrease in ignition delays.

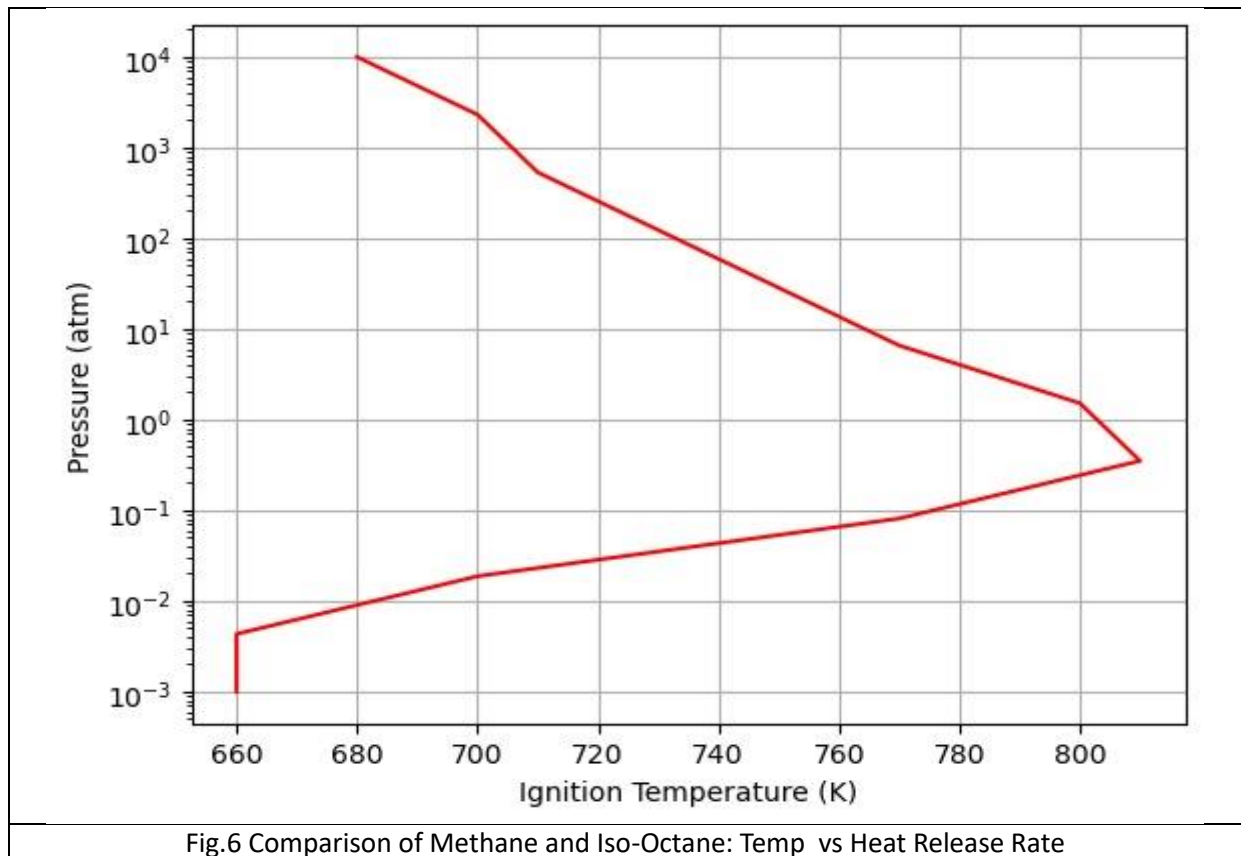
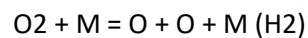
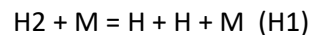
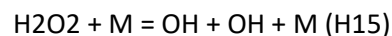
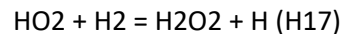
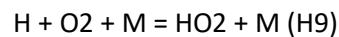


Fig.6 Comparison of Methane and Iso-Octane: Temp vs Heat Release Rate

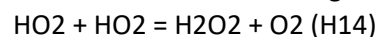
Reactions are at play: Reaction at Initiations



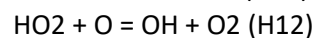
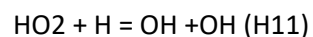
Third body collision will take place once pressure increases.



Reactions between Radicals HO_2 and HO_2 gives H_2O_2 at higher temperature.



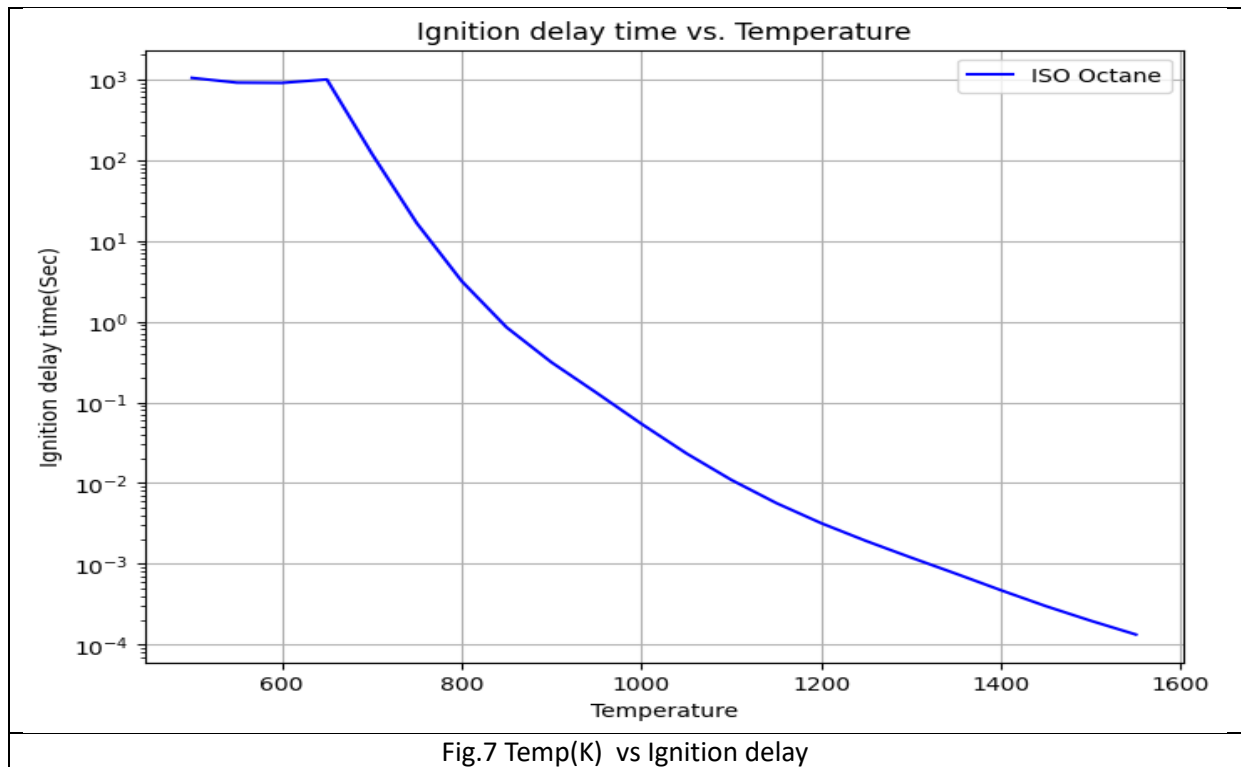
H and O radicals combined and make OH



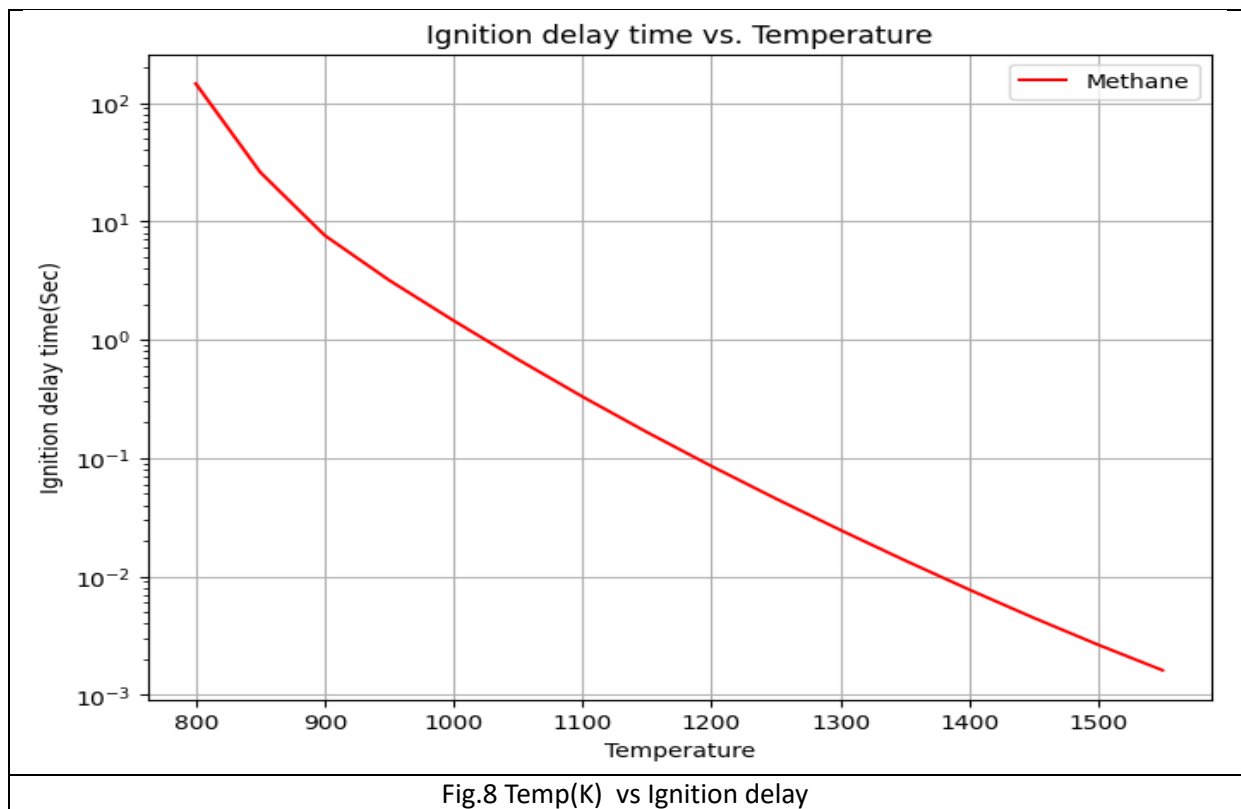
12. Low Pressure ignition involves complex chemical mechanisms including low temperature chemistry and radical formation. This difficulty can make it difficult to capture temperature and pressure. Also at low pressure condition ignition point and extinction point tries to come close as graph unwrapped and doesn't look like S Curve.

Question -4 (Ignition Delays vs Temperature)

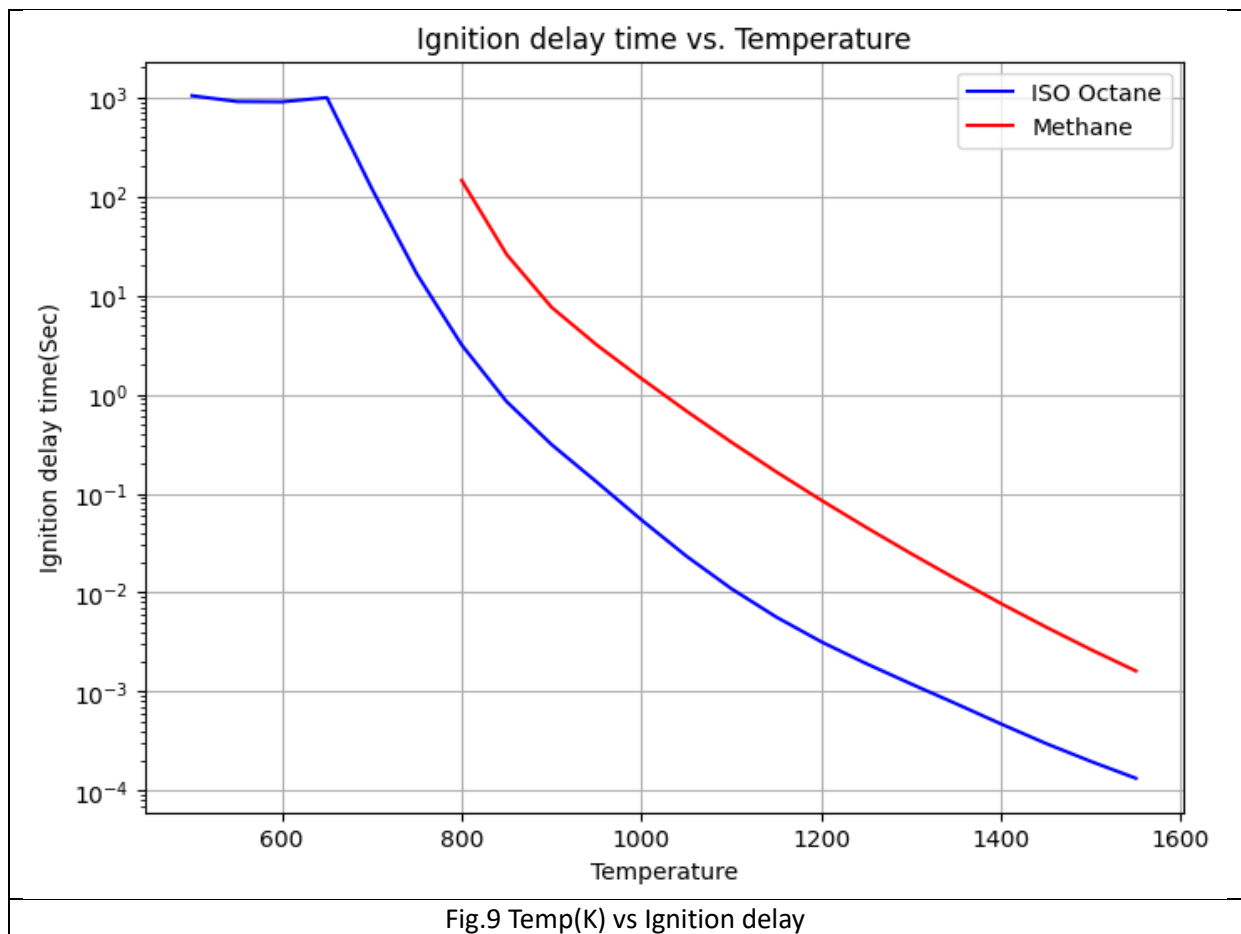
1. For Iso Octane :



2. For Methane:



3. Comment:



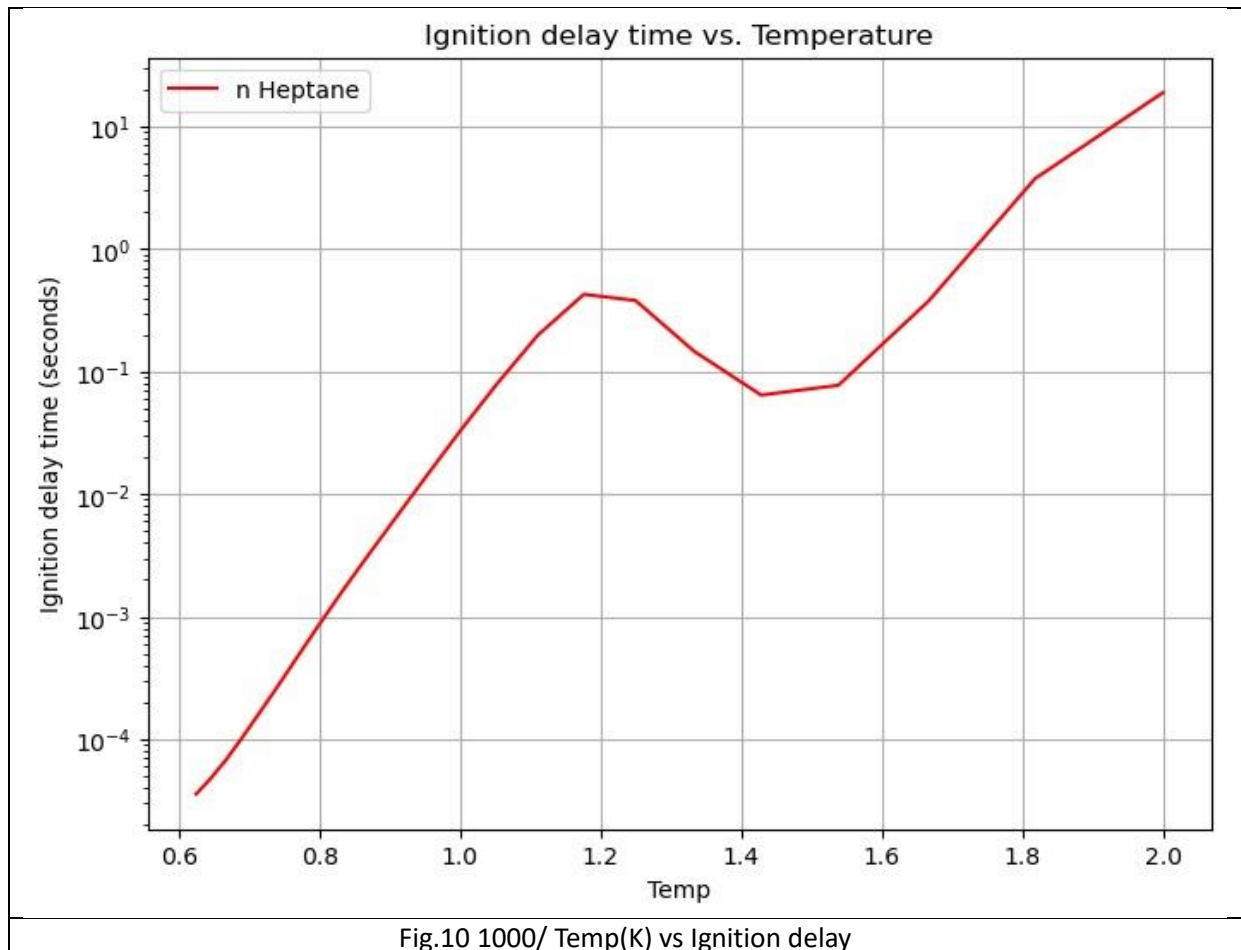
Ignition delays are high in the case of methane compared to iso octane because iso octane gives more free radicals during chain reaction which escalates the process of ignition and leads to lower ignition time. Also, Iso Octane contains a larger amount of chemical bond energy which is released during combustion process.

It is evident from the figures that Methane will not ignite during 500-800K methane will not ignite because autoignition temperature for methane is above 800K.

4. An increase in pressure would result in a decrease in ignition delay. Increase in Pressure results in more chances of collision which results in faster ignition. Also, an increase in pressure results in higher activation energy which affects the ignition delay.

5. N - Heptane :

Negative temperature Co-efficient of fuels is the phenomenon where the ignition delay times initially decrease with increase in temperature and then again increase at higher temperatures. In N-heptane case starts at 833 K. It signifies a balance between low-temperature reactions that promote ignition and high temperature reactions that resist ignition.



Question: 5 (Perfectly Stirred Mixture)

1. Calculation :

$$M_f = \frac{P \times 10^6}{0.42 \times 45 \times 10^6}$$

$$P = 120 \text{ MW}$$

$$M_f = 6.43 \text{ Kg/sec}$$

$$\text{Equivalence Ratio} = \frac{(F/A)_{\text{Actual}}}{(F/A)_{\text{Theory}}}$$

$$\text{Equivalence Ratio} = 0.394$$

2.

Equilibrium flame temperature at above condition is : 1713.78 K

Mole Fraction of CO = $1.973394334 \times 10^{-6}$

Mole Fraction of NO = 0.00231979

3. PSR Combustor:

Equilibrium flame temperature at PSR Condition is: 1719.1

Mole Fraction of CO = $3.7983394334 \times 10^{-6}$

Mole Fraction of NO = $1.113394334 \times 10^{-5}$

4. Residence Time: Residence time to reach steady state is 1.43×10^{-4} for Perfectly stirred reactor.

5. Difference in PSR Concentration and Equilibrium Condition:

PSR gives higher concentration value of CO as it allows mixtures to become homogeneously which eventually rise in Flame Temperature which results in higher CO concentration at the same time increase in temperature reduces NO concentration

6. Difference in PSR Temp and equilibrium Temp:

PSR gives a little higher temperature compared to equilibrium temperature as PSR returns exact temperature in case of perfectly mixed solution inside reactor whereas equilibrium calculates temperature by comparing Heat of Reaction for Products and Reactants.

7. Looping from Power 100MW to 350MW :

Power	Mass Flow Rate (Kg/sec)	Equivalence ratio	Residence Time
100	5.29100529100529	0.33402811180588954	5.15×10^{-4}
150	7.936507936507936	0.5010421677088344	2.87×10^{-5}
200	10.58201058201058	0.6680562236117791	6.22×10^{-6}
250	13.227513227513226	0.8350702795147239	3.45×10^{-6}
300	15.873015873015872	1.0020843354176687	2.57×10^{-6}
350	18.518518518518515	1.1690983913206134	1.98×10^{-6}

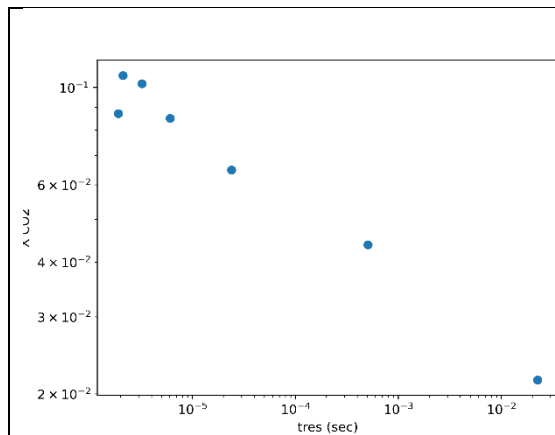


Fig.11 Residence Time vs CO2 Concern

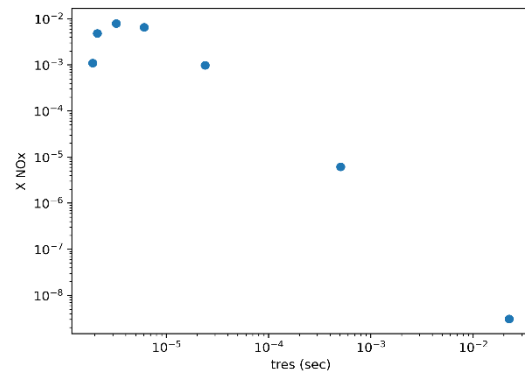
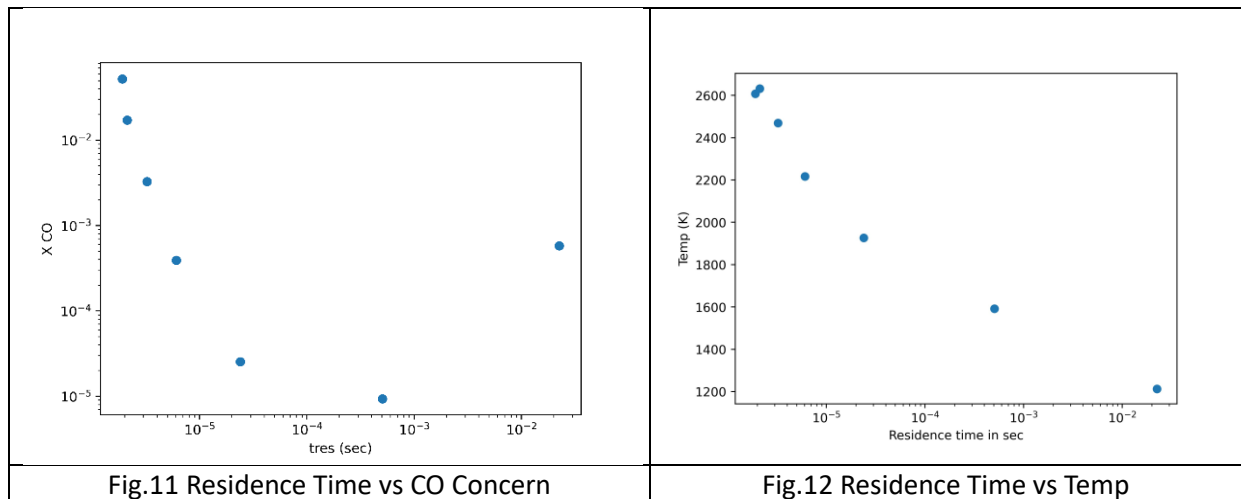


Fig.12 Residence Time vs NO Concern



Bonus Question: Script for PSR

1. Define gas with appropriate Reaction Mechanism.
2. Define Equivalence Ratio.
3. Define gas with initial pressure, temperature, and reactants.
4. Define Combustor Volume.
5. Define Inlet and outlet.
6. Define Mass flow rate in relation to residence time.
7. Define Inlet and Outlet Mass Flow Controller.
8. Give Initial Residence Time.
9. Run a loop with decrease in ignition times until flame distinguished.
10. Extract Values of concentration and equilibrium temperature.