

MECH 652: Dynamics of Combustion

PROJECT ASSIGNMENT #1: COMBUSTION THERMODYNAMICS

Name – Swadesh Suman

McGill ID – 261097252

Part I – Introduction to thermodynamics data

Problem - Write a code to extract the enthalpy (kJ/mol), $h^{\circ}(T)$, and the entropy (kJ/mol-K), $s^{\circ}(T)$, for O₂, N₂, CO₂, H₂O, CO, H₂, NO. Provide, without discussion, these data in a single table with proper units.

Species name	Molecular Weight(g/mol)	Enthalpy (KJ/mol)	Entropy (KJ/mol-K)
O ₂	32	59.201	0.269
N ₂	28	56.136	0.252
CO ₂	44	-302.071	0.309
H ₂ O	18	-168.782	0.265
CO	28	-53.799	0.259
H ₂	2	52.95	0.188
NO	30	149.147	0.273
C	12	752.108	0.198

Table 1 – Enthalpy and Entropy data for different species at 2000 K

Part II – Equilibrium constant

Consider the three following reactions:

- $H_2 + 1/2 O_2 \leftrightarrow H_2O$
- $1/2 N_2 + 1/2 O_2 \leftrightarrow NO$
- $CO + H_2O \leftrightarrow H_2 + CO_2$

Problem 1&2: Calculate the equilibrium constant $K_p(T)$ for temperatures from 300K to 3000K in steps of 100K, and Plot K_p (in log-scale) versus $1000/T$, for the three reactions, on the same graph.

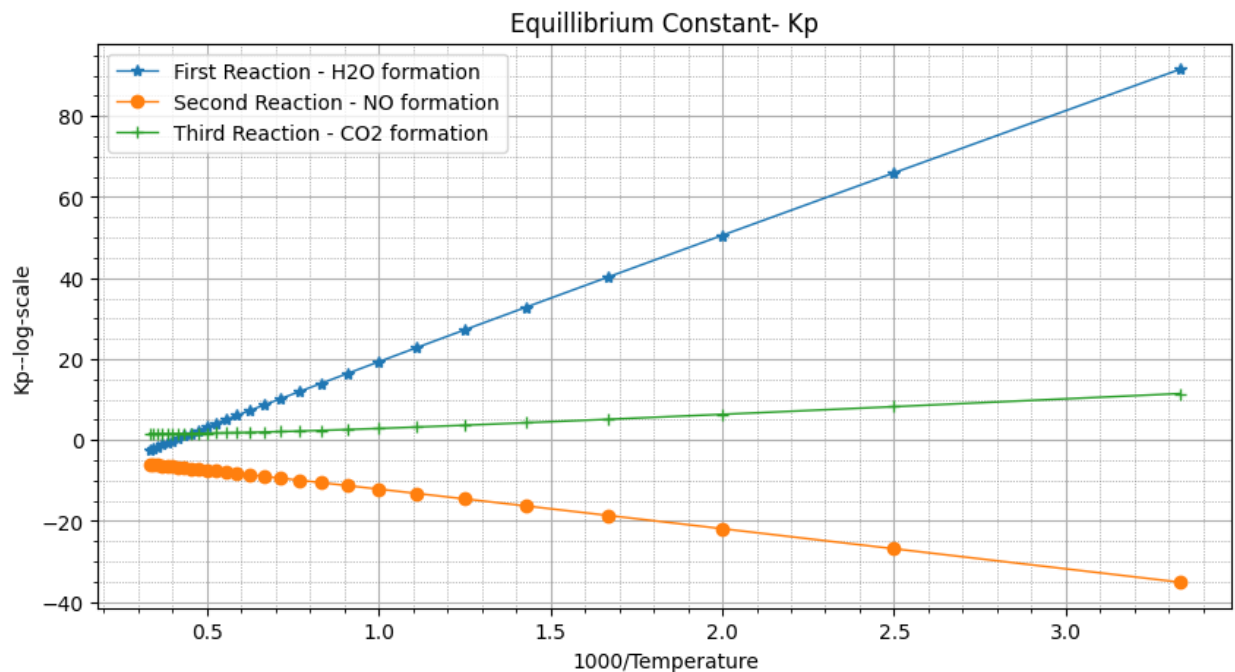


Fig 1 – Equilibrium Constant (K_p) vs $1000/T$ plot

Problem 3: What do the behaviors of the above graph indicate for each reaction?

- First reaction - $H_2 + 1/2 O_2 \leftrightarrow H_2O$
At lower temperatures, the K_p value is extremely positive, which means that the reaction favors the product (H_2O) at equilibrium.
whereas, at higher temperatures close to and beyond 3000 K, the K_p value is slightly negative, which means that as the temperature increases, the reaction favors the reactants at equilibrium.
- Second reaction - $1/2 N_2 + 1/2 O_2 \leftrightarrow NO$
At lower temperatures, the K_p value is negative, which means that the reaction favors the reactants (N_2 & O_2) at equilibrium.

Whereas, at higher temperatures close to 3000 K, the K_p value is slightly negative, which means at this temperature limit, the reaction still favors the reactants at equilibrium, but based on the trend of the graph, it may favor the product (NO) as temperature increases beyond a certain limit.

- Third reaction - $CO + H_2O \leftrightarrow H_2 + CO_2$

At lower temperatures, the K_p value is positive, which means that the reaction favors the product (CO_2) at equilibrium.

Whereas, at higher temperatures close to 3000 K, the K_p value is slightly positive, which means at this temperature limit, the reaction still favors the products at equilibrium, but based on the trend of the graph, it may favor the reactants (CO & H_2O) as temperature increases beyond a certain limit.

Problem 4: Using K_p , calculate X_{NO} for $N_2 + O_2 \leftrightarrow 2NO$, for normal air composition.

For calculating, the X_{NO} at the equilibrium, we know that from K_p definition -

$$K_p = (\chi_{NO}^2 / \chi_{N_2} \chi_{O_2}) * (\frac{P}{P^\circ})^2 \text{ --- (eq. - 0)}$$

As $P = P^\circ$, the pressure term cancels out. So, the eq. 0 can be written as -

$$K_p = (\chi_{NO}^2 / \chi_{N_2} \chi_{O_2}) \text{ --- (eq. - 1)}$$

Since there are three unknown mole fractions, we need three equations. The first equation is eq. 1.

The second equation comes from the conservation of elements before and after the reaction.

$$\frac{\text{No of Nitrogen atoms}}{\text{No of Oxygen Atomes}} = \frac{2\chi_{NO} + \chi_{N_2}}{2\chi_{NO} + \chi_{O_2}} \text{ --- (eq. 2)}$$

The N/O can be expressed as a parameter Z and can take any value based on the initial value of the mixture.

The third equation can be written as the sum of the mole fractions of all elements at equilibrium is equal to 1. i.e., $\sum \chi_i = 1$

$$\chi_{NO} + \chi_{N_2} + \chi_{O_2} = 1 \text{ --- (eq. 3)}$$

Using the above three equations, we get $\chi_{NO} = \frac{\sqrt{K_p}}{2 + \sqrt{K_p}} \text{ --- (eq. 4)}$

Using, the eq. 4, we can get mole fractions of NO at different value of different K_p value.

Temp (K)	300	400	500	600	700	800	900	1000	1100
Ln(K_p)	-35.125	-26.855	-21.904	-18.617	-16.283	-14.542	-13.198	-12.129	-11.2604
X_{NO}	2.78e-16	1.08e-12	1.53e-10	4.1e-09	4.23e-08	2.41e-07	9.27e-07	2.69e-06	6.43e-06

1200	1300	1400	1500	1600	1700	1800	1900	2000	2100
-10.54	-9.935	-9.419	-8.974	-8.587	-8.247	-7.946	-7.679	-7.44	-7.224
1.32e-05	2.42e-05	4.05e-05	6.33e-05	9.32e-05	1.31e-04	1.76e-04	2.31e-04	2.93e-04	3.63e-04

2200	2300	2400	2500	2600	2700	2800	2900	3000
-7.03	-6.853	-6.692	-6.545	-6.41	-6.286	-6.172	-6.065	-5.967
4.42e-04	5.27e-04	6.19e-04	7.17e-04	8.21e-04	9.28e-04	1.04e-03	1.15e-03	1.27e-03

Table 2. $\ln(K_p)$ and Mole fraction NO value at different temperatures

Problem 5 - Plot X_{NO} versus T. Comment.

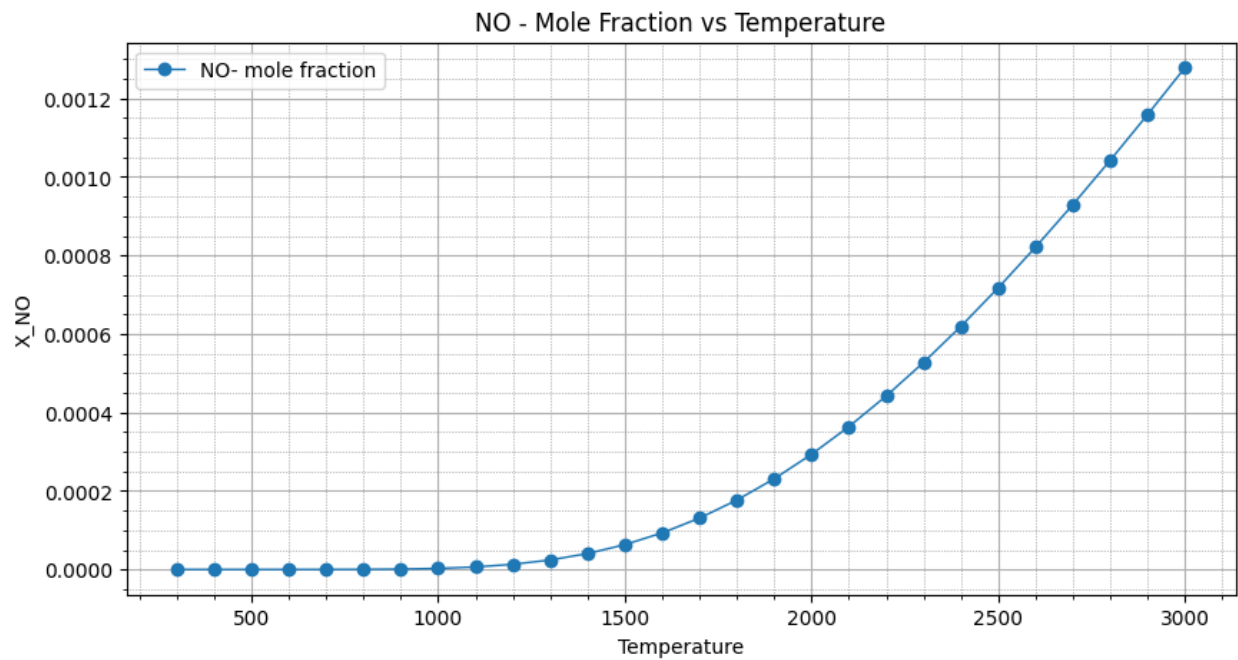


Fig 2 – X_{NO} vs Temperature plot

Fig 2 shows the mole fraction of NO at different temperatures ranging from 300 to 3000 K. As it can be clearly seen in the plot, the mole fraction of NO remains close to 0 till 800-1000 K. It starts increasing from 1000 K and increases with temperature as represented by a straight line in the plot. The highest concentration of NO is at 3000 K which is around 0.00127.

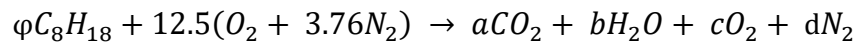
Part III – Incomplete combustion

For the reaction of iso-octane and air at initial temperature and pressure of $T_{in} = 300K$ and $P_{in} = 1atm$:

Problem 1: Write down the global reaction for the stoichiometric, the lean, and the rich conditions, as a function of the equivalence ratio ϕ .

Assumption: - $X_{CO_2} = 9 \cdot X_{CO}$ in the products to write down the global reaction for rich combustion.

Lean Condition:

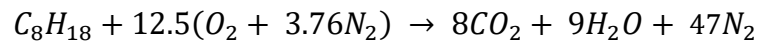


Here,

$$a = 8\phi, b = 9\phi, c = 12.5(1 - \phi), d = 47$$

ϕ – equivalence ratio, which is always less than 1.

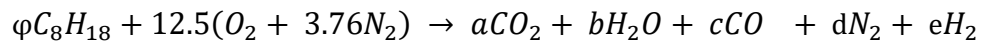
Stoichiometric Condition:



Here,

$$\phi = 1.$$

Rich Condition:



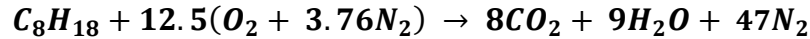
Here,

$$a = 7.2\phi, b = (25 - 15.2\phi), c = 0.8\phi, d = 47, e = (24.2\phi - 25)$$

ϕ – equivalence ratio, which is always greater than 1.

Problem 2: Calculate the lower and higher heating values in kJ/kg C₈H₁₈ (LHV and HHV) – comment and compare to other values in the literature.

For 1 mole of C₈H₁₈, the combustion equation can be written as,



HHV (Higher heating value), is the heat of combustion corresponds to when all of water in the product has condensed to liquid.

LHV (Lower heating value), is the heat of combustion calculated when none of the water is assumed to condense.

We know that, $\Delta H_c = -\Delta H_R = H_{reac} - H_{prod}$

Where, $H_{reac} = \sum N_i \bar{h}_i$ and $H_{prod} = \sum N_i \bar{h}_i$

$$\Delta H_{c,H_2O(l)} = \mathbf{HHV} = (1)\bar{h}^\circ_{f,C_8H_{18}} - [8\bar{h}^\circ_{f,CO_2} + 9\bar{h}^\circ_{f,H_2O(l)}] \text{ ---(eq. 1)}$$

$$\Delta H_{c,H_2O(g)} = \mathbf{LHV} = (1)\bar{h}^\circ_{f,C_8H_{18}} - [8\bar{h}^\circ_{f,CO_2} + 9\bar{h}^\circ_{f,H_2O(g)}] \text{ --- (eq. 2)}$$

To find, the enthalpy of formation for H₂O liquid, we can use enthalpy of formation of gaseous water, and enthalpy of vaporization \bar{h}_{fg} .

$$\bar{h}^\circ_{f,H_2O(l)} = \bar{h}^\circ_{f,H_2O(g)} - \bar{h}_{fg} \text{ --- (eq. 3)}$$

Where, $\bar{h}_{fg} = 44,010$ KJ/Kmol. (from Stephen Turns – An Introduction to Combustion Concepts and Applications, Appendix A, Table A.6).

Other data has been calculated by using ThermoPropertiesNASA using class Thermo.

Using the above three equations, we get $\Delta H_{c,H_2O(l)}$ (HHV) , $\Delta H_{c,H_2O(g)}$ (LHV) in KJ.

$$\Delta H_{c,H_2O(l)} = 5,495,803 \text{ KJ}$$

$$\Delta H_{c,H_2O(g)} = 5,099,713 \text{ KJ}$$

As 1 Kmole of C₈H₁₈ is present in the reaction, The same value can be written as KJ/Kmol of C₈H₁₈.

For finding, in terms of KJ/Kg of C₈H₁₈, we will divide the above values by Molecular weight of C₈H₁₈—114.232 Kg/Kmol.

$$\Delta h_c = HHV = \frac{\Delta H_{c,H_2O(l)}}{MW_{C_8H_{18}}} = \frac{5,495,803 \text{ kJ}}{114.232} = 47845 \frac{\text{KJ}}{\text{Kg } C_8H_{18}}$$

$$\Delta h_c = LHV = \frac{\Delta H_{c,H_2O(g)}}{MW_{C_8H_{18}}} = \frac{5,099,713 \text{ kJ}}{114.232} = 44371 \frac{\text{KJ}}{\text{Kg } C_8H_{18}}$$

Comparison with the literature –

In the course slides, (In Table A-27) –

HHV of C₈H₁₈ – 47870 KJ/Kg

LHV of C₈H₁₈ – 44430 KJ/Kg

Problem 3: Calculate the adiabatic temperature T_{ad} , estimation for ϕ ranging from 0.5 to 1.5, in step of 0.05, by assuming constant C_p for the reactants and products $C_p = 3.5R$, with $R = 8314.4621$ J/kmol/K. Indicate the maximum temperature, and for which equivalence ratio.

Temp (K)	0.5	0.55	0.6	0.65	0.7	0.75	0.8	0.85	0.9
$T_{ad,estimation}(K)$	1719.05	1855.29	1990.55	2124.83	2258.14	2390.5	2521.91	2652.4	2781.95

0.95	1	1.05	1.1	1.15	1.2	1.25	1.3	1.35	1.4
2910.6	3038.34	2993.98	2934.41	2876.31	2819.63	2764.31	2710.3	2657.57	2606.07

1.45	1.5
2555.75	2506.57

The maximum temperature is 3038 K, at equivalence ratio 1.

Problem 4: Compute the adiabatic temperature T_{ad} , integration for ϕ ranging from 0.5 to 1.5, in step of 0.05 by iterating the integration of $C_{pi}(T)$. Indicate the maximum temperature, and for which equivalence ratio.

Temp (K)	0.5	0.55	0.6	0.65	0.7	0.75	0.8	0.85	0.9
$T_{ad,integration}(K)$	1497.5	1602.5	1702.5	1797.5	1892.5	1982.5	2072.5	2157.5	2242.5

0.95	1	1.05	1.1	1.15	1.2	1.25	1.3	1.35	1.4
2322.5	2387.5	2357.5	2317.5	2282.5	2245	2207.5	2172.5	2137.5	2102.5

1.45	1.5
2070.5	2035

The maximum temperature is 2387.5 K, at equivalence ratio 1.

Problem 5: Plot the result T_{ad} vs. ϕ for both question 3 and 4 on the same graph.

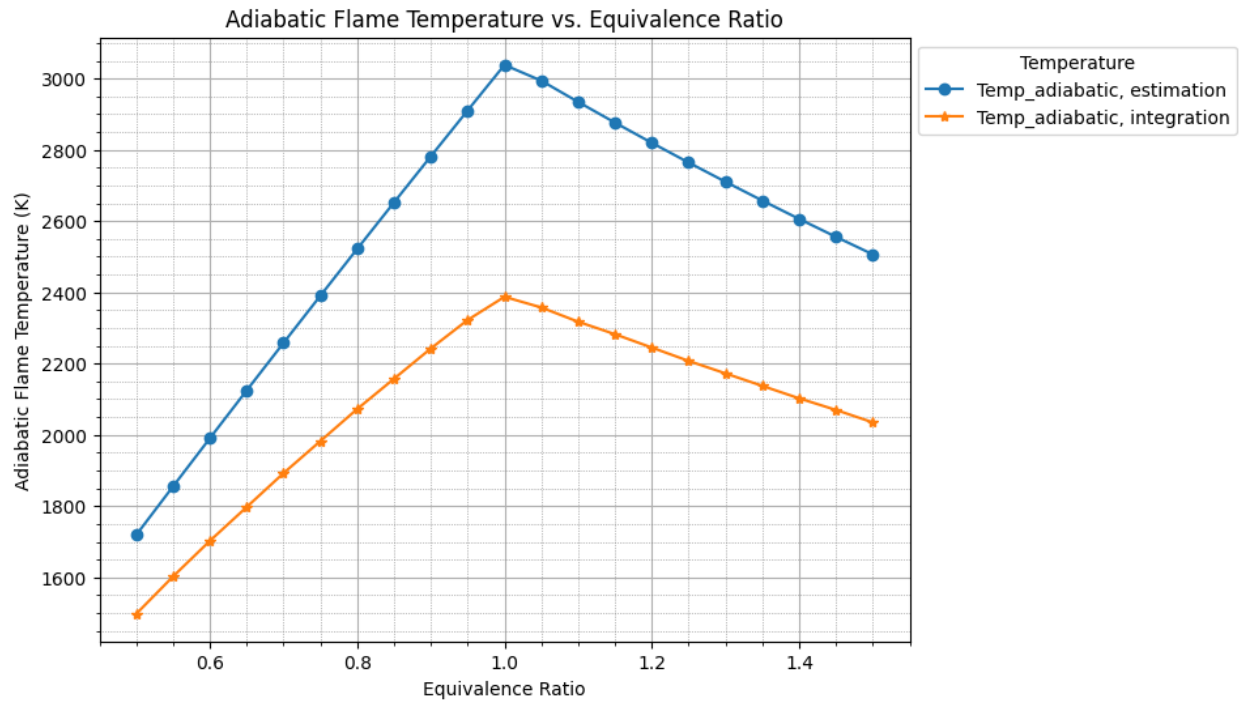


Fig 3 – Temperature adiabatic (estimation, integration) vs Equivalence ratio plot

Problem 6: Compare and explain the results.

For the calculation of T adiabatic estimation – the main assumption is the constant $C_p = 3.5 \cdot R_u$, which underpredicts the C_p of the species at different temperatures and therefore the T adiabatic obtained using this C_p is higher.

For the calculation of T adiabatic integration, NASA Glenn coefficients were used to calculate the enthalpy of products at different temperatures, which accurately predicts the C_p and enthalpy of the species at the temp range of 300 to 5000 K. Therefore, we get relatively higher enthalpy of products. And hence the lower T adiabatic.

Part IV – Chemical equilibrium using Cantera

For the reaction of iso-octane and air1 at initial temperature and pressure of $T_{in} = 300K$ and $P_{in} = 1atm$:

Problem 1: Calculate and plot T_{ad} , equilibrium for ϕ ranging from 0.5 to 2 in steps of 0.05.

Temp (K)	0.5	0.55	0.6	0.65	0.7	0.75	0.8	0.85	0.9
$T_{ad, integration}(K)$	1511.34	1609.69	1704.82	1796.72	1885.17	1969.68	2049.31	2122.5	2186.82

0.95	1	1.05	1.1	1.15	1.2	1.25	1.3	1.35	1.4
2238.78	2273.56	2285.63	2273.85	2245.77	2210.24	2171.95	2132.87	2093.8	2055.07

1.45	1.5	1.55	1.6	1.65	1.7	1.75	1.8	1.85
2016.83	1979.15	1942.04	1905.49	1869.51	1834.06	1799.14	1764.72	1730.78

1.9	1.95	2
1697.32	1664.3	1631.73

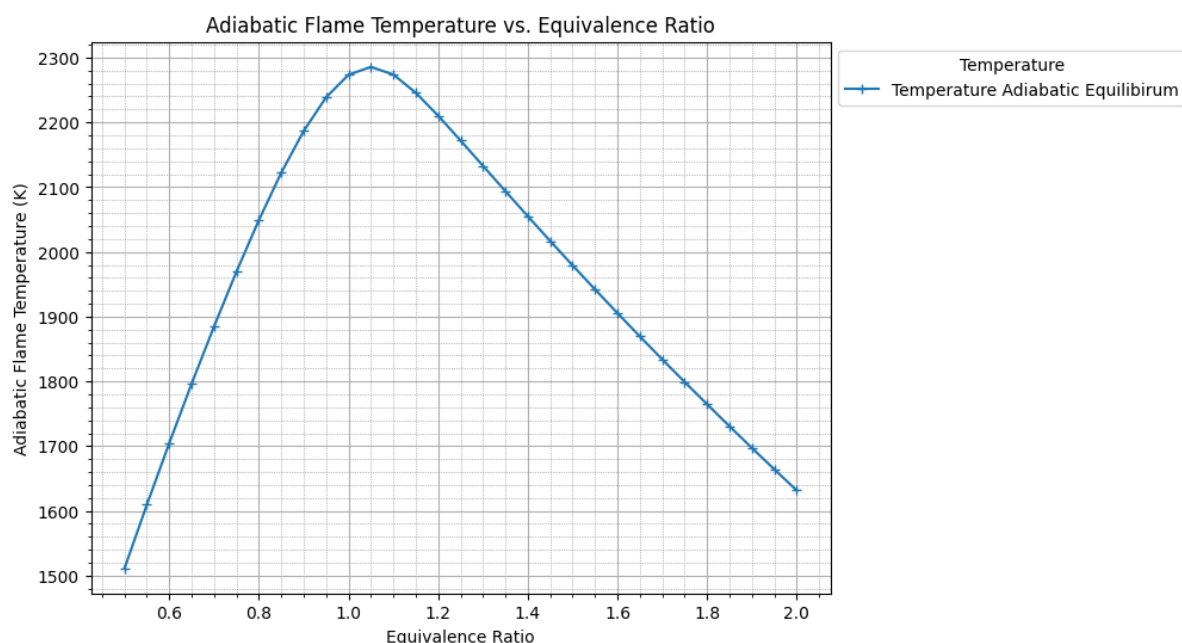


Fig 4 – Temperature adiabatic equilibrium vs Equivalence ratio plot

Problem 2: Indicate the maximum temperature and at which equivalence ratio it occurs, explain.

The maximum temperature is 2285.63 K and it occurs at equivalence ratio of 1.05.

The adiabatic flame temperature (T_{ad} , equilibrium) is highest at an equivalence ratio of 1.05, it indicates that the combustion process is most efficient at this fuel-to-air ratio. At an equivalence ratio of 1.05, we are slightly on the fuel-rich side, which means there is a bit more fuel than the ideal stoichiometric ratio. However, this slight deviation from stoichiometry may be not so significant enough to cause a substantial decrease in combustion efficiency or flame temperature. Therefore, we observe the highest adiabatic flame temperature at $\phi = 1.05$.

Problem 3: Compare $T_{ad, equilibrium}$, $T_{ad, estimation}$, and $T_{ad, integration}$.

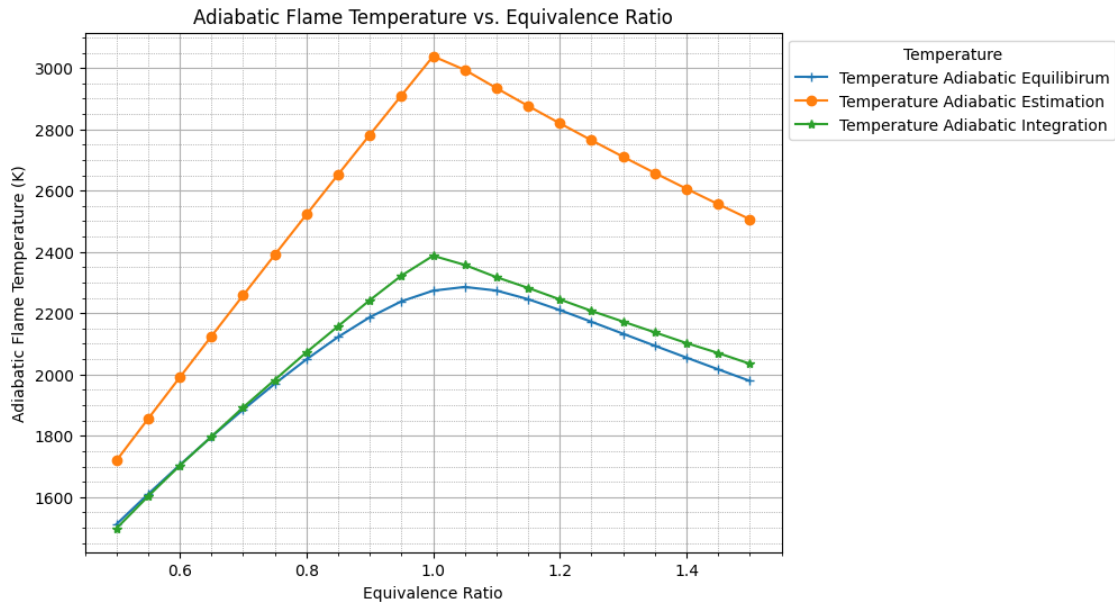


Fig 5 – Temperature adiabatic (equilibrium, estimation, integration) vs Equivalence ratio plot

Bonus Question – Repeating parameters from question IV.1, calculate and plot T_{ad} vs. ϕ for hydrogen (H_2) combustion. Compare and explain the difference in temperature.

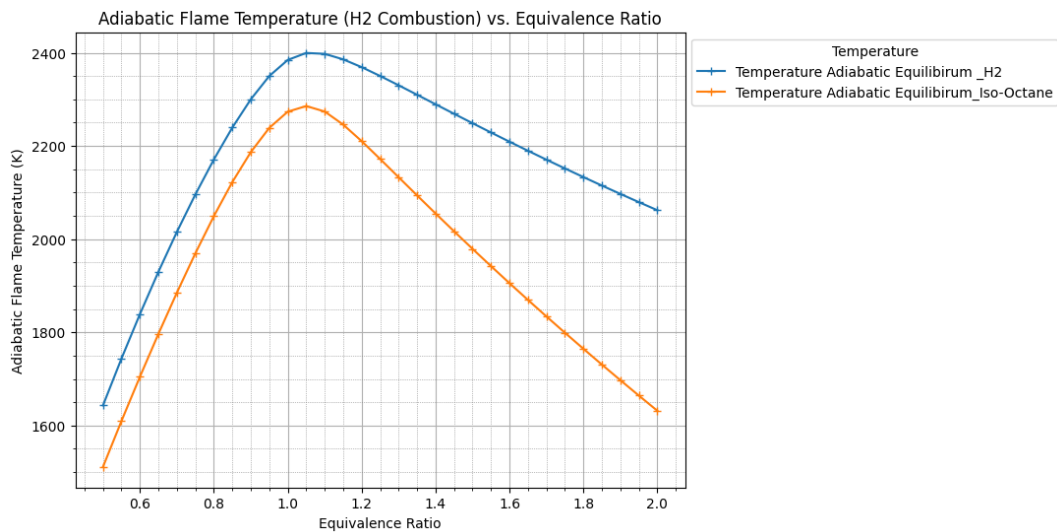


Fig 6 – Temperature adiabatic (equilibrium) for H_2 and Iso-Octane vs Equivalence ratio plot

The highest temperature in H_2 combustion case is 2399 K, at 1.05 equivalence ratio.

Hydrogen has higher heat of combustion as compared to Iso-Octane, so the amount of heat released per Kg of the fuel is higher than Iso-octane. Therefore, the adiabatic flame temperature of H_2 is higher than Iso-octane. Moreover, Hydrogen, being a diatomic molecule, has much lower specific heat capacity than iso-octane, this means Hydrogen can heat-up to higher temperature during combustion.

Part V – Parameters affecting T adiabatic

For the reaction of iso-octane and air, and using results from Part IV as a reference case:

For the species: [O,CO,CO₂,H₂,H₂O,H,OH,NO]

Problem 1 & 4: Keeping $P_{in} = 1\text{atm}$ and $T_{in} = 300\text{K}$ constant, compute T_{ad} and the equilibrium composition of the specified species for ϕ ranging from 0.5 to 2 in steps of 0.05. Plot the effect of equivalence ratio on T_{ad} and the equilibrium composition of the specified species.

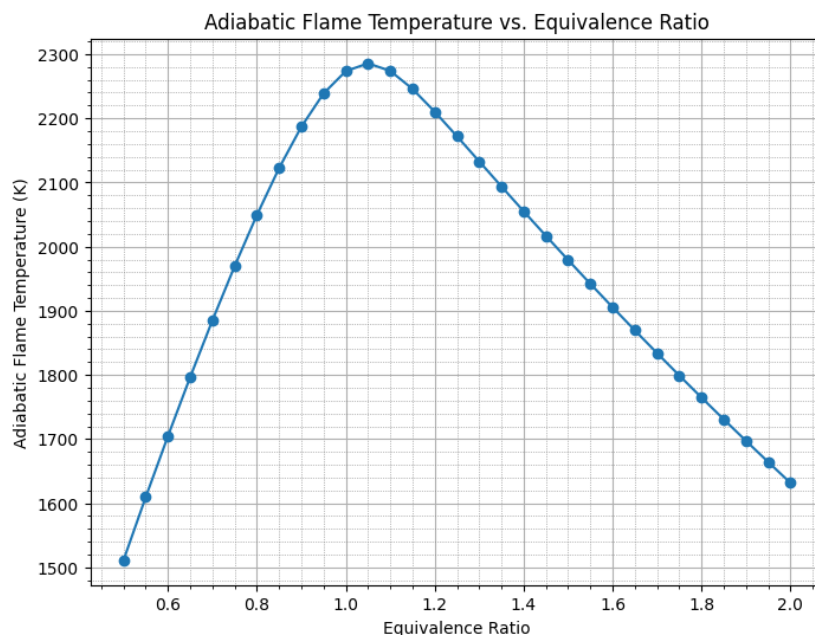


Fig 7 – Temperature adiabatic (equilibrium) vs Equivalence ratio plot

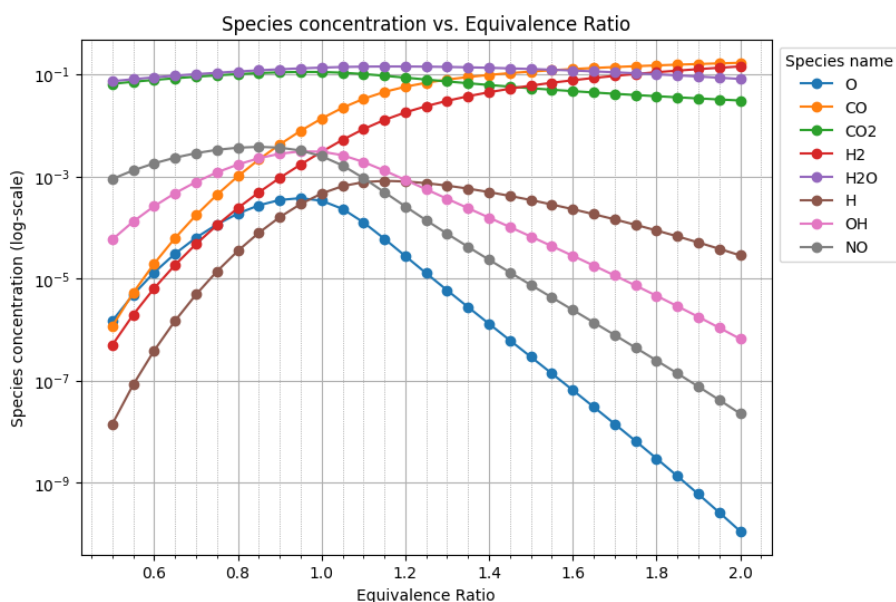


Fig. 8 – Species Concentration (Mole fraction) in log-scale vs Equivalence ratio plot

Problem 2 & 4: Keeping $\phi = 1$ and $T_{in} = 300K$ constant, compute T_{ad} and the equilibrium composition of the specified species for pressures ranging from 1 to 36atm in steps of 5atm. Plot the effect of pressure on T_{ad} and the equilibrium composition of the specified species.

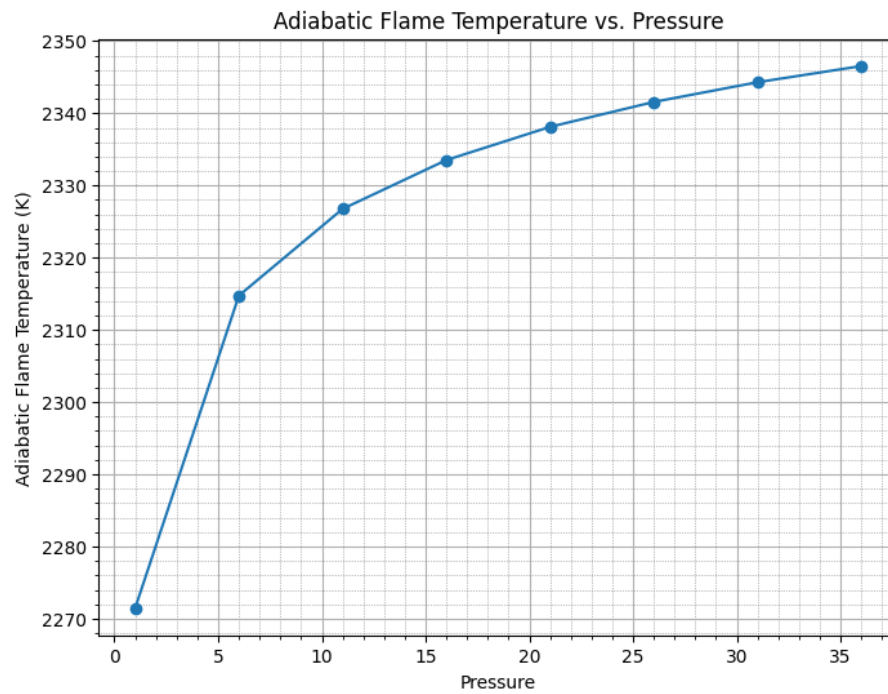


Fig 9 – Temperature adiabatic (equilibrium) vs Pressure plot

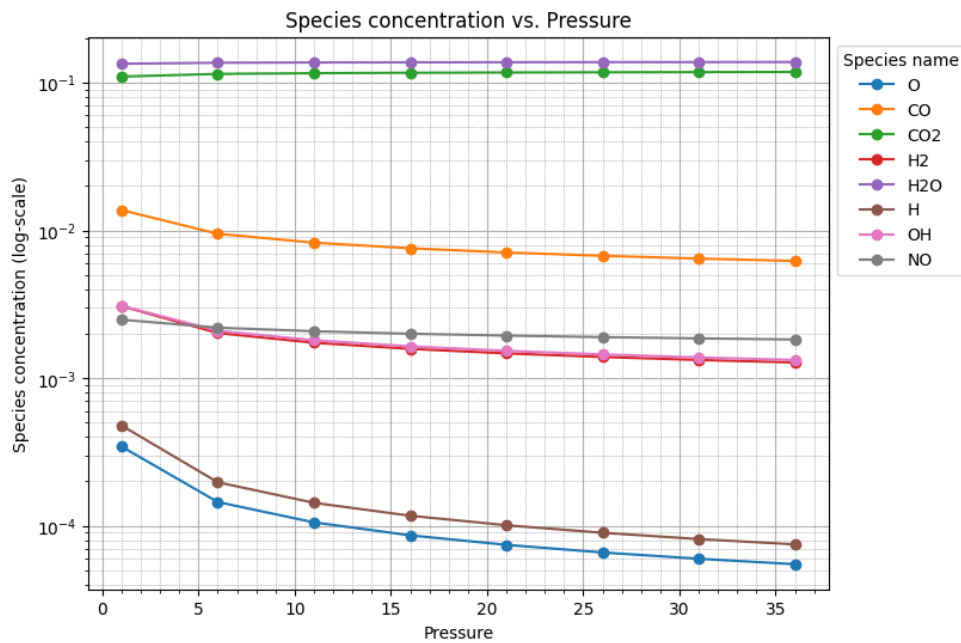


Fig. 10 – Species Concentration (Mole fraction) in log-scale vs Pressure plot

Problem 3 & 4: Keeping $\phi = 1$ and $P_{in} = 1\text{atm}$ constant, find T_{ad} and the equilibrium composition of the specified species for initial temperatures ranging from 300K to 900K in increments of 100K. Plot the effect of initial temperature on T_{ad} and the equilibrium composition of the specified species.

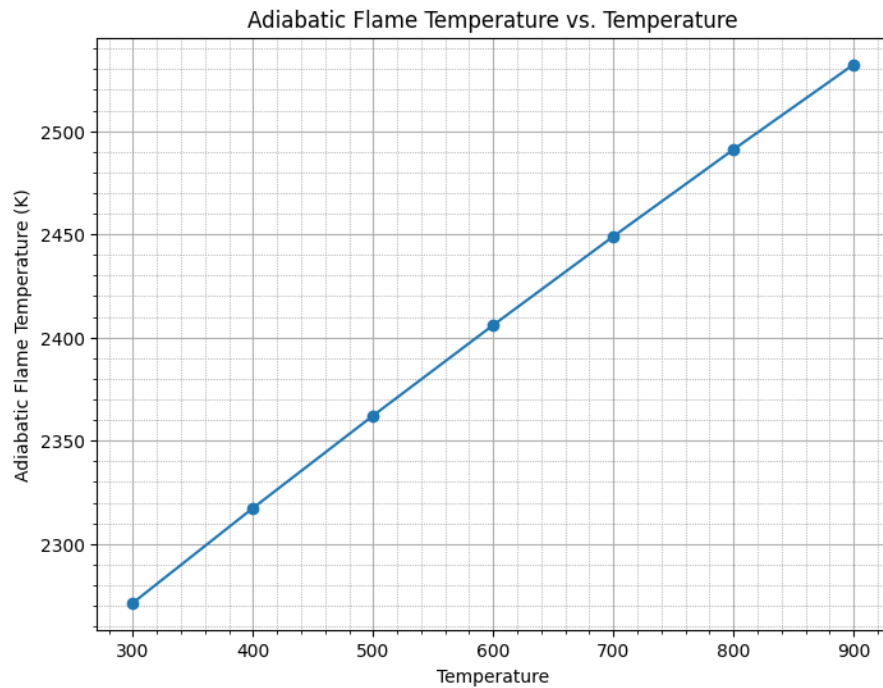


Fig 11 – Temperature adiabatic (equilibrium) vs Initial Temperature plot

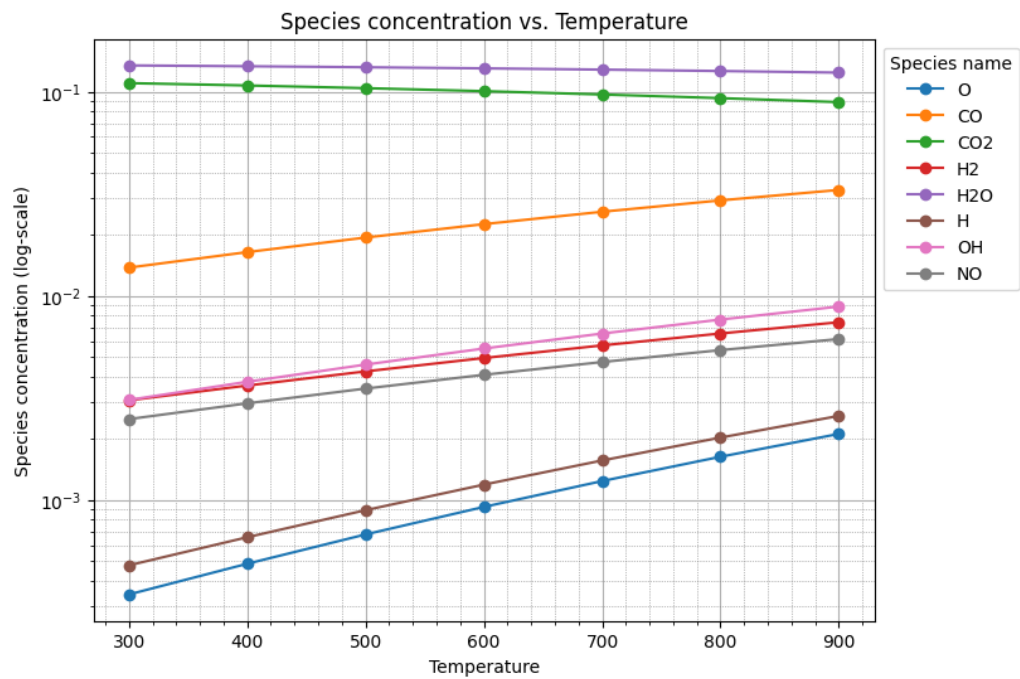


Fig. 12 – Species Concentration (Mole fraction) in log-scale vs Initial temperature plot

Problem 5: Comment on the effect of the initial temperature, pressure, and equivalence ratio on T_{ad} and the equilibrium composition.

Effect of Equivalence ratio on T_{ad} and the equilibrium composition –

Temperature Adiabatic Equilibrium = as ϕ increases from 0.5 to 2, T_{ad} increases from $\phi = 0.5$ ($T_{ad} = 1511.34$ K) to $\phi = 1.05$ ($T_{ad} = 2285.63$ K) and then decreases till $\phi = 2$ ($T_{ad} = 1631.73$ K).

Mole_fraction_O = as ϕ increases from 0.5 to 2, X_O increases from $\phi = 0.5$ ($X_O = 1.48E-6$) to $\phi = 0.95$ ($X_O = 3.73E-4$) and then decreases till $\phi = 2$ ($X_O = 1.12E-10$).

Mole_fraction_CO = as ϕ increases from 0.5 to 2, X_{CO} increases from $\phi = 0.5$ ($X_{CO} = 1.165E-6$) to $\phi = 2$ ($X_{CO} = 1.67E-1$).

Mole_fraction_CO2 = as ϕ increases from 0.5 to 2, X_{CO2} increases from $\phi = 0.5$ ($X_{CO2} = 0.0647$) to $\phi = 0.95$ ($X_{CO2} = 0.1106$) and then decreases till $\phi = 2$ ($X_{CO2} = 0.03049$).

Mole_fraction_H2 = as ϕ increases from 0.5 to 2, X_{H2} increases from $\phi = 0.5$ ($X_{H2} = 5.0011E-7$) to $\phi = 2$ ($X_{CO} = 1.415E-1$).

Mole_fraction_H2O = as ϕ increases from 0.5 to 2, X_{H2O} increases from $\phi = 0.5$ ($X_{H2O} = 0.0728$) to $\phi = 1.15$ ($X_{H2O} = 0.1415$) and then decreases till $\phi = 2$ ($X_{H2O} = 0.0806$).

Mole_fraction_H = as ϕ increases from 0.5 to 2, X_H increases from $\phi = 0.5$ ($X_H = 1.41E-8$) to $\phi = 1.15$ ($X_H = 8.138E-4$) and then decreases till $\phi = 2$ ($X_H = 2.827E-5$).

Mole_fraction_OH = as ϕ increases from 0.5 to 2, X_{OH} increases from $\phi = 0.5$ ($X_{OH} = 5.798E-8$) to $\phi = 0.95$ ($X_{OH} = 3.079E-3$) and then decreases till $\phi = 2$ ($X_{OH} = 6.55E-7$).

Mole_fraction_NO = as ϕ increases from 0.5 to 2, X_{NO} increases from $\phi = 0.5$ ($X_{NO} = 8.888E-4$) to $\phi = 0.85$ ($X_{NO} = 3.774E-3$) and then decreases till $\phi = 2$ ($X_{NO} = 2.259E-8$).

Effect of Pressure on T_{ad} and the equilibrium composition –

Temperature Adiabatic Equilibrium = as pressure increases from 1 to 36 atm, T_{ad} increases from $T_{ad} = 2271.47$ K at ($p=1$) to $T_{ad} = 2346.54$ K (at $p = 36$ atm).

Mole_fraction_O = as pressure increases from 1 to 36 atm, X_O decreases from $p = 1$ atm ($X_O = 3.4409E-4$) till $p = 36$ atm ($X_O = 5.499E-5$).

Mole_fraction_CO = as pressure increases from 1 to 36 atm, X_{CO} decreases from $p = 1$ atm ($X_{CO} = 0.01373$) till $p = 36$ atm ($X_{CO} = 0.00621$).

Mole_fraction_CO2 = as pressure increases from 1 to 36 atm X_{CO2} increases from $p = 1$ atm ($X_{CO2} = 0.11$) till $p = 36$ atm ($X_{CO2} = 0.1182$).

Mole_fraction_H2 = as pressure increases from 1 to 36 atm, X_{H2} decreases from $p = 1$ atm ($X_{H2} = 0.00307$) till $p = 36$ atm ($X_{H2} = 0.00127$).

Mole_fraction_H2O = as pressure increases from 1 to 36 atm X_{H2O} increases from $p = 1$ atm ($X_{H2O} = 0.1344$) till $p = 36$ atm ($X_{H2O} = 0.13806$).

Mole_fraction_H = as pressure increases from 1 to 36 atm, X_H decreases from $p = 1$ atm ($X_H = 4.778E-4$) till $p = 36$ atm ($X_H = 7.487E-4$).

Mole_fraction_OH = as pressure increases from 1 to 36 atm, X_{OH} decreases from $p = 1$ atm ($X_{OH} = 0.00308$) till $p = 36$ atm ($X_{OH} = 0.00132$).

Mole_fraction_NO = as pressure increases from 1 to 36 atm, X_{NO} decreases from $p = 1$ atm ($X_{NO} = 0.00248$) till $p = 36$ atm ($X_{NO} = 0.00182$).

Effect of Initial Temperature on T_{ad} and the equilibrium composition –

Temperature Adiabatic Equilibrium = as initial temperature increases from 300 to 900 K, T_{ad} increases from 2271.47 K to 2532.23 K, respectively.

Mole_fraction_O = as initial temperature increases from 300 to 900 K, X_O increases from 0.000344 to 0.002104, respectively.

Mole_fraction_CO = as initial temperature increases from 300 to 900 K, X_{CO} increases from 0.01373 to 0.03298, respectively.

Mole_fraction_CO2 = as initial temperature increases from 300 to 900 K, X_{CO2} decreases from 0.11005 to 0.08883, respectively.

Mole_fraction_H2 = as initial temperature increases from 300 to 900 K, X_{H2} increases from 0.00307 to 0.00741, respectively.

Mole_fraction_H2O = as initial temperature increases from 300 to 900 K, X_{H2O} decreases from 0.134402 to 0.12392, respectively.

Mole_fraction_H = as initial temperature increases from 300 to 900 K, X_H increases from 0.000477 to 0.002578, respectively.

Mole_fraction_OH = as initial temperature increases from 300 to 900 K, X_{OH} increases from 0.00308 to 0.00885, respectively.

Mole_fraction_NO = as initial temperature increases from 300 to 900 K, X_{NO} increases from 0.002486 to 0.006135, respectively.

Part VI - Effect of dilution on T_{ad} - Exhaust Gas Recirculation (EGR)

In practice, the exhaust gas (which is mainly composed of CO_2) is recirculated back to the engine to control the temperature and stabilize the flame. EGR is a feature of advanced low-emission gas turbine engines. In this section, we will simulate EGR through Cantera by using dilution:

For the reaction of iso-octane and air:

Problem 1: For fixed values of $\phi = 0.9$, $P_{in} = 30\text{atm}$, and $T_{in} = 800\text{K}$, vary the mole fraction of CO_2 in the reactant mixture from 0 to 0.95, in steps of 0.05. Compute and plot T_{ad} and X_{NO} , X_{NO_2} , X_{CO} , and X_{CO_2} . How and why are these parameters affected by increasing dilution of CO_2 ? What would happen if we were to increase CO_2 dilution to 100%?

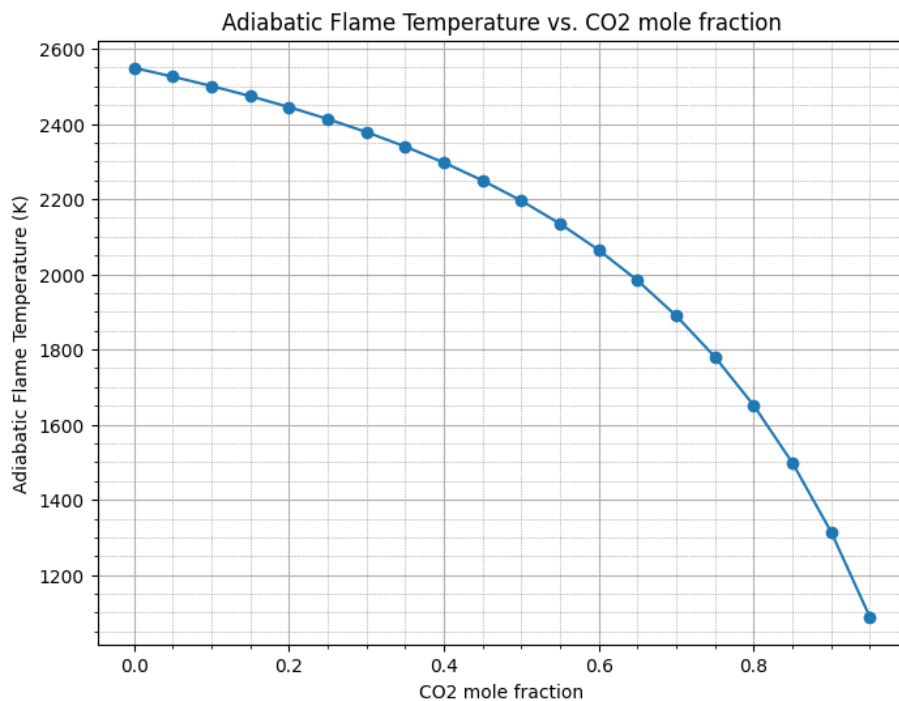


Fig. 13 – Adiabatic Flame Temperature vs CO_2 mole fraction plot

Temperature Adiabatic Equilibrium = as the mole fraction of CO_2 in the reactant increases from 0 to 0.95, T_{ad} decreases from 2548.79 K to 1088.63 K, respectively.

- This is primarily due to the dilution effect. It occupies the space in the reaction mixture, thus bringing down the rate of forward reaction and hence the less adiabatic temperature.
- CO_2 being the product of combustion, adding CO_2 in the reactant side forces the reaction equilibrium position towards the reactant side according to Le Chatelier's principle. And therefore, the adiabatic equilibrium temperature reduces.
- Being a triatomic molecule, the specific heat capacity of CO_2 is higher than other reactants like O_2 and N_2 . Hence, it can absorb more heat compared to O_2 & N_2 for the same temperature change, thus preventing the increase in temperature.

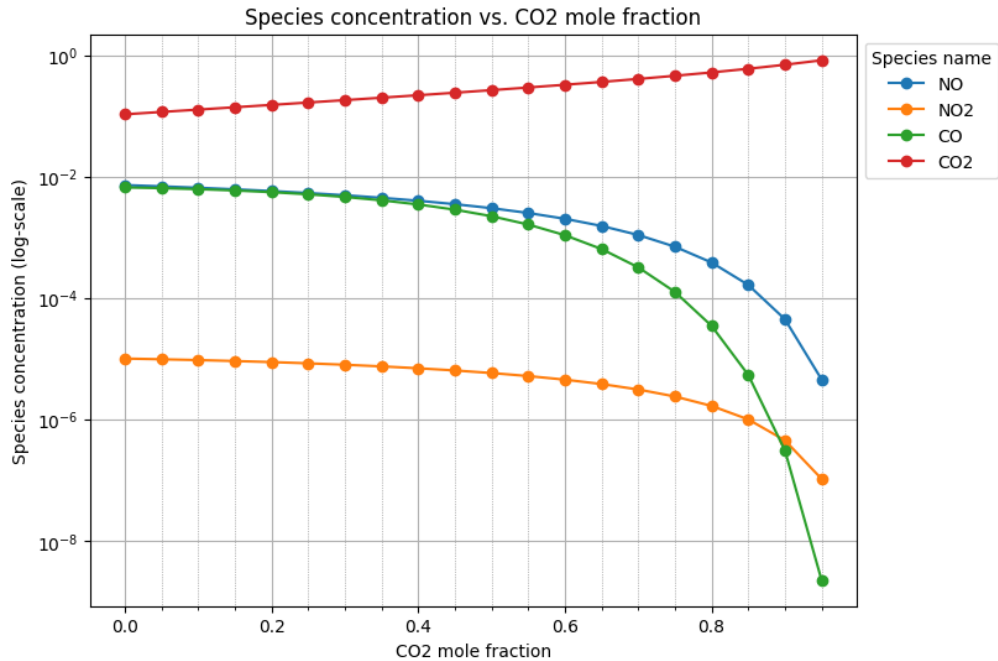


Fig. 14 – Species Concentration vs CO2 mole fraction plot

Mole_fraction_NO = as the mole fraction of CO2 in the reactant increases from 0 to 0.95, X_{NO} decreases from $7.25E-3$ to $4.58E-6$, respectively.

- NO being the temperature dependent species (higher the temperature higher the concentration). As the adiabatic equilibrium temperature reduces, the concentration of NO in the product side reduces.

Mole_fraction_NO2 = as the mole fraction of CO2 in the reactant increases from 0 to 0.95, X_{NO2} decreases from $1.011E-5$ to $1.057E-7$, respectively.

- NO2 being the temperature dependent species (higher the temperature higher the concentration). As the adiabatic equilibrium temperature reduces, the concentration of NO2 in the product side reduces.

Mole_fraction_CO = as the mole fraction of CO2 in the reactant increases from 0 to 0.95, X_{CO} decreases from $6.637E-3$ to $2.284E-9$, respectively.

- CO is generally produced in the product due to incomplete combustion. Being a fuel lean reactant-mixture, the combustion reaction will be complete. Hence the CO concentration is less in the product.
- With the increase in CO2 mole fraction in the reactant, the equilibrium position shift towards the reactant side according to Le Chatelier's principle. As a result the concentration of CO reduces further.

Mole_fraction_CO2 = as the mole fraction of CO2 in the reactant increases from 0 to 0.95, X_{CO2} increases from 0.10605 to 0.82288, respectively.

- This is because of the addition of CO2 in the reactant side. CO2 is further produced as a part of combustion products. Hence the concentration of CO2 in the product increases.

Increasing CO2 dilution to 100% -

Increasing CO2 dilution to 100% basically stops the combustion process due to significantly reduced oxygen supply. During this process of increasing CO2 concentration to 100%, incomplete combustion may occur resulting in the formation of soot or unburned hydrocarbons.

Problem 2: Repeat the process with H2O, instead of CO2. Comment on the difference between the two gases.

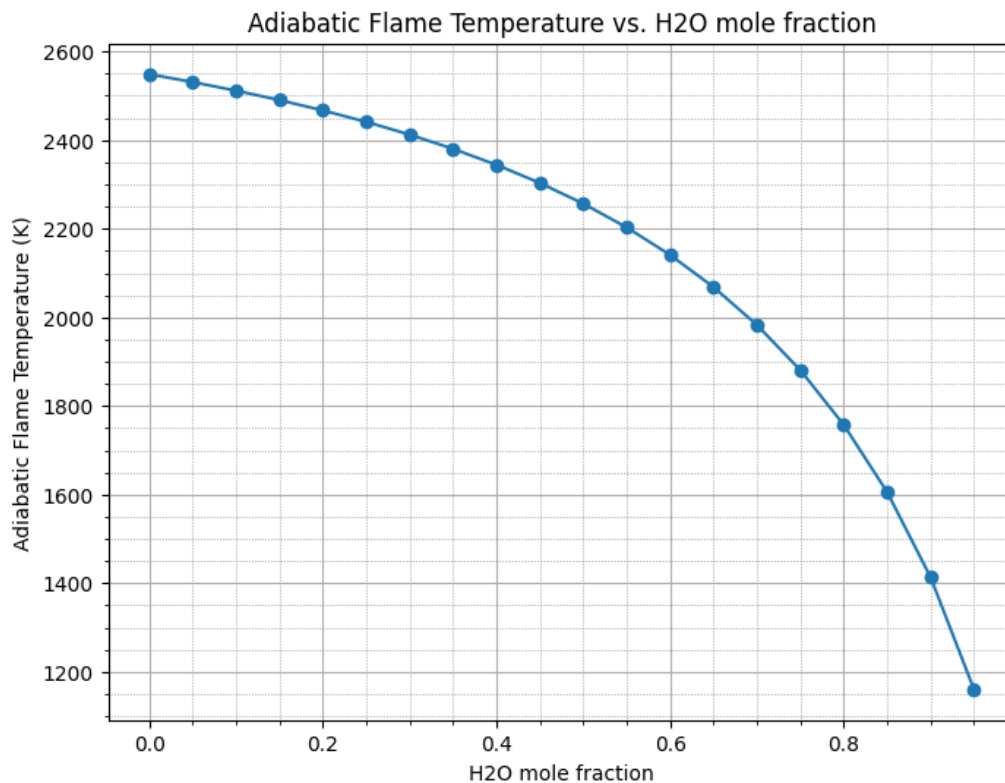


Fig. 15 – Adiabatic Flame Temperature vs H2O mole fraction plot

Temperature Adiabatic Equilibrium = as the mole fraction of H2O in the reactant increases from 0 to 0.95, T_{ad} decreases from 2548.79 K to 1160.82 K, respectively.

- Other reasons remain the same as the CO2 addition. However, the difference in the T_{ad} may be because of lower specific heat capacity of H2O as compared to specific heat capacity of CO2. This will result in higher adiabatic temperatures compared to CO2 addition.

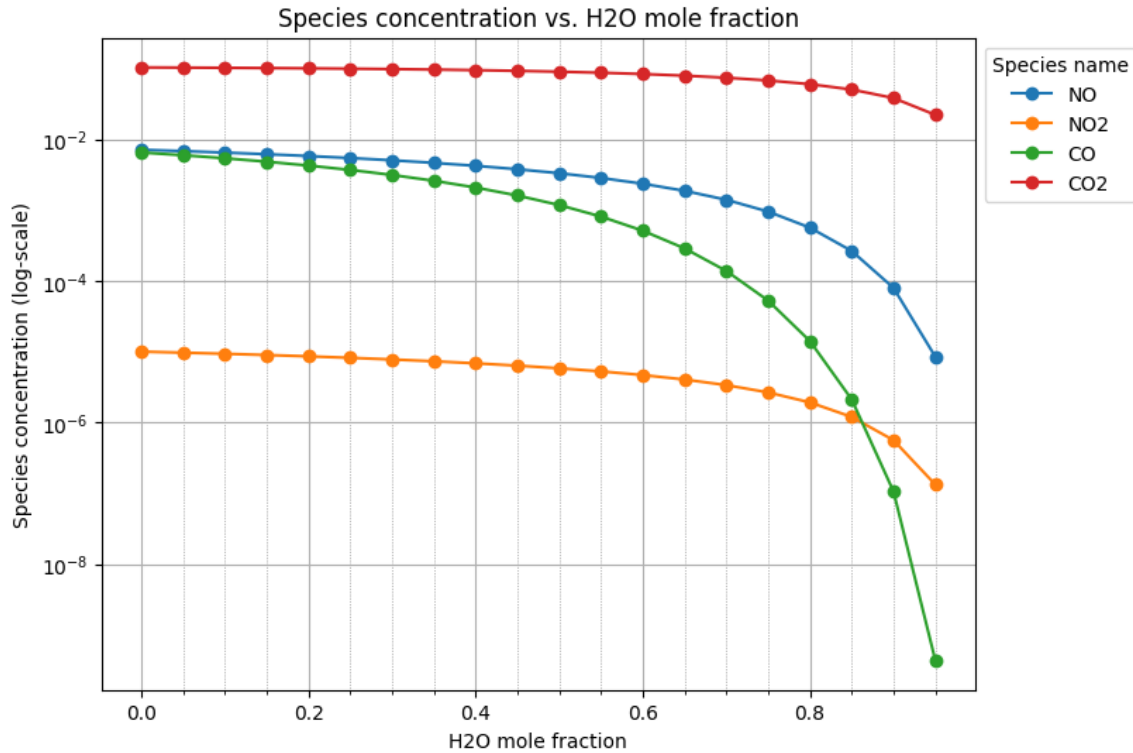


Fig. 16 – Species Concentration vs H2O mole fraction plot

Mole_fraction_NO = as the mole fraction of H2O in the reactant increases from 0 to 0.95, X_NO decreases from 7.25E-3 to 8.588E-6 , respectively.

- Compared to CO2 case, there is a little higher X_NO concentration, which is the result of little higher adiabatic equilibrium temperature in H2O case.

Mole_fraction_NO2 = as the mole fraction of H2O in the reactant increases from 0 to 0.95, X_NO2 decreases from 1.011E-5 to 1.331E-7, respectively.

- Compared to CO2 case, there is a little higher X_NO2 concentration, which is the result of little higher adiabatic equilibrium temperature in H2O case.

Mole_fraction_CO = as the mole fraction of CO2 in the reactant increases from 0 to 0.95, X_CO decreases from 6.637E-3 to 4.366E-10, respectively.

- Compared to CO2 case, the concentration of X_CO reduces further as H2O increases. This is due to the case of water-gas shift reaction, in which water molecule reacts with the CO and produces CO2 and H2. Hence the X_CO reduces further.

Mole_fraction_CO2 = as the mole fraction of CO2 in the reactant increases from 0 to 0.95, X_CO2 decreases from 0.10605 to 0.0226, respectively.

- Compared to CO₂ case, the concentration of X_{CO₂} reduces as the mole fraction of H₂O increases. However, the decrease is not that significant because CO₂ is produced from the combustion product and water-gas shift reaction.

Problem 3: What would happen if we were to remove N₂ from air in the combustion of iso-octane and air?

If we remove N₂ from air in the combustion process, the following will happen –

- Removing the N₂ from combustion air, results in oxygen-enriched environment. This will result in complete and efficient combustion.
- The adiabatic flame temperature will increase significantly. For example in the above case, for $\phi = 0.9$, the adiabatic flame temperature in the absence of N₂ is around 3658.11 K.
- N₂ being the inert gas, helps in diluting the combustion products. Removing N₂ from the air may result in vigorous combustion and changed flame behavior.

Problem 4: Repeat question VI.1 with the dilution of an inert Ar and explain your results

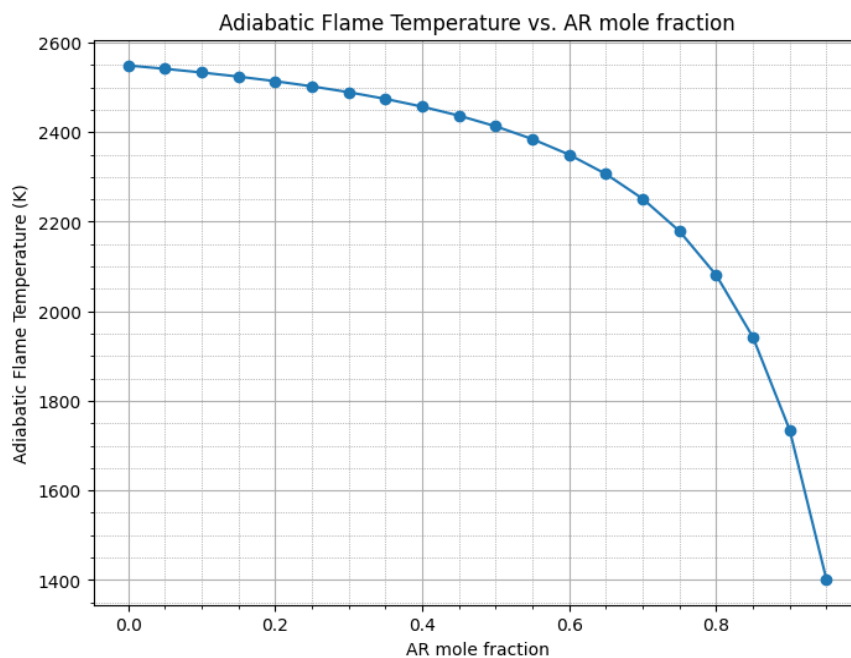


Fig. 17 – Adiabatic Flame Temperature vs Ar mole fraction plot

Temperature Adiabatic Equilibrium = as the mole fraction of Ar in the reactant increases from 0 to 0.95, T_{ad} decreases from 2548.79 K to 1401.86 K, respectively.

- Ar being an inert gas does not take part in the reaction. Hence, the reduction on the adiabatic flame temperature is primarily due to dilution effect and an addition of species which can absorb some amount of heat and hence the T_{ad} reduces. However, this decrease in temperature is not as high as in case of CO₂ and H₂O addition.

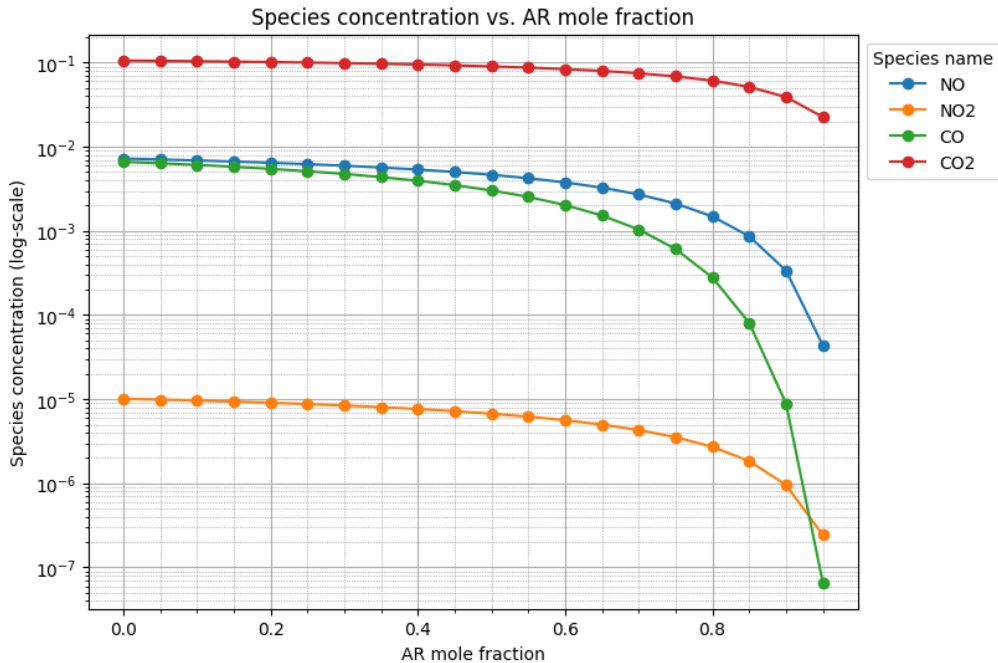


Fig. 18 – Species Concentration vs Ar mole fraction plot

Mole_fraction_NO = as the mole fraction of Ar in the reactant increases from 0 to 0.95, X_{NO} decreases from $7.25E-3$ to $4.368E-5$, respectively.

- Compared to CO2 and H2O case, there is higher X_{NO} concentration, which is the result of higher adiabatic equilibrium temperature.

Mole_fraction_NO2 = as the mole fraction of Ar in the reactant increases from 0 to 0.95, X_{NO2} decreases from $1.011E-5$ to $2.429E-7$, respectively.

- Compared to CO2 and H2O cases, there is higher X_{NO2} concentration, which is the result of higher adiabatic equilibrium temperature.

Mole_fraction_CO = as the mole fraction of Ar in the reactant increases from 0 to 0.95, X_{CO} decreases from $6.637E-3$ to $6.596E-8$, respectively.

- Compared to CO2 and H2O cases, the concentration of X_{CO} is higher in Ar case. This is primarily due to because Ar does not take part in the reaction, hence the effect on CO is only due to dilution effect.

Mole_fraction_CO2 = as the mole fraction of Ar in the reactant increases from 0 to 0.95, X_{CO2} decreases from 0.10605 to 0.0226, respectively.

- The effect on CO2 is similar to the effect on CO. However, compared to H2O case, the CO2 concentration is slightly lower.