Project Assignment 1: Combustion Thermodynamics

Part I : Introduction to Thermodynamics Data

Ans 1:

1. Entropy of N2 at 298.15 K: 191.60855931163846 J/mol
2. Entropy of O2 at 298.15 K: 205.14823368386573 J/mol
3. Entropy of CO2 at 298.15 K: 213.78611511544437 J/mol
4. Entropy of H2O at 298.15 K: 188.8279799776917 J/mol
5. Entropy of CO at 298.16 K: 197.6596085379824 J/mol
6. Entropy of H2 at 298.15 K: 130.68022841674744 J/mol
7. Entropy of xNO at 298.15 K: 210.74669282421232 J/mol
8. Entropy of C at 298.15 K: 158.1000070393054 J/mol

Ans 2:

1. Entropy of N2 at 2000 K: 252.0731314099827 J/mol
2. Entropy of O2 at 2000 K: 268.7704738895574 J/mol
3. Entropy of CO2 at 2000 K: 309.2879623388743 J/mol
4. Entropy of H2O at 2000 K: 264.9168012902104 J/mol
5. Entropy of CO at 2000 K: 258.71217188508786 J/mol
6. Entropy of H2 at 2000 K: 188.4172331388416 J/mol
7. Entropy of xNO at 2000 K: 273.1332461258387 J/mol
8. Entropy of C at 2000 K: 197.71349783750927 J/mol
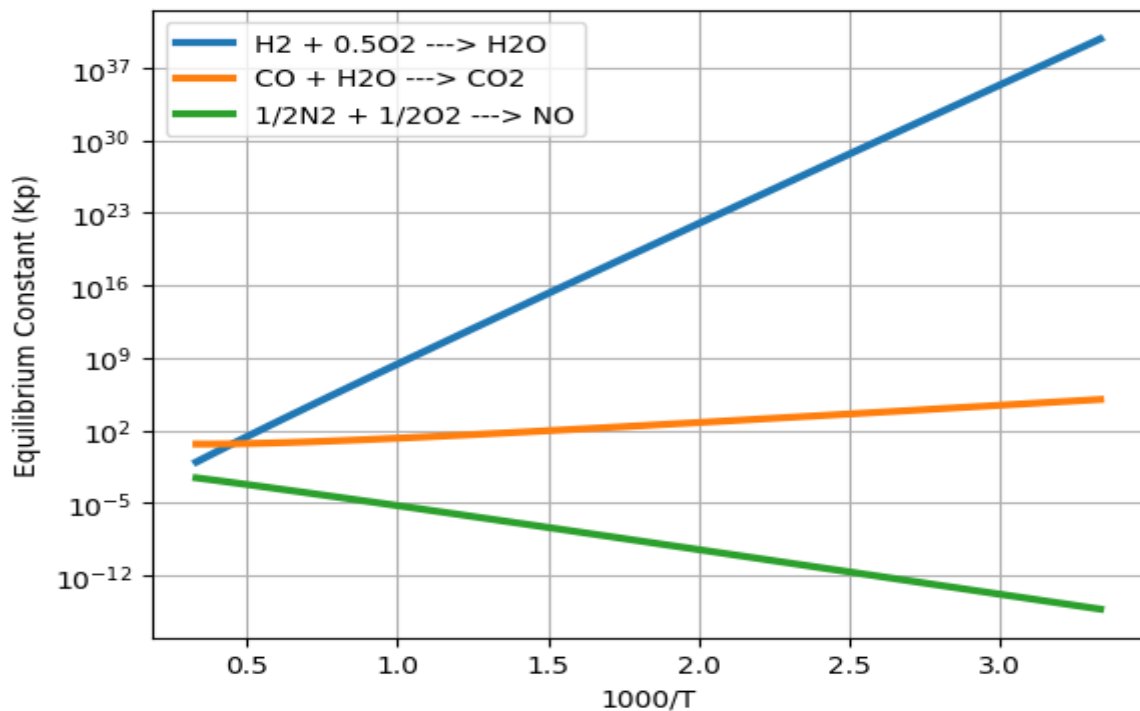
Part II – Equilibrium constant

Fig 1. Kp (in log-scale) versus 1000/T, for the three reactions

3. These reaction indicates that for exothermic reaction, Equilibrium constant decrease with increase in temperature and While for an endothermic reaction, Equilibrium constant Increase with increase in temperature.

4. $XNO = (Kp*XN2*XO2)^{1/2}$
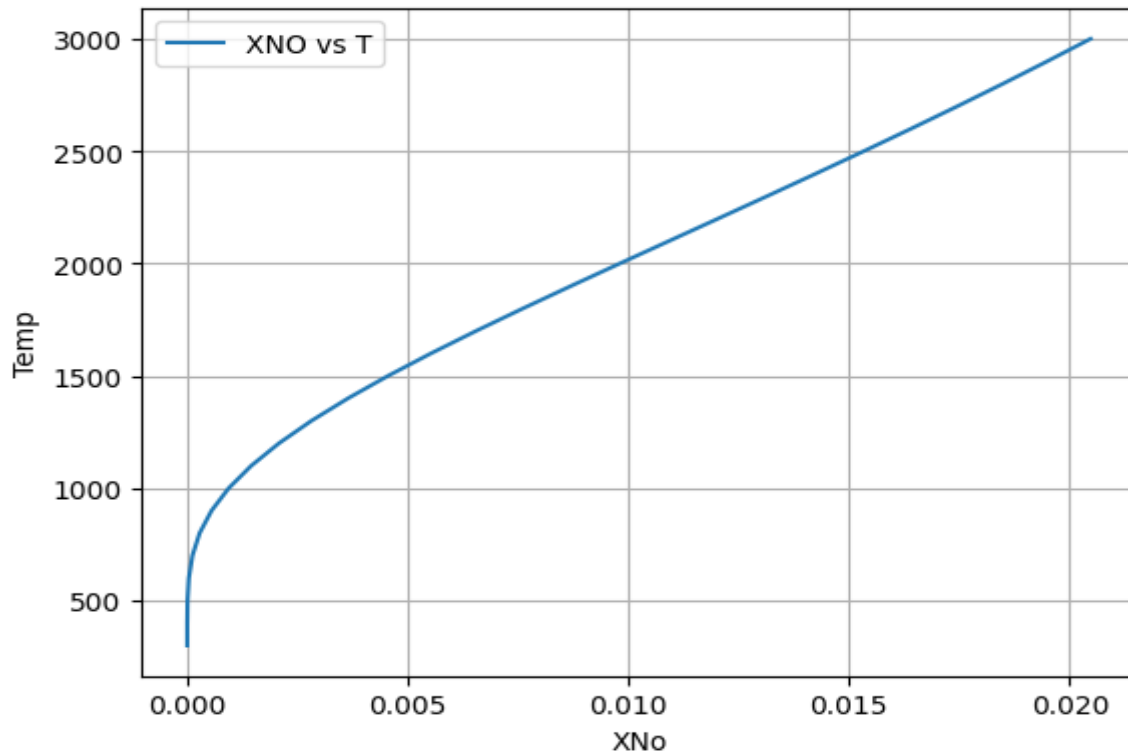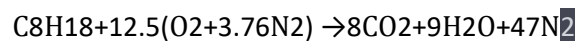
$\quad\quad = (Kp*0.78*0.21)^{1/2}$

5.

Fig 2. XNo versus T
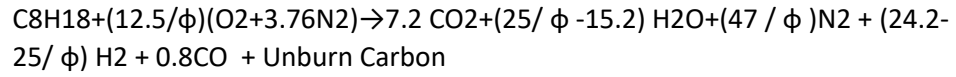
Part III – Incomplete combustion

1. Global Reaction :
    1. For Stoichiometric(Complete Combustion) :

        $$C8H18+12.5(O2+3.76N2) \rightarrow 8CO2+9H2O+47N2$$

    2. Incomplete Combustion (ϕ<1 Fuel Lean)

        $$C8H18+(12.5/ϕ)(O2+3.76N2) \rightarrow 7.2\ CO2+(25/ϕ -15.2)\ H2O+(47 / ϕ)N2 + (24.2- 25/ ϕ)\ H2 + 0.8CO$$

    3. For Fuel Rich (ϕ>1 Fuel Rich)

C8H18+(12.5/φ)(O2+3.76N2)→7.2 CO2+(25/ φ -15.2) H2O+(47 / φ)N2 + (24.2-25/ φ) H2 + 0.8CO + Unburn Carbon
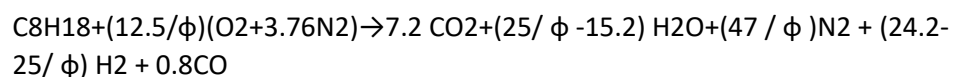
2. LHV and HHV for Fuel :

$$Delta_{hrp} = \sum_{i=1}^{n} h°_{f_p} - \sum_{i=1}^{n} h°_{f_R}$$

$$xDelta_{hrp} = n \times h°_{fCO_2} + n \times h°_{fH_2O} + n \times h°_{fN_2} - n \times h°_{fC_8H_{12}} - n \times h°_{fO_2} - n \times h°_{fN_2}$$

$$\because h°_{fN_2} = h°_{fO_2} = \phi(0)$$

$$= 8(-393,500) + 9(-241,820) - 1(-249,910)$$

$$= -5074630 \ KJ/mol$$

For LHV: $= h°_{RF} \times \dfrac{1}{Molecular \ Mass \ of \ Fuel}$

$$= 5074630 \times \frac{1}{114}$$

$$\therefore L \cdot H \cdot V = \ 44430 \ KJ/kg$$

$$\frac{(n_{H_2O} * \mu_{H_2O})}{(n_f * \mu_f)} * h_{fg}$$

$$44430 + \frac{(9 \times 18.02)}{(1 \times 114.14)}$$

$$\therefore H \cdot H \cdot V = 47900 KJ/Kg$$

3. Maximum Adiabatic Temperature occurs at Equivalence ratio of 0.9736
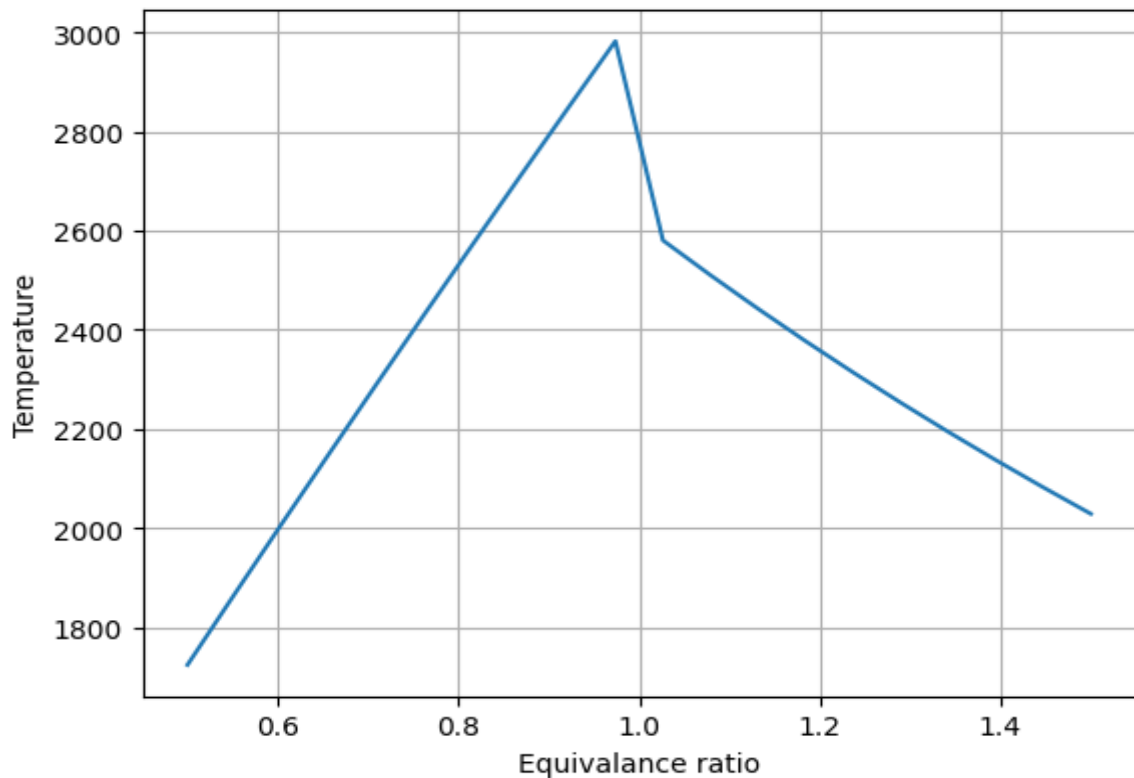

Fig 3. For Constant Cp Equivalence ratio vs Temp

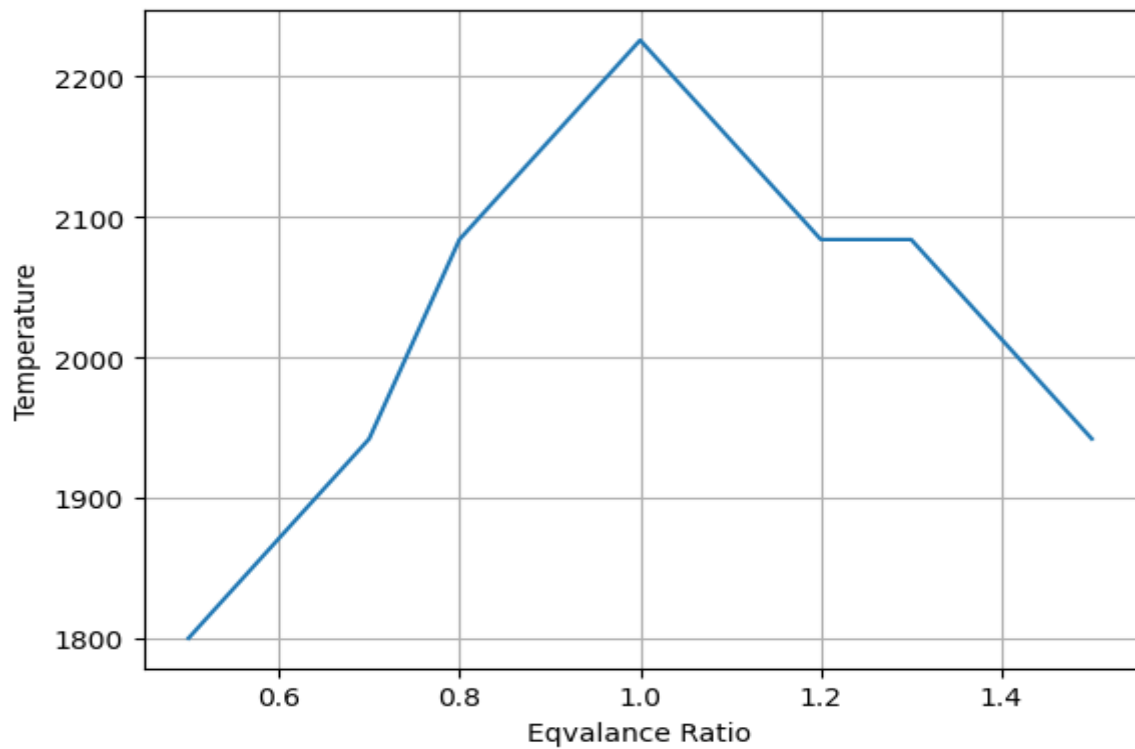4. Maximum Adiabatic Temperature occurs at Equivalence ratio of 0.9736

Fig 4. For Variable Cp Equivalence ratio vs Temp

5. Comparison : Variable Cp will give the more accurate Adiabatic flame Temp than constant Cp.

Part IV – Chemical equilibrium using Cantera:
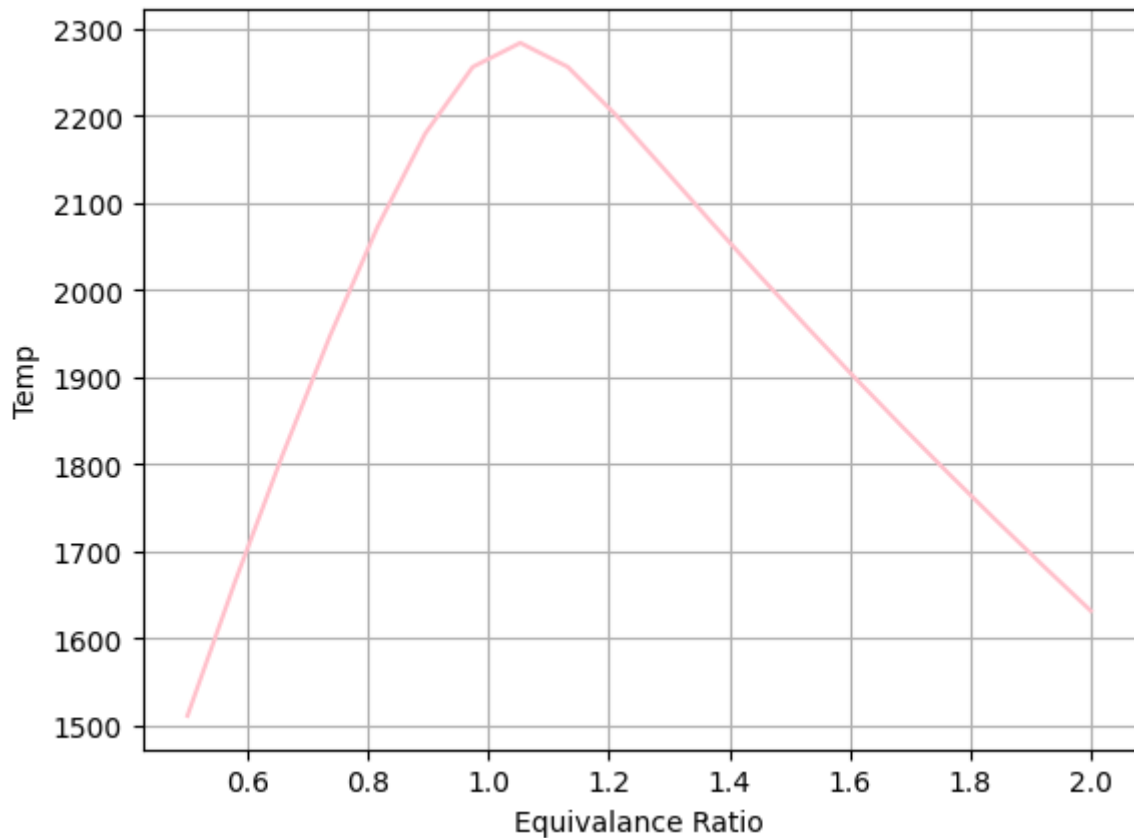
1. Plot of Tad vs Equivalence Ratio

Fig 5. Equivalence ratio vs Temp using Cantera

2. Maximum Adiabatic Temperature occurs at Equivalence ratio of 1.089
3. Comparison of Tad,equilibrium,Tad,estimation, and Tad,integration

    1. Tad Equilibrium : 2287.876072K
    2. Tad,estimation : 2982.072324K
    3. Tad,integration : 2226.000 K

    Comments : Tad,integration and Tad Equilibrium are the accurate values as it gives from Cp values which are dependent to temperature and Cantera mechanism respectively.

Part V – Parameters affecting Tad:

1. Maximum Adiabatic Temperature is 2287K at 1.19 equivalence ratio
2. Maximum Adiabatic Temperature is 2347K at 36atm inlet Pressure
3. Maximum Adiabatic Temperature is 2698K at 900K inlet Temperature
4.
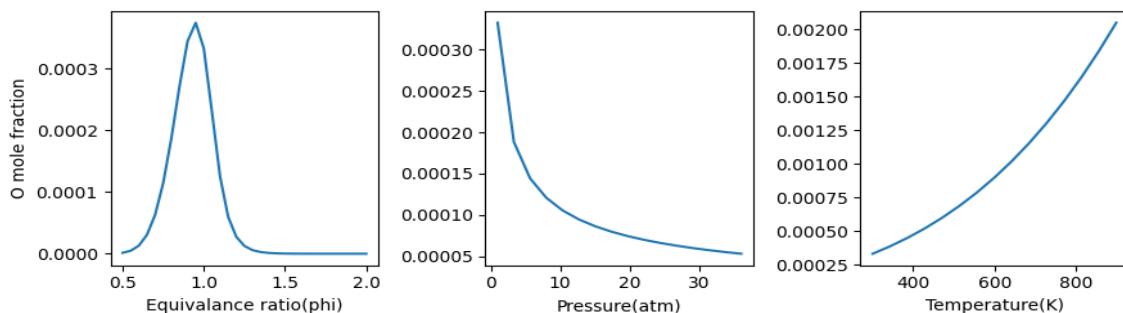
Fig 6. Variation of mole fraction of O with phi,pressure,temperature
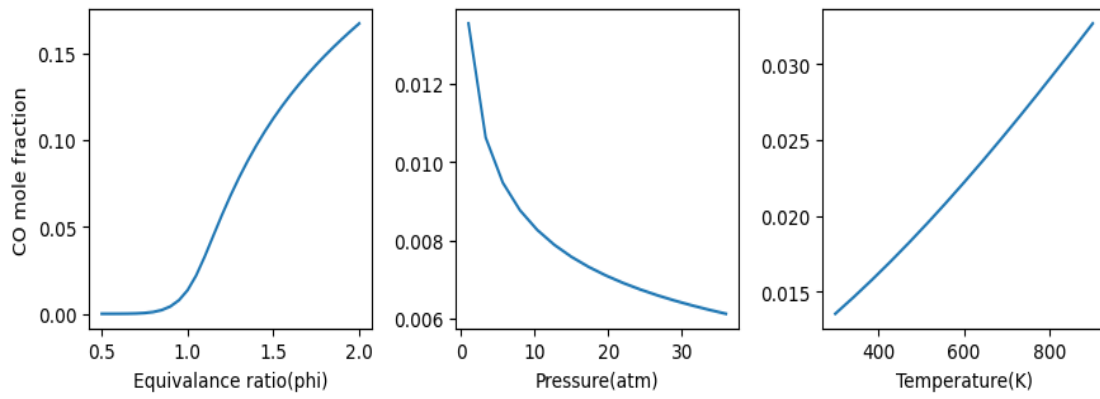
Fig 7. Variation of mole fraction of CO with phi,pressure,temperature
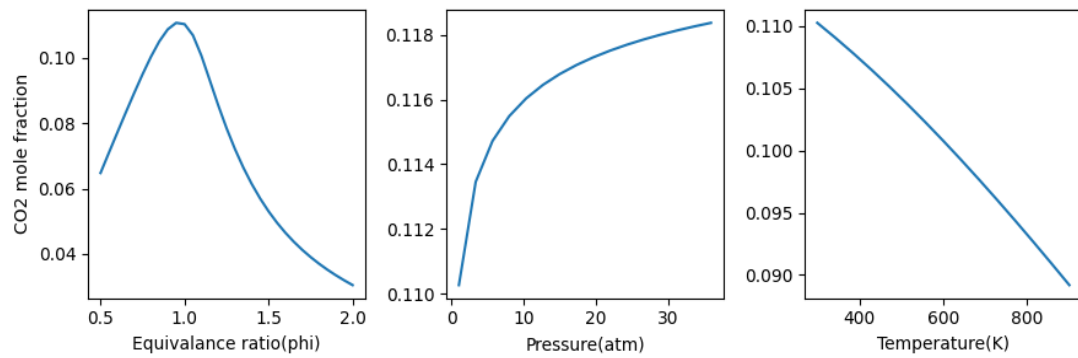
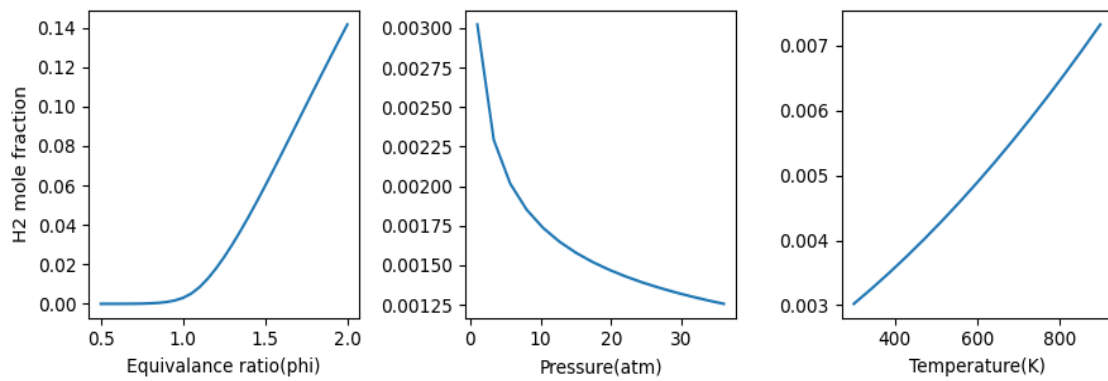Fig 8. Variation of mole fraction of CO2 with phi,pressure,temperature

Fig 9. Variation of mole fraction of H2 with phi,pressure,temperature

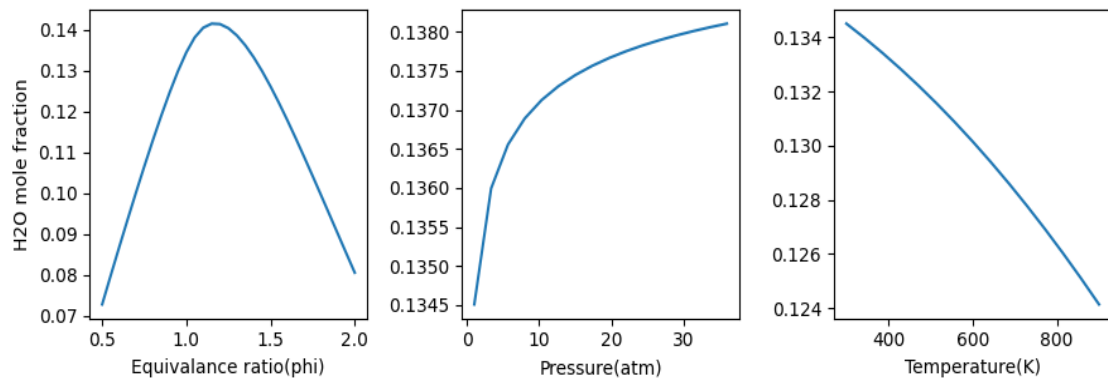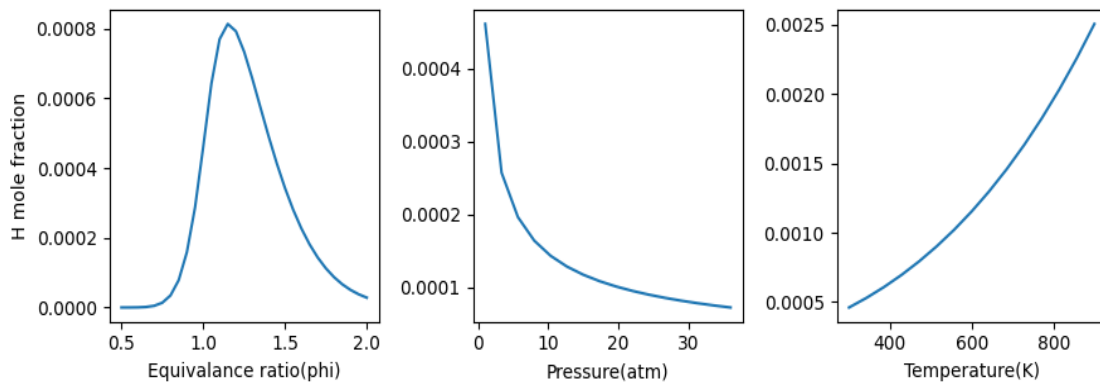Fig 10. Variation of mole fraction of H2O with phi,pressure,temperature

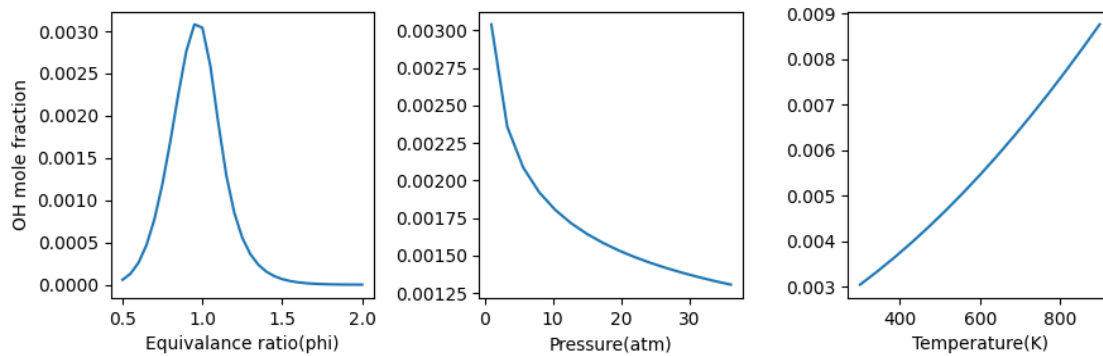Fig 10. Variation of mole fraction of H with phi,pressure,temperature

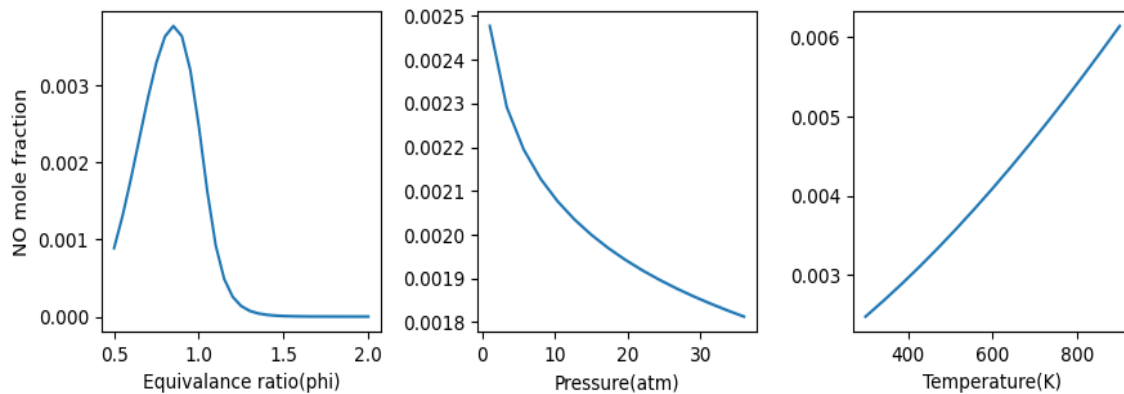Fig 11. Variation of mole fraction of OH with phi,pressure,temperature

Fig 12. Variation of mole fraction of NO with phi,pressure,temperature

5. Comments :
   a. Adiabatic Flame Temperature reaches maximum at an equivalence ratio of 1.091 and get reduces with further increment (Fuel Rich Condition) and same with decrement (Fuel Lean Condition).
   b. Adiabatic Flame Temperature Reaches peak at maximum of inlet pressure.
   c. Adiabatic Flame Temperature Reaches peak at maximum of inlet temperature.
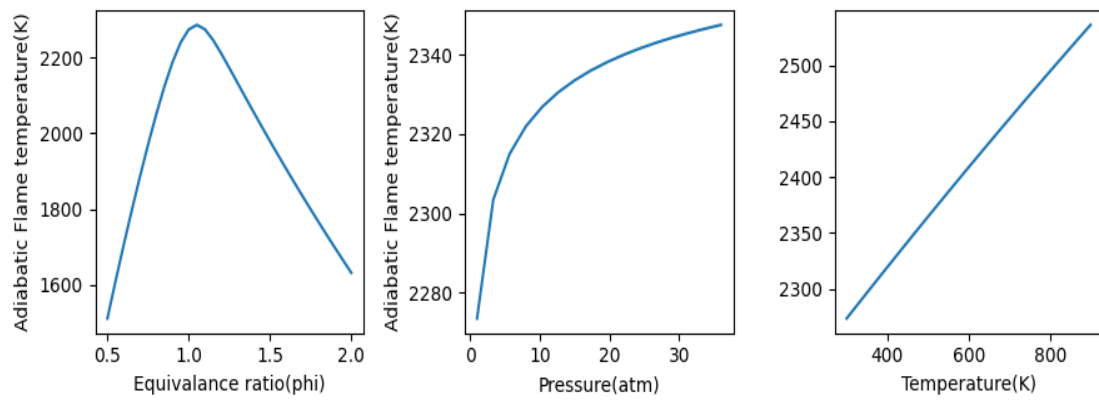
Fig 13. Variation of mole Adiabatic Flame Temp with phi, inlet pressure , inlet temp

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

1. Dilution of CO2 :
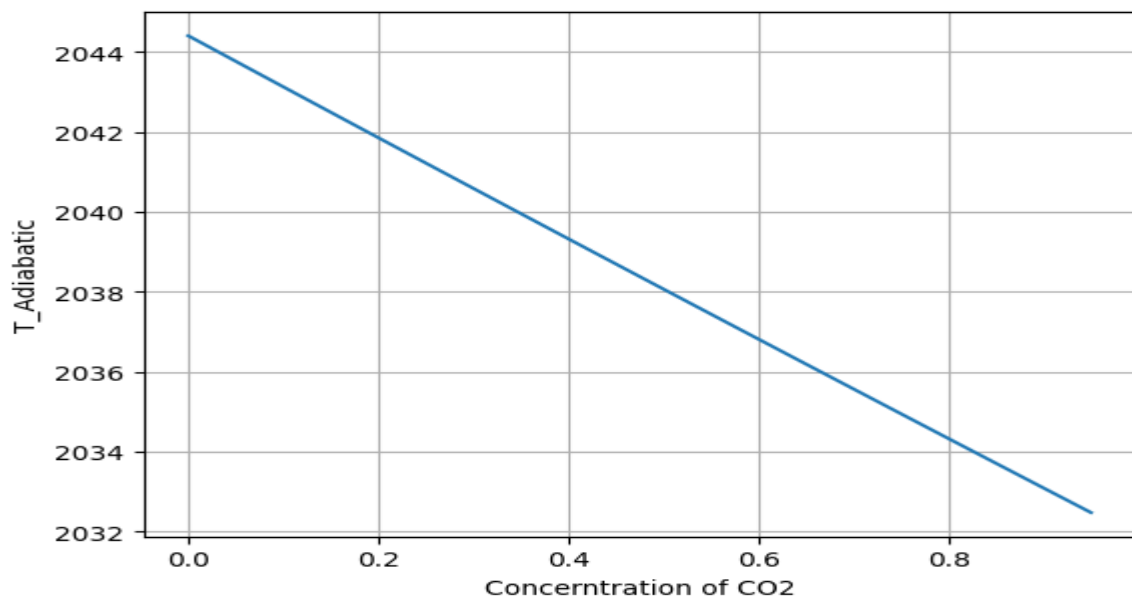
Fig 14. Variation of mole Adiabatic Flame Temp with Concentration of CO2
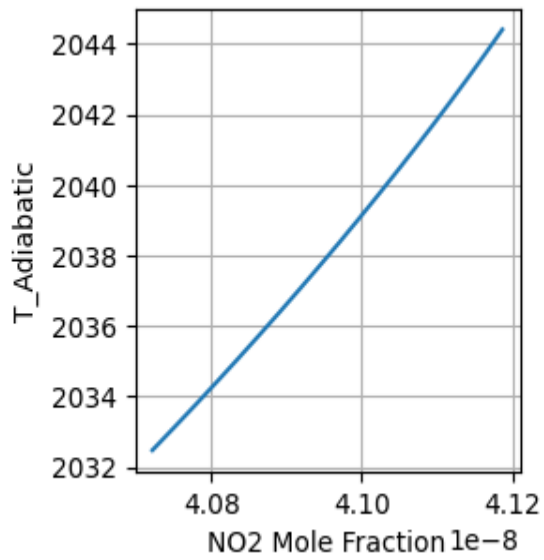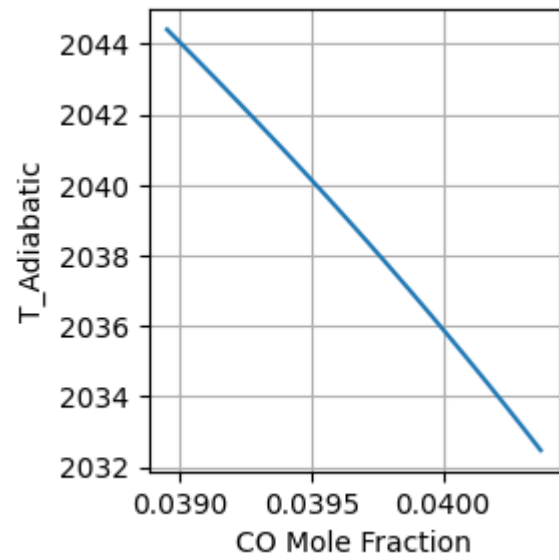
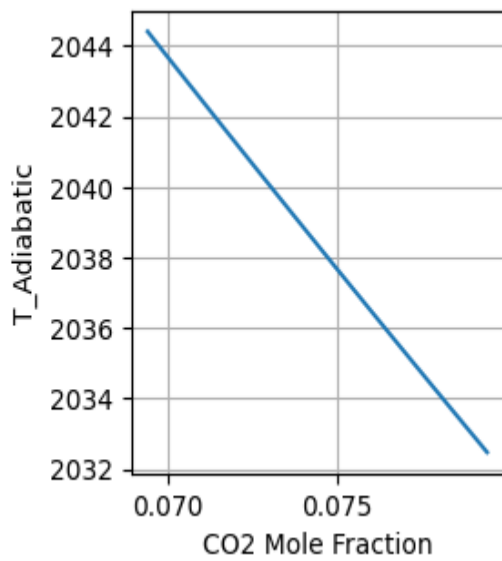Fig 15. XNO2 vs T_Adiabatic

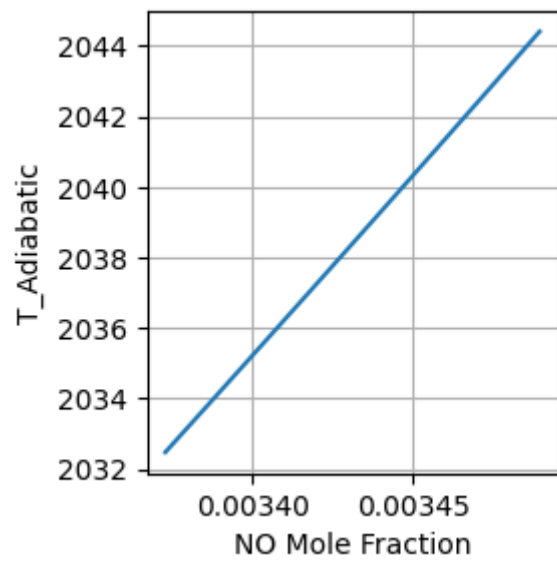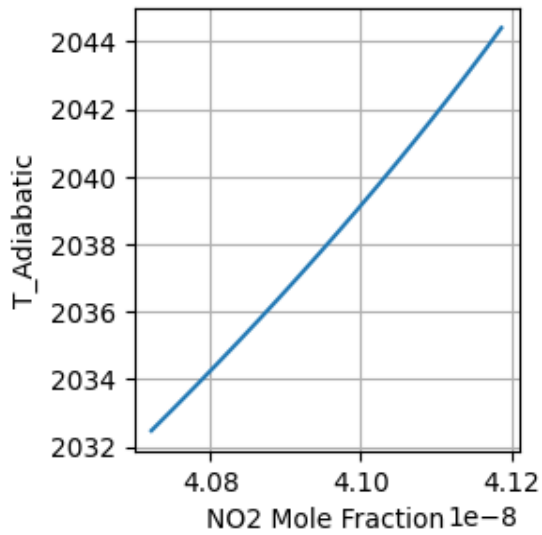

Fig 16. XCO vs T_Adiabatic

Fig 17. XCO2 vs T_Adiabatic

Fig 18. XNO vs T_Adiabatic

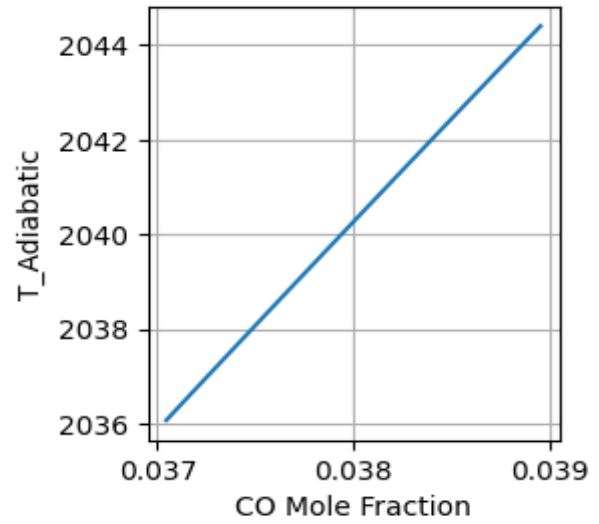2. Dilution of H20 :

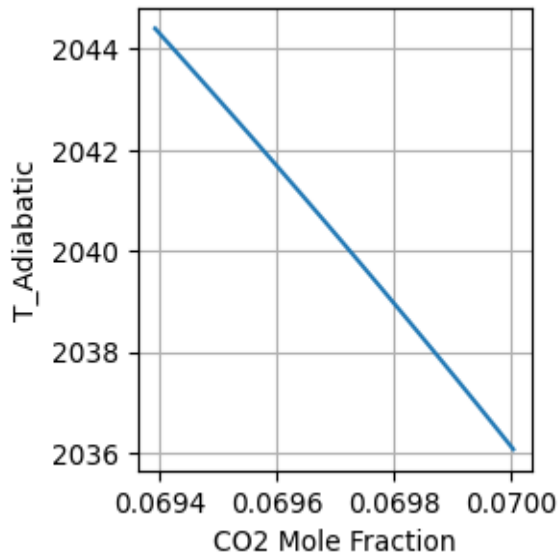Fig 19. XNO2 vs T_Adiabatic

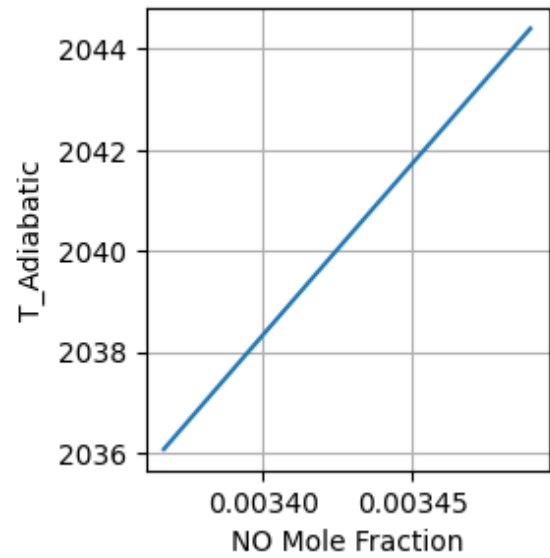Fig 20. XCO vs T_Adiabatic

Fig 21. XCO2 vs T_Adiabatic

Fig 22. XCO vs T_Adiabatic

3. Reduction of N2 from standard air : Reduction of N2 from standard air will lead to neglect the production of Nox and no dissociation will occur . in this case formation of CO2 and H20 dominant the product side.
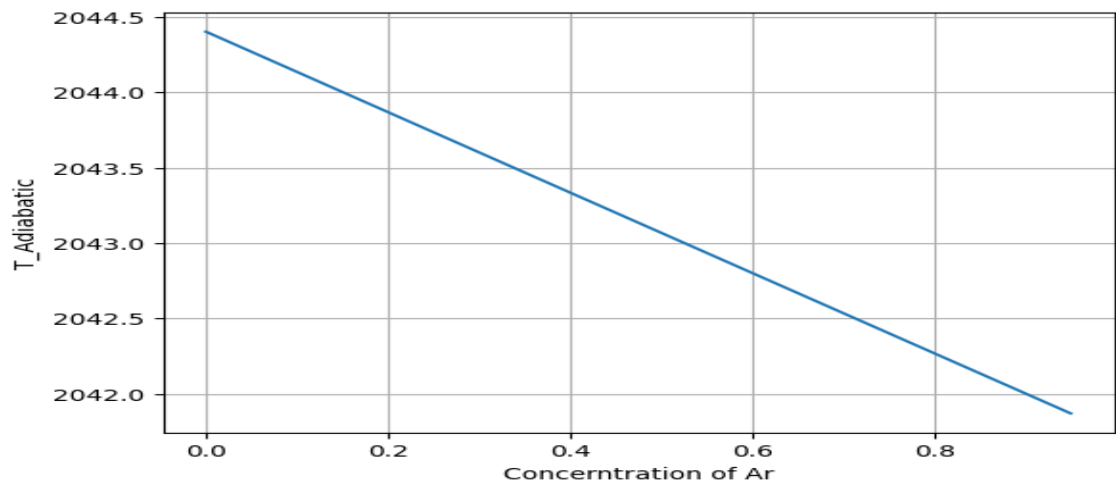
4. Dilution of Ar :

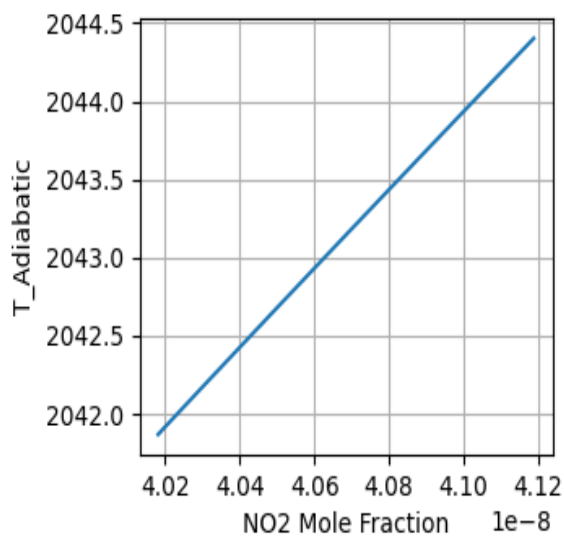Fig 23. Variation of Adiabatic Flame Temp with Concentration of Ar
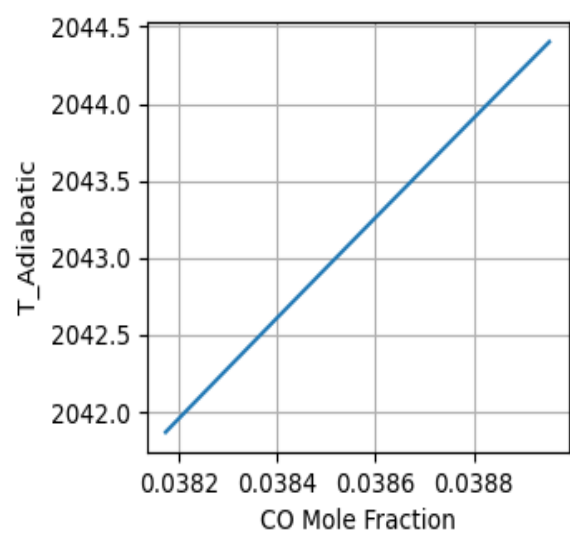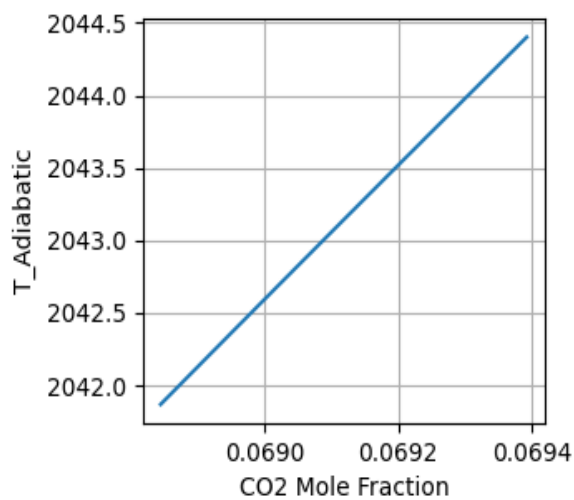

Fig 24. XNO2 vs T_Adiabatic

Fig 25. XCO vs T_Adiabatic

Fig 26. XCO2 vs T_Adiabatic
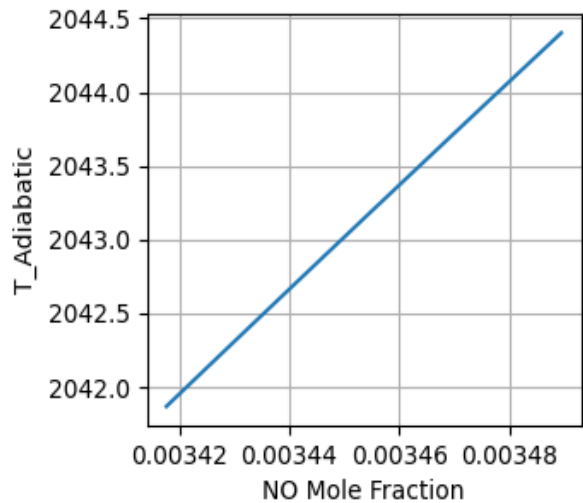

Fig 27. XNO vs T_Adiabatic

Comments : From fig 23 (Dilution of Argon) and fig 14 (Dilution of CO2), It can be suggested that to reach the same adiabatic temperature Argon requires more concentration than CO2.