

MECH 447/652
DYNAMICS OF COMBUSTION



PROJECT ASSIGNMENT 1

**COMBUSTION
THERMODYNAMICS**

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Part I – Introduction to thermodynamics data

1. Find the enthalpy (kJ/mol), $h^\circ(T)$, and the entropy (kJ/mol-K), $s^\circ(T)$, at 298.15K for C_8H_{18} , O_2 , N_2 , CO_2 , H_2O , CO , and H_2 .
2. Using the code provided, find the enthalpy (kJ/mol), $h^\circ(T)$, and the entropy (kJ/mol-K), $s^\circ(T)$, at 2000K for C_8H_{18} , O_2 , N_2 , CO_2 , H_2O , CO , and H_2 .
3. Provide, without discussion, these data in a single table with units.

Table I: Enthalpy and entropy of selected species at specified temperatures.

| Species | Enthalpy, h° [kJ/mol] | | Entropy, $s^\circ(T)$ [kJ/mol-K] | |
|-------------|------------------------------|----------|----------------------------------|----------|
| | At 298.15K | At 2000K | At 298.15K | At 2000K |
| C_8H_{18} | -224.010 | 552.096 | 0.423 | 1.171 |
| O_2 | 0.000 | 59.201 | 0.205 | 0.269 |
| N_2 | 0.000 | 56.136 | 0.192 | 0.252 |
| CO_2 | -393.510 | -302.071 | 0.214 | 0.309 |
| H_2O | -241.826 | -168.782 | 0.189 | 0.265 |
| CO | -110.535 | -53.799 | 0.198 | 0.259 |
| H_2 | 0.000 | 52.950 | 0.131 | 0.188 |

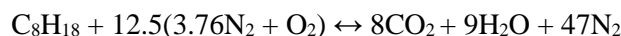
Part II – Complete combustion

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

1. Write down the global reaction (using the equivalence ratio ϕ) for the stoichiometric, the lean, and the rich conditions

Stoichiometric ($\phi = 1$):

Since complete combustion was assumed, the products were assumed to be only CO_2 , H_2O and N_2 . Balancing was done for each species (C, H, O) to produce:



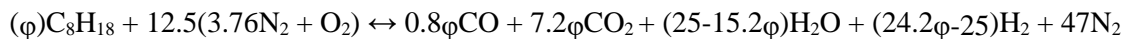
Fuel Lean ($\phi < 1$):

On the fuel lean side, O_2 was included in the products since it was in excess:



Fuel Rich ($\phi > 1$):

On the fuel rich side, CO and H_2 was included in the products. Since there were 4 unknowns, and only three equations for balancing C, H, and O, the last equation was induced from the hint ($X_{CO_2} = 9 \cdot X_{CO}$) to fully solve the system:



2. Calculate the lower and higher heating values in $kJ/kg_{C_8H_{18}}$ (LHV and HHV) – comment, and compare to other values in the literature.

From the stoichiometric chemical equation written and the enthalpy values tabulated previously,

The lower heating value of C_8H_{18} , q_{LHV} :

$$\tilde{q}_{LHV} = (0 - 1)(h^\circ_{C_8H_{18}}) + (47 - 47)(h^\circ_{N_2}) + (0 - 12.5)(h^\circ_{O_2}) + (8 - 0)(h^\circ_{CO_2}) + (9 - 0)(h^\circ_{H_2O(g)})$$

$$\tilde{q}_{LHV} = -5100.504 \text{ kJ/mol}$$

$$q_{LHV} = -\frac{\tilde{q}_{LHV}}{\text{Molar Mass of } C_8H_{18}} = -44,651 \text{ kJ/kg}$$

Similarly, the higher heating value of C_8H_{18} , q_{HHV} , was found by using enthalpy of H_2O as liquid:

$$\tilde{q}_{HHV} = (0 - 1)(h^\circ_{C_8H_{18}}) + (47 - 47)(h^\circ_{N_2}) + (0 - 12.5)(h^\circ_{O_2}) + (8 - 0)(h^\circ_{CO_2}) + (9 - 0)(h^\circ_{H_2O(l)})$$

$$\tilde{q}_{HHV} = -5496.540 \text{ kJ/mol}$$

$$q_{HHV} = -\frac{\tilde{q}_{HHV}}{\text{Molar Mass of } C_8H_{18}} = -48,118 \text{ kJ/kg}$$

On the other hand, the documented literature values were -44,430 kJ/kg and -47,890 kJ/kg for the lower and higher heating values respectively. As observed, the difference was very small (<less than 0.5% of percentage error for both cases) and almost negligible. Generally, it could be presumed that these deviations were caused by rounding error, or by having slightly different values of enthalpy/molar mass from different sources, or both.

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 $R = 8314.4621 \text{ J/kmol}\cdot\text{K}$. Indicate the maximum temperature, and for which equivalence ratio.

The adiabatic temperature is defined by the following equation:

$$\Delta H_{f, T=300K}^{\circ} + \int_{300K}^T \sum v''_i c_{p_i}(T) dT = 0$$

In the above equation $\Delta H_{f, T=300K}^{\circ}$ represents the chemical heat released by the reaction, which can be found by taking the difference in enthalpy values. Taking $\phi = 1$ as example,

$$\Delta H_{f, T=300K}^{\circ} = \sum (v''_i - v'_i) h_i^{\circ}$$

$$\Delta H_{f, T=300K}^{\circ} = (0 - 1)(h_{C_8H_{18}}^{\circ}) + (47 - 47)(h_{N_2}^{\circ}) + (0 - 12.5)(h_{O_2}^{\circ}) + (8 - 0)(h_{CO_2}^{\circ}) + (9 - 0)(h_{H_2O(g)}^{\circ})$$

$$\Delta H_{f, T=300K}^{\circ} = -5100393 \text{ kJ/kmol}$$

Note: v''_i and v'_i are the coefficients of the i -species at the products' side and the reactants' respectively.

$\int_{300K}^T \sum n_i c_{p_i}(T) dT$ then represents the temperature rise in the products due to the amount of heat absorbed.

In this case the c_p is a constant and equal to $3.5R$. Again taking $\phi = 1$:

$$\int_{300K}^T \sum v''_i c_{p_i}(T) dT = c_p \int_{300K}^T (8 + 9 + 47) dT = 64c_p(T - 300) \text{ kJ/kmol}$$

Substituting both expressions into the first equation yields:

$$-5100393 + 64c_p(T - 300) = 0$$

$$\rightarrow T = 3039K$$

Similar steps can be taken to solve for fuel lean and fuel rich conditions by substituting different ϕ values, where:

For fuel lean ($\phi < 1$):

$$\Delta H_{f, T=300K}^{\circ} = -5100393\phi \text{ kJ/kmol}$$

$$\int_{300K}^T \sum v''_i c_{p_i}(T) dT = (4.5\phi + 59.5)(c_p)(T - 300) \text{ kJ/kmol}$$

For fuel rich ($\phi > 1$):

$$\Delta H_{f, T=300K}^{\circ} = (978578\phi - 6046050) \text{ kJ/kmol}$$

$$\int_{300K}^T \sum v''_i c_{p_i}(T) dT = (17\phi + 47)(c_p)(T - 300) \text{ kJ/kmol}$$

With the above expressions, T_{ad} was solved for all ϕ and the results are tabulated below.

Table IIa: ϕ and corresponding T_{ad} for constant C_p .

| ϕ | T_{ad} [K] |
|--------|--------------------------|
| 0.50 | 1719.17014268 |
| 0.55 | 1855.41963601 |
| 0.60 | 1990.68340149 |
| 0.65 | 2124.97209778 |
| 0.70 | 2258.29623041 |
| 0.75 | 2390.66615453 |
| 0.80 | 2522.09207761 |
| 0.85 | 2652.58406203 |
| 0.90 | 2782.15202768 |
| 0.95 | 2910.80575445 |
| 1.00 | 3038.55488471 (Max Temp) |
| 1.05 | 2959.29180482 |
| 1.10 | 2899.29490273 |
| 1.15 | 2840.83060370 |
| 1.20 | 2783.84092348 |
| 1.25 | 2728.27076644 |
| 1.30 | 2674.06774784 |
| 1.35 | 2621.18202920 |
| 1.40 | 2569.56616539 |
| 1.45 | 2519.17496268 |
| 1.50 | 2469.96534680 |

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

The same equation as the previous part can be used to define the adiabatic temperature. While $\Delta H^\circ_{f, T=300K}$ remains unchanged, the same $\int_{300K}^T \sum v''_i c_{p_i}(T) dT$ can no longer be used, as in this situation, C_p is not a constant. To simplify the process, the 't.cp_mole(T)' function was used to call C_p values at different temperatures for different molecules from 'thermoDataNASA-9.yaml'. The values were then integrated numerically with the 'scipy.integrate.quad' function to give the expression for $\int_{300K}^T \sum v''_i c_{p_i}(T) dT$. The equation was then solved with 'scipy.optimize.fsolve' and the results were tabulated below.

Table IIb: ϕ and corresponding T_{ad} for varying C_p .

| ϕ | T_{ad} [K] |
|--------|--------------------------|
| 0.50 | 1513.40701494 |
| 0.55 | 1612.94670428 |
| 0.60 | 1709.78219873 |
| 0.65 | 1804.07948874 |
| 0.70 | 1895.98333458 |
| 0.75 | 1985.62176086 |
| 0.80 | 2073.10927481 |
| 0.85 | 2158.54924261 |
| 0.90 | 2242.03572302 |
| 0.95 | 2323.65482650 |
| 1.00 | 2403.48581969 (Max Temp) |
| 1.05 | 2358.48838601 |
| 1.10 | 2321.28060681 |
| 1.15 | 2284.69408916 |
| 1.20 | 2248.71288450 |
| 1.25 | 2213.32160778 |
| 1.30 | 2178.50548105 |
| 1.35 | 2144.25023442 |
| 1.40 | 2110.54213105 |
| 1.45 | 2077.36789078 |
| 1.50 | 2044.71472962 |

5. Plot the result $T_{ad, integration}$ vs. ϕ for both question 3 and 4.

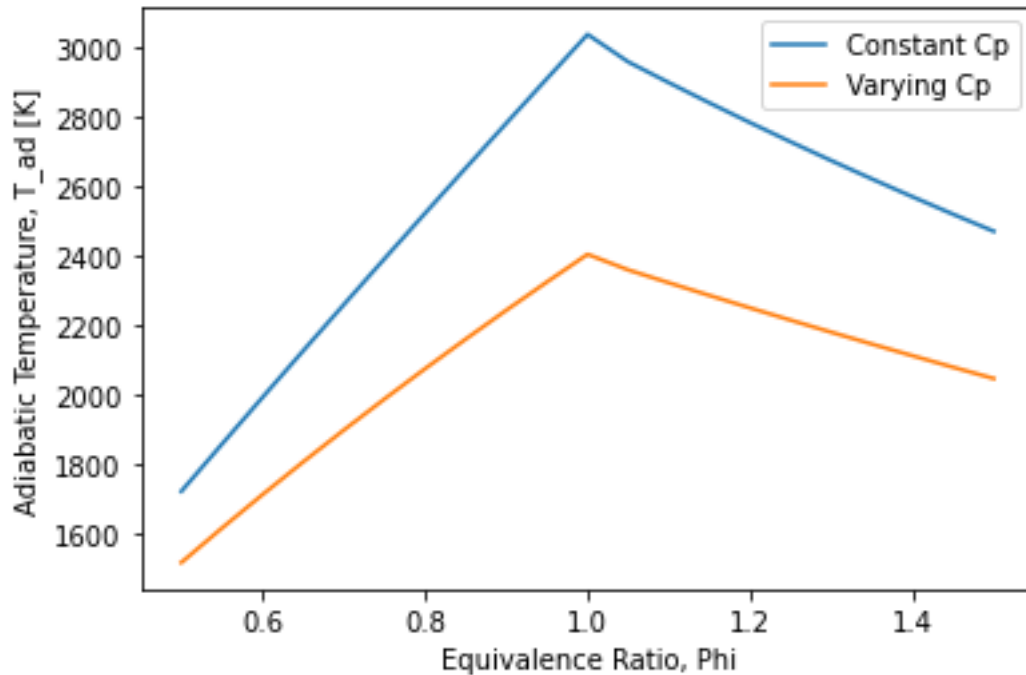


Figure IIa: T_{ad} vs ϕ for constant and varying C_p

6. Compare and explain the results.

From the graph, it can be clearly observed that the maximum adiabatic temperature was found at $\phi = 1$ for both cases. This was theoretical expected as at $\phi=1$, the fuel should be fully oxidized without producing any excess products.

The adiabatic temperatures found using varying C_p (ie: $C_p = C_p(T)$) was significantly lower compared to the ones found assuming constant C_p . The phenomenon was expected as C_p increases with temperature in the varying C_p model, which mean that more heat is required to raise the temperature of the products. In mathematical terms, $dH = C_p(T) dT$. Since dH is fixed being defined as the amount of chemical heat released, as C_p was increased, dT must decrease.

Part III: Chemical Equilibrium using Cantera

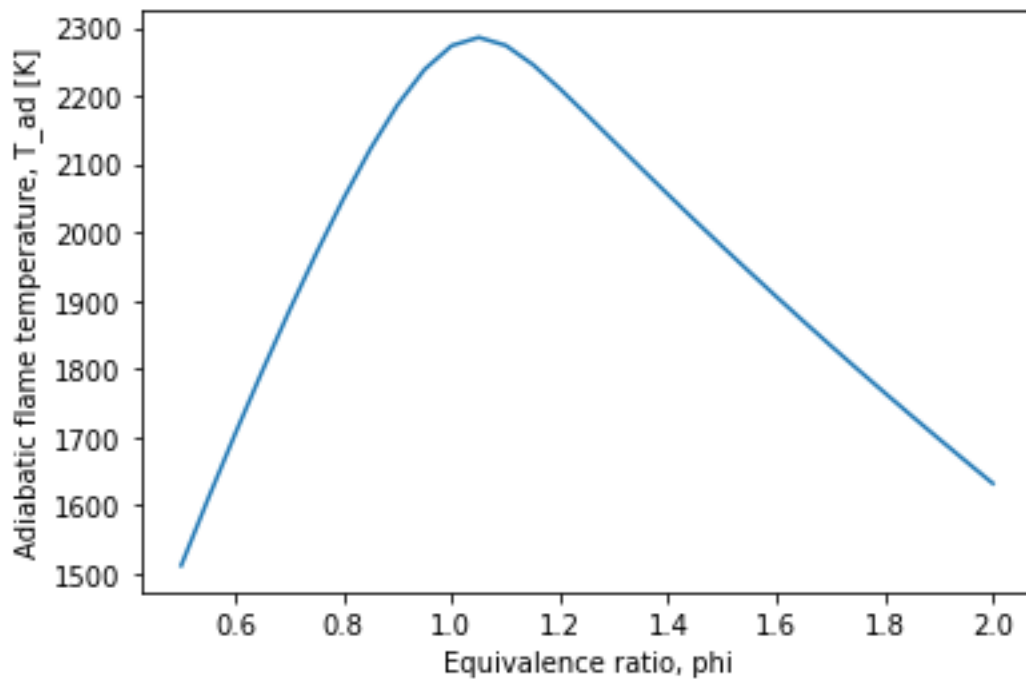
For the same conditions than in Part II, but using Cantera:

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

With the codes from 'adiatic.py' from Cantera as basis, assuming initial temperature of 300K and initial pressure of 101,325Pa, the adiabatic temperatures for ϕ values ranging from 0.5 to 2 were tabulated and the variation was plotted.

Table III: ϕ and corresponding T_{ad} using Cantera.

| ϕ | T_{ad} [K] |
|--------|--------------|
| 0.50 | 1511.34 |
| 0.55 | 1609.688 |
| 0.60 | 1704.824 |
| 0.65 | 1796.718 |
| 0.70 | 1885.167 |
| 0.75 | 1969.678 |
| 0.80 | 2049.315 |
| 0.85 | 2122.501 |
| 0.90 | 2186.819 |
| 0.95 | 2238.783 |
| 1.00 | 2273.56 |
| 1.05 | 2285.633 |
| 1.10 | 2273.849 |
| 1.15 | 2245.773 |
| 1.20 | 2210.236 |
| 1.25 | 2171.953 |
| 1.30 | 2132.874 |
| 1.35 | 2093.799 |
| 1.40 | 2055.069 |
| 1.45 | 2016.832 |
| 1.50 | 1979.149 |
| 1.55 | 1942.037 |
| 1.60 | 1905.495 |
| 1.65 | 1869.509 |
| 1.70 | 1834.063 |
| 1.75 | 1799.139 |
| 1.80 | 1764.718 |
| 1.85 | 1730.784 |
| 1.90 | 1697.318 |
| 1.95 | 1664.305 |
| 2.00 | 1631.727 |

Figure IIIa: T_{ad} vs ϕ using Cantera

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

The maximum adiabatic temperature was found at $\phi = 1.05$ due to incomplete combustion. At the pressure level of 1 atm, some products may dissociate to fill up more space, absorbing the part of the energy that was released by oxidation. As the result, the adiabatic temperature decreases. As the extent of dissociation is usually greater on the lean side, it pushes the peak slightly to the rich side. To obtain a peak that is closer to $\phi = 1$, the pressure of the reaction can be increased to reduce the likelihood of dissociation.

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

$T_{ad, equilibrium} < T_{ad, integration} < T_{ad, estimation}$. The reason of why $T_{ad, estimation}$, where constant C_p was assumed, was greater than $T_{ad, integration}$ was explained previously. The reason behind $T_{ad, equilibrium}$ being the lowest value is because in the chemical equilibrium created by Cantera, the possible formation of a variety of other species was taken into consideration (will be shown in more details in the next part). This leads to some reduction in energy to form other molecules, causing it to be slightly lower compared to $T_{ad, integration}$.

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

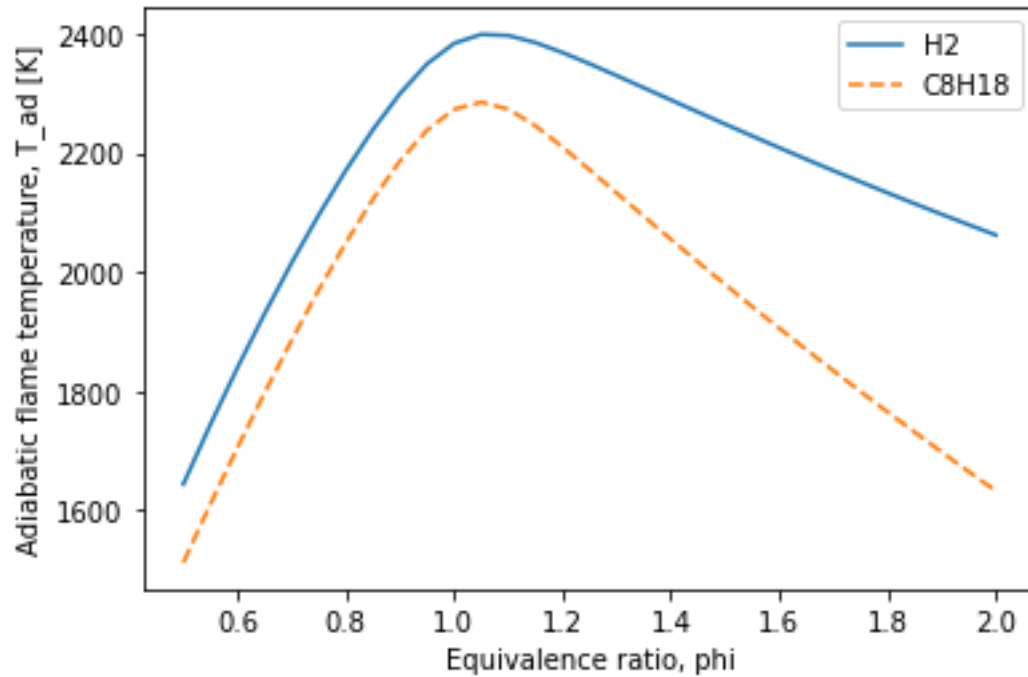


Figure IIIb: T_{ad} vs ϕ using Cantera, for H_2 and C_8H_{18}

The adiabatic temperatures of H_2 are slightly higher than those of C_8H_{18} . This may be attributed to the fact that H_2 is at a higher energy state compared to C_8H_{18} , so less energy is needed to dissociate it.

Part IV – Parameters affecting T_{ad}

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

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

1. 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.

Again using 'adiabatic.py' as basis, the adiabatic temperatures for ϕ values ranging from 0.5 to 2 were computed. At the chemical equilibrium, mole fractions of the selected species, χ_i , were extracted using 'mix.species_moles' and the data was written to an Excel file.

Table IVa: ϕ , T_{ad} , and χ_i of selected species.

| ϕ | T_{ad} [K] | Equilibrium Composition, χ_i | | | | | | | |
|--------|--------------|-----------------------------------|----------|-----------------|----------------|------------------|----------|----------|----------|
| | | O | CO | CO ₂ | H ₂ | H ₂ O | H | OH | NO |
| 0.50 | 1511.34 | 1.53E-06 | 1.20E-06 | 0.066665 | 5.15E-07 | 0.07497 | 1.46E-08 | 5.97E-05 | 0.000915 |
| 0.55 | 1609.688 | 4.99E-06 | 5.44E-06 | 0.073267 | 2.02E-06 | 0.082362 | 8.65E-08 | 0.000135 | 0.001351 |
| 0.60 | 1704.824 | 1.36E-05 | 2.03E-05 | 0.079847 | 6.67E-06 | 0.089709 | 4.03E-07 | 0.000269 | 0.001859 |
| 0.65 | 1796.718 | 3.18E-05 | 6.45E-05 | 0.086386 | 1.92E-05 | 0.096993 | 1.55E-06 | 0.000487 | 0.002409 |
| 0.70 | 1885.167 | 6.54E-05 | 0.000181 | 0.092842 | 4.92E-05 | 0.104195 | 5.05E-06 | 0.000809 | 0.002957 |
| 0.75 | 1969.678 | 0.00012 | 0.000456 | 0.099129 | 0.000115 | 0.111287 | 1.44E-05 | 0.001246 | 0.003448 |
| 0.80 | 2049.315 | 0.000196 | 0.001052 | 0.105084 | 0.000251 | 0.118241 | 3.64E-05 | 0.001785 | 0.003811 |
| 0.85 | 2122.501 | 0.000284 | 0.002243 | 0.110433 | 0.000511 | 0.12502 | 8.25E-05 | 0.002377 | 0.003969 |
| 0.90 | 2186.819 | 0.000363 | 0.004451 | 0.114754 | 0.000984 | 0.131576 | 0.000168 | 0.002922 | 0.003846 |
| 0.95 | 2238.783 | 0.000397 | 0.008273 | 0.117451 | 0.001813 | 0.137838 | 0.000305 | 0.003269 | 0.003397 |
| 1.00 | 2273.56 | 0.000355 | 0.014456 | 0.117775 | 0.003228 | 0.143662 | 0.000492 | 0.003248 | 0.002646 |
| 1.05 | 2285.633 | 0.000248 | 0.023687 | 0.115041 | 0.005569 | 0.148761 | 0.000692 | 0.002787 | 0.001755 |
| 1.10 | 2273.849 | 0.000136 | 0.035785 | 0.10943 | 0.009144 | 0.152767 | 0.000837 | 0.002074 | 0.001004 |
| 1.15 | 2245.773 | 6.56E-05 | 0.049357 | 0.102333 | 0.013955 | 0.155539 | 0.000895 | 0.00142 | 0.000537 |
| 1.20 | 2210.236 | 3.05E-05 | 0.063098 | 0.095057 | 0.019826 | 0.157185 | 0.000881 | 0.000944 | 0.000285 |
| 1.25 | 2171.953 | 1.42E-05 | 0.076407 | 0.088202 | 0.026613 | 0.157848 | 0.000826 | 0.000624 | 0.000154 |
| 1.30 | 2132.874 | 6.66E-06 | 0.089091 | 0.081961 | 0.034214 | 0.15764 | 0.000747 | 0.000412 | 8.51E-05 |
| 1.35 | 2093.799 | 3.15E-06 | 0.101118 | 0.076367 | 0.042545 | 0.15666 | 0.00066 | 0.000273 | 4.77E-05 |
| 1.40 | 2055.069 | 1.50E-06 | 0.112518 | 0.07139 | 0.051522 | 0.154998 | 0.000571 | 0.00018 | 2.70E-05 |
| 1.45 | 2016.832 | 7.21E-07 | 0.123345 | 0.066975 | 0.061066 | 0.152741 | 0.000486 | 0.000119 | 1.54E-05 |
| 1.50 | 1979.149 | 3.46E-07 | 0.133662 | 0.063059 | 0.071101 | 0.149967 | 0.000407 | 7.85E-05 | 8.85E-06 |
| 1.55 | 1942.037 | 1.65E-07 | 0.143531 | 0.059581 | 0.081556 | 0.14675 | 0.000337 | 5.16E-05 | 5.10E-06 |
| 1.60 | 1905.495 | 7.89E-08 | 0.153011 | 0.056481 | 0.092369 | 0.143155 | 0.000276 | 3.37E-05 | 2.94E-06 |
| 1.65 | 1869.509 | 3.74E-08 | 0.162155 | 0.053707 | 0.103485 | 0.139237 | 0.000223 | 2.20E-05 | 1.69E-06 |
| 1.70 | 1834.063 | 1.76E-08 | 0.17101 | 0.051212 | 0.114856 | 0.135047 | 0.000178 | 1.42E-05 | 9.68E-07 |
| 1.75 | 1799.139 | 8.21E-09 | 0.179615 | 0.048956 | 0.12644 | 0.130626 | 0.000141 | 9.10E-06 | 5.53E-07 |
| 1.80 | 1764.718 | 3.78E-09 | 0.188007 | 0.046903 | 0.138204 | 0.126011 | 0.00011 | 5.80E-06 | 3.13E-07 |
| 1.85 | 1730.784 | 1.72E-09 | 0.196215 | 0.045023 | 0.150115 | 0.121232 | 8.53E-05 | 3.66E-06 | 1.77E-07 |
| 1.90 | 1697.318 | 7.72E-10 | 0.204267 | 0.04329 | 0.162148 | 0.116317 | 6.54E-05 | 2.28E-06 | 9.85E-08 |
| 1.95 | 1664.305 | 3.41E-10 | 0.212186 | 0.041679 | 0.174279 | 0.11129 | 4.96E-05 | 1.41E-06 | 5.45E-08 |
| 2.00 | 1631.727 | 1.48E-10 | 0.219992 | 0.040171 | 0.18649 | 0.10617 | 3.72E-05 | 8.63E-07 | 2.98E-08 |

2. 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

The same code was modified to vary pressure, P , and the same procedure was repeated.

Table IVb: P , T_{ad} , and χ_i of selected species.

| P [atm] | T_{ad} [K] | Equilibrium Composition, χ_i | | | | | | | |
|------------|-----------------|-----------------------------------|----------|-----------------|----------------|------------------|----------|----------|----------|
| | | O | CO | CO ₂ | H ₂ | H ₂ O | H | OH | NO |
| 1 | 2273.56 | 0.000355 | 0.014456 | 0.117775 | 0.003228 | 0.143662 | 0.000492 | 0.003248 | 0.002646 |
| 6 | 2316.117 | 0.000149 | 0.009954 | 0.122277 | 0.002117 | 0.145446 | 0.000203 | 0.002191 | 0.002325 |
| 11 | 2327.92 | 0.000109 | 0.008665 | 0.123567 | 0.001818 | 0.145923 | 0.000147 | 0.00189 | 0.002195 |
| 16 | 2334.583 | 8.87E-05 | 0.00793 | 0.124301 | 0.001651 | 0.146189 | 0.00012 | 0.001718 | 0.002111 |
| 21 | 2339.126 | 7.64E-05 | 0.007427 | 0.124805 | 0.001538 | 0.146369 | 0.000104 | 0.001601 | 0.002049 |
| 26 | 2342.524 | 6.78E-05 | 0.007049 | 0.125183 | 0.001454 | 0.146503 | 9.22E-05 | 0.001513 | 0.002 |
| 31 | 2345.214 | 6.14E-05 | 0.006749 | 0.125483 | 0.001388 | 0.146608 | 8.36E-05 | 0.001444 | 0.00196 |
| 36 | 2347.425 | 5.64E-05 | 0.006502 | 0.12573 | 0.001334 | 0.146694 | 7.69E-05 | 0.001387 | 0.001925 |

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

Similarly, data for different initial temperatures, T , was obtained.

Table IVc: T , T_{ad} , and χ_i of selected species.

| T [K] | T_{ad} [K] | Equilibrium Composition, χ_i | | | | | | | |
|----------|-----------------|-----------------------------------|----------|-----------------|----------------|------------------|----------|----------|----------|
| | | O | CO | CO ₂ | H ₂ | H ₂ O | H | OH | NO |
| 300 | 2273.56 | 0.000355 | 0.014456 | 0.117775 | 0.003228 | 0.143662 | 0.000492 | 0.003248 | 0.002646 |
| 400 | 2319.446 | 0.000506 | 0.017306 | 0.114926 | 0.003832 | 0.142584 | 0.000682 | 0.004006 | 0.003171 |
| 500 | 2364.538 | 0.000706 | 0.02045 | 0.111781 | 0.004507 | 0.14135 | 0.000927 | 0.004877 | 0.003757 |
| 600 | 2408.753 | 0.000967 | 0.023867 | 0.108365 | 0.005256 | 0.139952 | 0.001241 | 0.005863 | 0.004402 |
| 700 | 2452.094 | 0.001298 | 0.02753 | 0.104701 | 0.006077 | 0.138382 | 0.001634 | 0.006965 | 0.005104 |
| 800 | 2494.585 | 0.001713 | 0.03141 | 0.100822 | 0.006974 | 0.136633 | 0.002122 | 0.008183 | 0.005859 |
| 900 | 2536.215 | 0.002224 | 0.035462 | 0.09675 | 0.007944 | 0.134679 | 0.002718 | 0.009512 | 0.006663 |

4. Plot the effects of equivalence ratio, pressure, and initial temperature on T_{ad} and the equilibrium composition of the specified species.

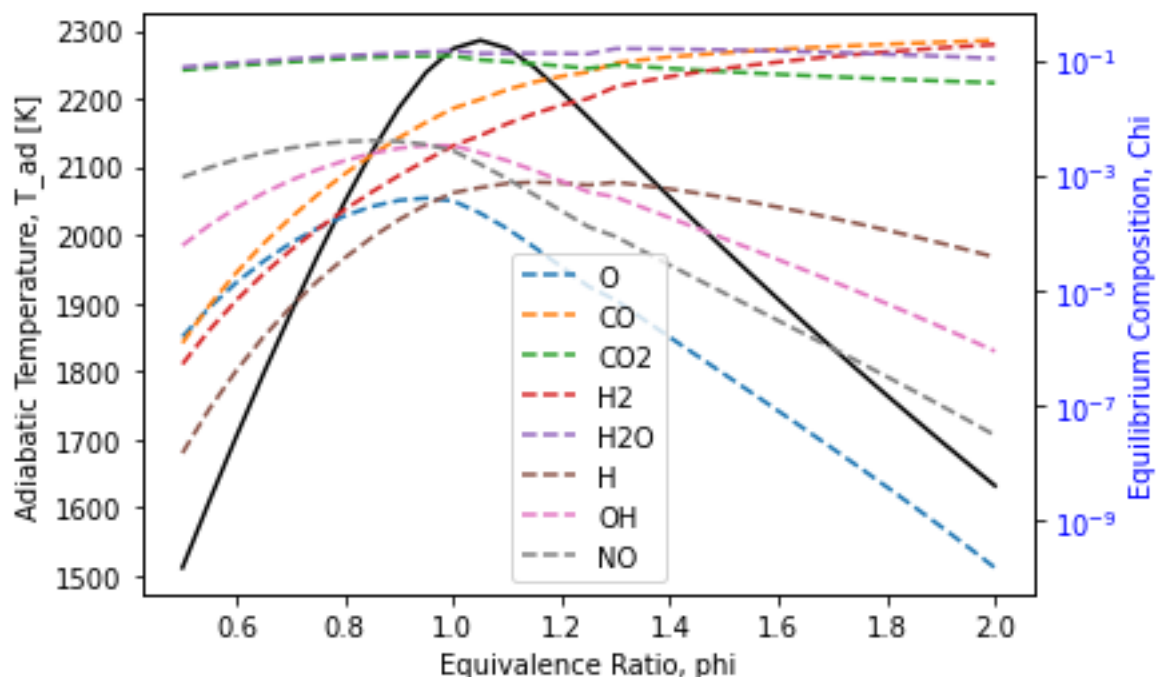


Figure IVa: Effects of ϕ on T_{ad} and the equilibrium composition of the specified species.

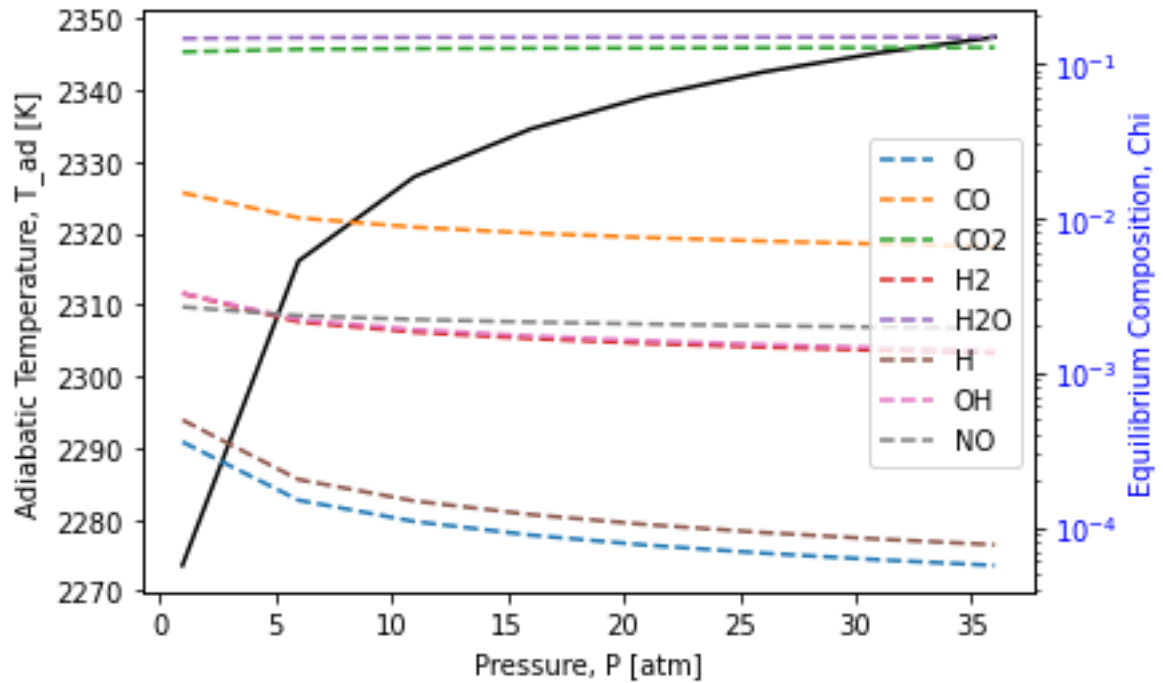


Figure IVb: Effects of P on T_{ad} and the equilibrium composition of the specified species.

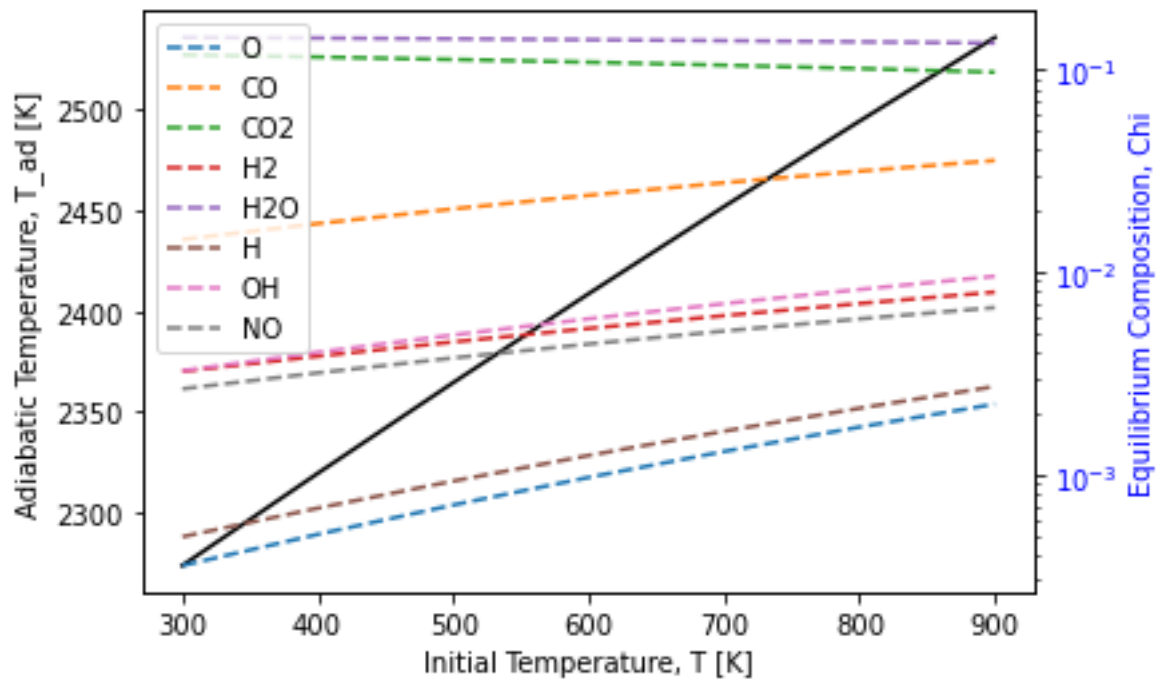


Figure IVc: Effects of T on T_{ad} and the equilibrium composition of the specified species.

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

As observed before, T_{ad} peaks at $\phi = 1.05$, and decreases going away from it. The main combustion products, CO_2 and H_2O have their mole fractions maintained at relatively higher percentage. The amount of CO and H_2 increases significantly after the fuel becomes rich, even surpassing CO_2 and H_2O at $\phi = 2$. This is expected as the complete oxidation cannot be reached due to insufficient oxygen. As for the minor species, the mole fraction O , H , OH , and NO all peaked at around the stoichiometric ratio. It must be noted that the amount of O , OH , and NO decreases drastically at fuel rich conditions with the lack of O , while there are significantly less H at fuel lean conditions.

Although the effect may be weak, T_{ad} is observed to increase with increasing pressure. While the increase is large at lower pressures, it slowly flattens out at higher pressures. It is expected that there is a theoretical limit to the increase. The mole fraction of CO_2 and H_2O increases with increasing pressure (not obvious with plot; readable from Table IVb), while the amount of all other species decreases. This phenomenon reinforces the previous claim of having higher pressures forces more complete combustion by reducing the likelihood of product dissociation. This also explains the increase in T_{ad} .

Increasing the initial temperature causes a linear increase in T_{ad} as well. This was expected as a higher initial temperature naturally means a higher final temperature given the same amount of heat added to the system. Interestingly, while the mole fraction of selected species also showed linear relationship with initial temperature, only the amount of CO_2 and H_2O was shown to decrease while the others increase. This suggests that the higher the flame temperature, the more likely the 'less stable' products are formed. This concept will be explored further in the next part.

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

Any combustion with air will lead to the emission of Nitrogen Oxides (NO_x), an important combustion pollutant

For the reaction of iso-octane and air:

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%?

To vary the mole fraction of CO_2 in the reactants, two additional arguments was added when inputting 'gas.set_equivalence_ratio'. 'diluent' was specified to be CO_2 and 'fraction = {'diluent': X_{CO_2} }' was used to set the mole fraction of CO_2 , where X represents the CO_2 mole fraction. The mole fractions of NO , NO_2 , CO and CO_2 in the product mixture was also obtained with 'mix.species_moles'. The results were tabulated and plotted below.

Table Va: Data for dilution with CO_2 .

| X_{CO_2} | T_{ad} [K] | Equilibrium Composition, Y_i | | | |
|------------|--------------|--------------------------------|----------|----------|----------|
| | | NO | NO2 | CO | CO2 |
| 0 | 2548.791 | 0.007211 | 1.01E-05 | 0.006601 | 0.105471 |
| 0.05 | 2449.63 | 0.005842 | 8.89E-06 | 0.005604 | 0.149026 |
| 0.1 | 2352.663 | 0.004503 | 7.47E-06 | 0.004143 | 0.187845 |
| 0.15 | 2256.331 | 0.003514 | 6.38E-06 | 0.002884 | 0.232254 |
| 0.2 | 2159.989 | 0.002684 | 5.39E-06 | 0.001839 | 0.277333 |
| 0.25 | 2063.644 | 0.001973 | 4.44E-06 | 0.001058 | 0.317945 |
| 0.3 | 1967.712 | 0.001429 | 3.65E-06 | 0.000564 | 0.361654 |
| 0.35 | 1872.761 | 0.001007 | 2.96E-06 | 0.000276 | 0.405544 |
| 0.4 | 1779.304 | 0.000689 | 2.36E-06 | 0.000124 | 0.4497 |
| 0.45 | 1687.692 | 0.000455 | 1.84E-06 | 5.08E-05 | 0.49417 |
| 0.5 | 1598.104 | 0.000289 | 1.41E-06 | 1.89E-05 | 0.539023 |
| 0.55 | 1510.588 | 0.000176 | 1.04E-06 | 6.35E-06 | 0.584254 |
| 0.6 | 1425.105 | 0.000102 | 7.50E-07 | 1.89E-06 | 0.629892 |
| 0.65 | 1341.569 | 5.54E-05 | 5.17E-07 | 4.95E-07 | 0.675943 |
| 0.7 | 1259.863 | 2.81E-05 | 3.39E-07 | 1.11E-07 | 0.72294 |
| 0.75 | 1179.863 | 1.30E-05 | 2.09E-07 | 2.09E-08 | 0.769546 |
| 0.8 | 1101.435 | 5.39E-06 | 1.18E-07 | 3.19E-09 | 0.816983 |
| 0.85 | 1024.444 | 1.92E-06 | 5.85E-08 | 3.84E-10 | 0.865336 |
| 0.9 | 948.7379 | 5.44E-07 | 2.33E-08 | 3.50E-11 | 0.910292 |
| 0.95* | 874.039 | 1.01E-07 | 5.76E-09 | 2.42E-12 | 0.955453 |

Note: At $X_{CO_2} = 0.95$, T does not converge with Gibbs Free Energy Minimization. Hence, the solver was set to auto to try other algorithms and convergence was obtained.

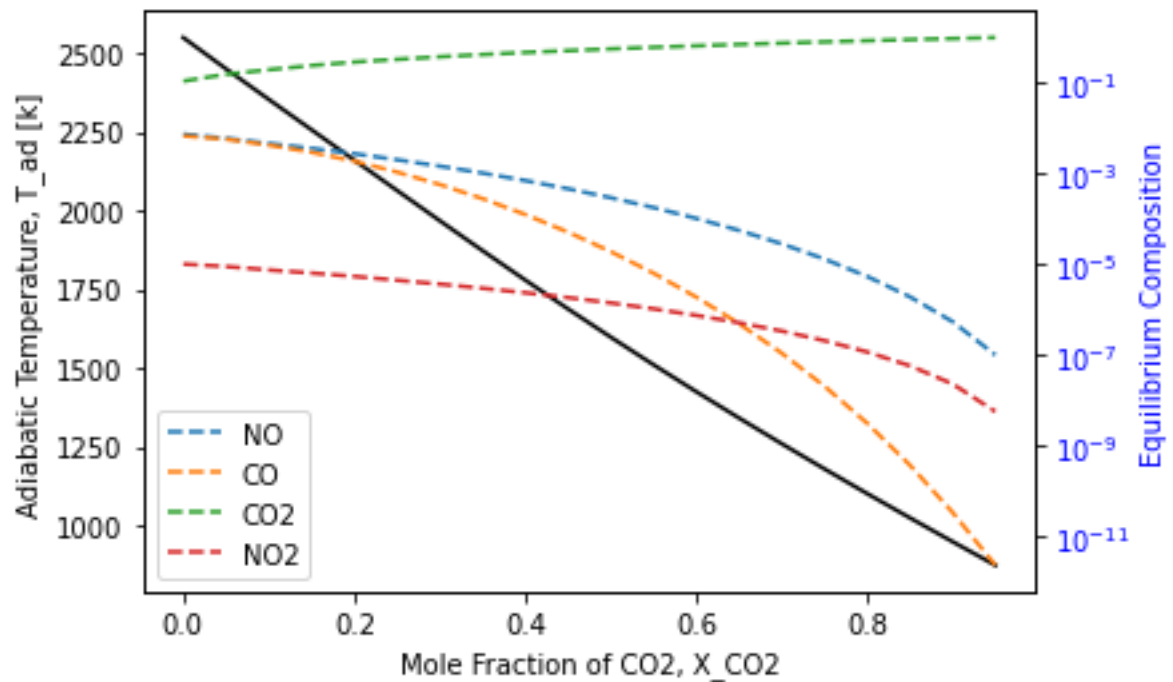


Figure Va: Effect of dilution with CO₂ on T_{ad} (black) and equilibrium composition of certain species.

From the figure it is clear that T_{ad} decreases linearly as the mole fraction of CO₂ in reactant increases. This is expected as the heat released from the fuel is now used to increase the temperature of larger amount of products. Naturally, the percentage of CO₂ at equilibrium also increases as a result of having more CO₂ in the mixture initially. The equilibrium composition of NO, CO, and NO₂ decreases with increasing dilution. This supports the previous claim that these ‘less stable’ products are less likely to form at lower temperatures. This is especially true for NO_x products as N₂ has very strong triple covalent bond.

If, theoretically speaking, the mole fraction of CO₂ at reactant mixture was raised to 100%, then no fuel will be present. As a result, combustion will not occur and the temperature of the mixture (now containing only CO₂) will maintain at 800K.

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

The same procedure was repeated using H₂O as the diluent.

Table Vb: Data for dilution with H₂O.

| X_{H_2O} | T_{ad} [K] | Equilibrium Composition, z_i | | | |
|------------|--------------|--------------------------------|-----------------|----------|-----------------|
| | | NO | NO ₂ | CO | CO ₂ |
| 0 | 2548.791 | 0.007211 | 1.01E-05 | 0.006601 | 0.105471 |
| 0.05 | 2471.041 | 0.006057 | 8.85E-06 | 0.004492 | 0.104395 |
| 0.1 | 2391.226 | 0.004997 | 7.73E-06 | 0.002893 | 0.101943 |
| 0.15 | 2309.33 | 0.004026 | 6.67E-06 | 0.001749 | 0.097886 |
| 0.2 | 2225.597 | 0.003154 | 5.66E-06 | 0.000986 | 0.092296 |
| 0.25 | 2140.419 | 0.002443 | 4.80E-06 | 0.000527 | 0.087109 |
| 0.3 | 2054.228 | 0.001852 | 4.03E-06 | 0.000265 | 0.081709 |
| 0.35 | 1967.408 | 0.001369 | 3.34E-06 | 0.000124 | 0.076199 |
| 0.4 | 1880.249 | 0.000983 | 2.72E-06 | 5.39E-05 | 0.070516 |
| 0.45 | 1792.934 | 0.000682 | 2.17E-06 | 2.15E-05 | 0.064733 |
| 0.5 | 1705.549 | 0.000455 | 1.69E-06 | 7.83E-06 | 0.058926 |
| 0.55 | 1618.097 | 0.000291 | 1.28E-06 | 2.55E-06 | 0.053207 |
| 0.6 | 1530.514 | 0.000176 | 9.30E-07 | 7.29E-07 | 0.047355 |
| 0.65 | 1442.681 | 9.99E-05 | 6.50E-07 | 1.78E-07 | 0.041481 |
| 0.7 | 1354.429 | 5.20E-05 | 4.29E-07 | 3.56E-08 | 0.035458 |
| 0.75 | 1265.541 | 2.46E-05 | 2.65E-07 | 5.61E-09 | 0.029598 |
| 0.8 | 1175.747 | 1.02E-05 | 1.49E-07 | 6.50E-10 | 0.023723 |
| 0.85 | 1084.721 | 3.48E-06 | 7.27E-08 | 4.99E-11 | 0.017817 |
| 0.9 | 992.0621 | 9.02E-07 | 2.81E-08 | 2.19E-12 | 0.011895 |
| 0.95 | 897.2897 | 1.40E-07 | 6.49E-09 | 4.13E-14 | 0.005955 |

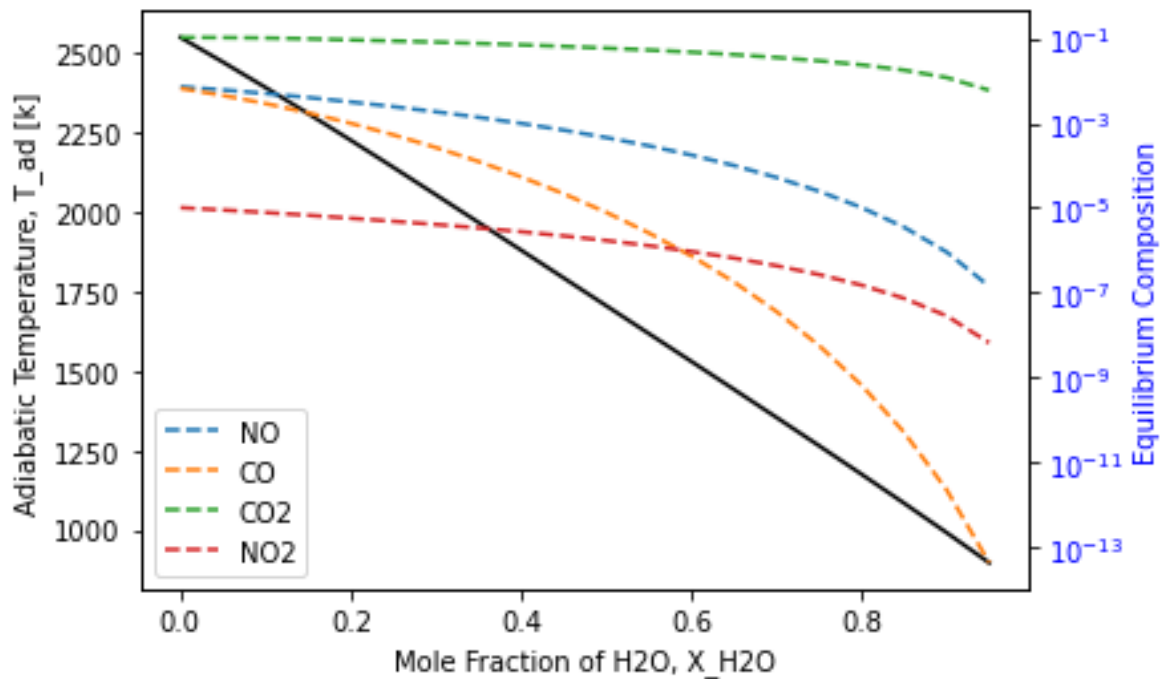


Figure Vb: Effect of dilution with H₂O on T_{ad} (black) and equilibrium composition of certain species.

It was observed that the dilution with both CO₂ and H₂O decreases the adiabatic temperature linearly. The adiabatic temperatures were slightly lower when CO₂ was used as the diluent, this is likely due to CO₂ having greater C_p values on mole basis when compared to H₂O. Hence, it was able to lower the temperature more. Both diluents have similar effects on decreasing the mole fraction of NO, NO₂, and CO. When diluting with H₂O, the equilibrium composition of CO₂ drops, as opposite to the situation when CO₂ was used as the diluent. The observation was expected as using CO₂ as the diluent obviously increases the equilibrium composition of CO₂.

3. What would happen if we were to remove N_2 from air in the combustion of iso-octane and air?

If N_2 was removed, it was expected that the adiabatic temperature will increase. In the previously established chemical equation for combustion of iso-octane and air, N_2 does not participate in the chemical reaction, therefore it is effectively acting as a diluent. If the diluent was removed, the adiabatic temperature increases due to having less product to distribute the heat. Additionally, it was predicted that the by-products of nitrogen (NO_x etc.) will not be formed in the absence of nitrogen.

Bonus points – Repeat question V.1 with the dilution of an inert Ar and explain your results.

Table Vc: Data for dilution with Ar.

| X_{AR} | T_{ad} [K] | Equilibrium Composition, z_i | | | |
|----------|--------------|--------------------------------|----------|----------|----------|
| | | NO | NO2 | CO | CO2 |
| 0 | 2548.791 | 0.007669 | 1.07E-05 | 0.007021 | 0.112184 |
| 0.05 | 2515.501 | 0.006853 | 9.61E-06 | 0.005825 | 0.10742 |
| 0.1 | 2479.296 | 0.006067 | 8.58E-06 | 0.004726 | 0.102558 |
| 0.15 | 2439.819 | 0.005315 | 7.61E-06 | 0.003735 | 0.097589 |
| 0.2 | 2396.674 | 0.004601 | 6.70E-06 | 0.002861 | 0.092503 |
| 0.25 | 2349.434 | 0.003926 | 5.85E-06 | 0.002112 | 0.087292 |
| 0.3 | 2297.645 | 0.003296 | 5.06E-06 | 0.001491 | 0.081953 |
| 0.35 | 2240.843 | 0.002713 | 4.32E-06 | 0.000999 | 0.076485 |
| 0.4 | 2178.563 | 0.002182 | 3.65E-06 | 0.000628 | 0.070895 |
| 0.45 | 2110.349 | 0.001705 | 3.03E-06 | 0.000366 | 0.065197 |
| 0.5 | 2035.751 | 0.001287 | 2.46E-06 | 0.000195 | 0.059408 |
| 0.55 | 1954.306 | 0.000929 | 1.95E-06 | 9.27E-05 | 0.05355 |
| 0.6 | 1865.51 | 0.000636 | 1.49E-06 | 3.85E-05 | 0.047644 |
| 0.65 | 1768.785 | 0.000405 | 1.09E-06 | 1.34E-05 | 0.041708 |
| 0.7 | 1663.445 | 0.000235 | 7.52E-07 | 3.70E-06 | 0.035758 |
| 0.75 | 1548.685 | 0.000121 | 4.79E-07 | 7.49E-07 | 0.029801 |
| 0.8 | 1423.579 | 5.19E-05 | 2.73E-07 | 9.83E-08 | 0.023841 |
| 0.85 | 1287.117 | 1.72E-05 | 1.31E-07 | 6.84E-09 | 0.017881 |
| 0.9 | 1138.268 | 3.75E-06 | 4.74E-08 | 1.78E-10 | 0.011921 |
| 0.95 | 976.1015 | 3.77E-07 | 9.32E-09 | 8.83E-13 | 0.00596 |

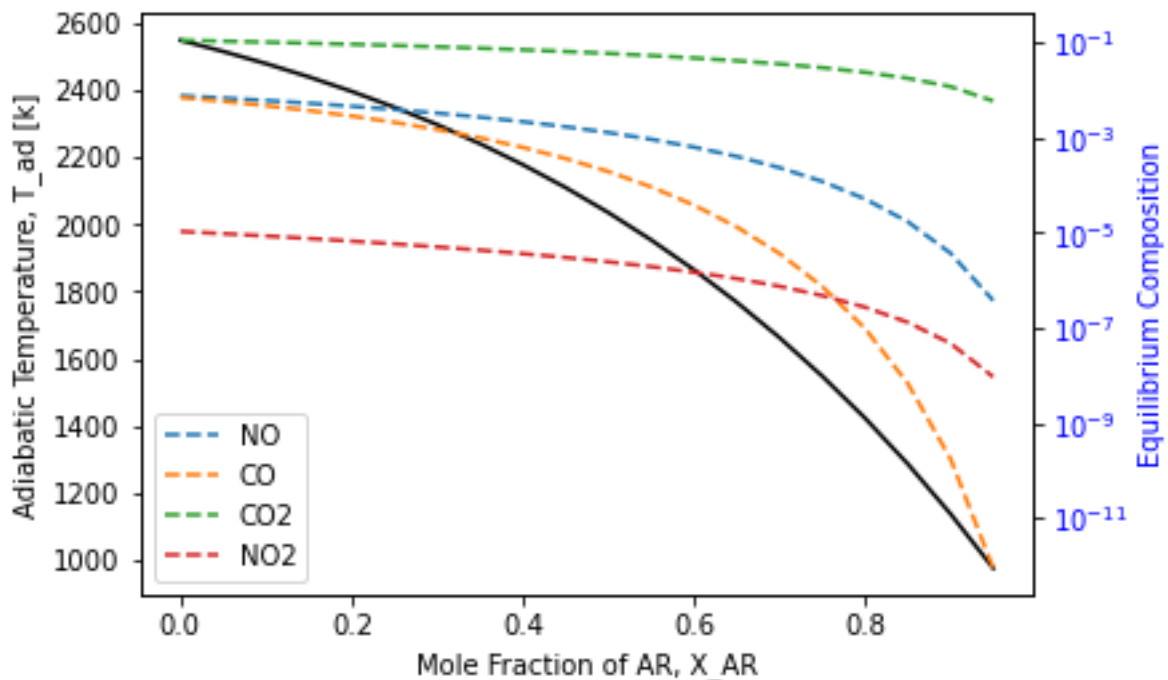


Figure Vc: Effect of dilution with Ar on T_{ad} (black) and equilibrium composition of certain species

The temperature does not decrease as much compared to the other two diluents as argon is a monoatomic gas and therefore has only 3 activation modes. Nevertheless, the equilibrium composition of selected molecules still showed the same behavior as when diluted with H_2O .

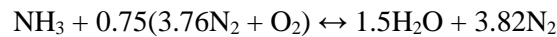
Part VI – Relate this assignment to your design project

Using the alternative fuel that you have selected for your group's design project, and following this assignment as a guideline, determine:

- The chemical model you will need to use Cantera

Our group chose ammonia, NH_3 as the topic of interest.

- The complete reaction (with air)



- The adiabatic temperature with varying equivalence ratio, initial temperature, and pressure.

The codes from Part IV were reused using NH_3 as fuel. When not varied, ϕ was kept at 1, initial temperature was kept at 300K and initial pressure was kept at 1 atm.

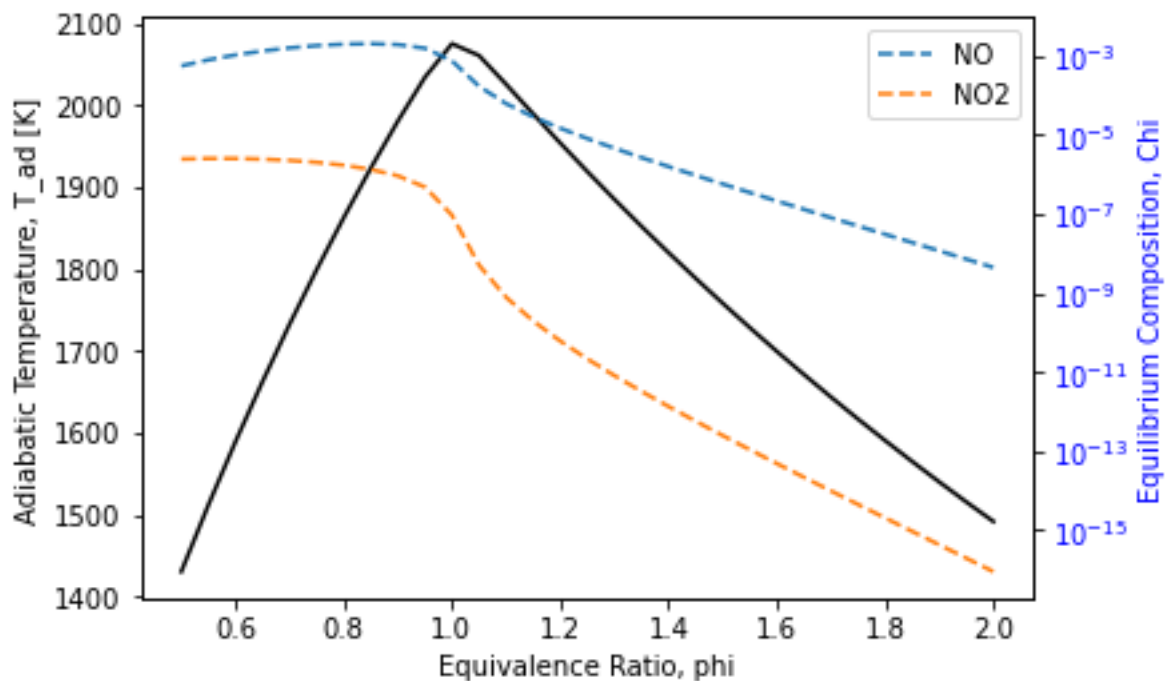
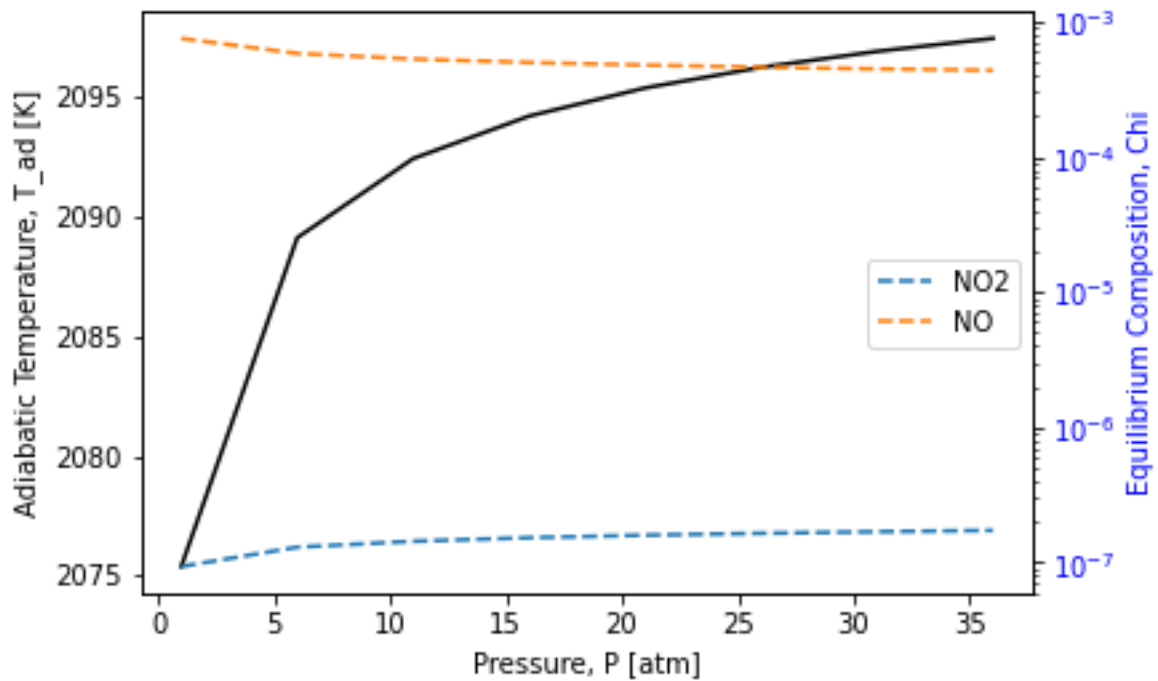
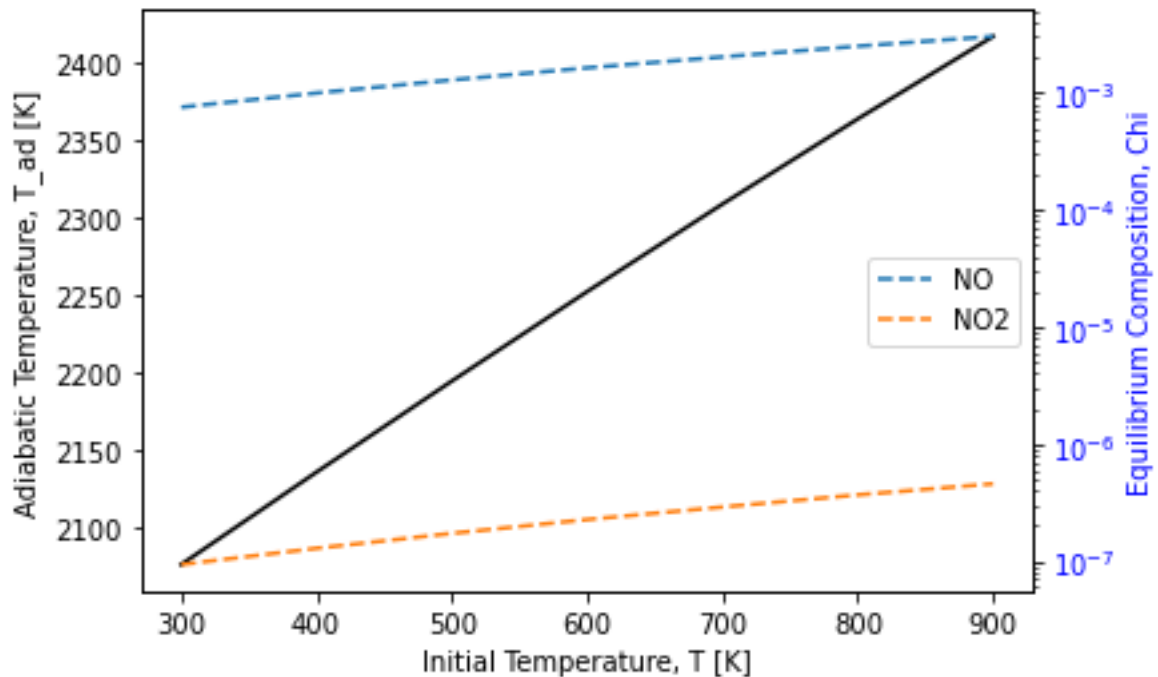


Figure VIa: Effects of ϕ on T_{ad} and the equilibrium composition NO_x .

Figure VIb: Effects of P on T_{ad} and the equilibrium composition NO_x .Figure VIc: Effects of T on T_{ad} and the equilibrium composition NO_x .

- **The concentration of the main pollutants after equilibrium**

Without any C present in the reactants, the main pollutant of this reaction will be NO and NO_2 . Their concentration at equilibrium was shown at previous figures with varying ϕ , pressure, and temperature.