PROJECT ASSIGNMENT #1: COMBUSTION THERMODYNAMICS

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Submitted to:
Professor. Jeffrey Bergthorson
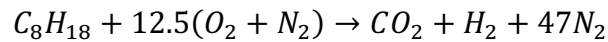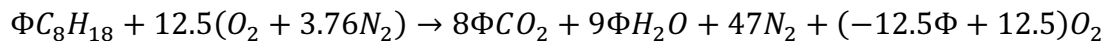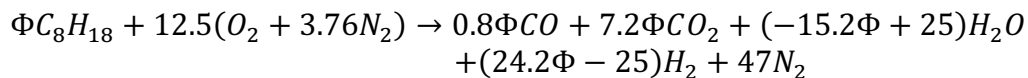
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Part I – Introduction to thermodynamics data:

Results from using the report of McBride et al.:

	C8H18	O2	N2	CO2	H2O	CO	H2
Enthalpy at 298.15K (KJ/mol)	-224.009	0.000	0.000	-393.508	-241.825	-110.535	0.000
Entropy at 298.15K (KJ/mol-K)	0.423	0.205	0.192	0.214	0.189	0.198	0.131
Enthalpy at 2000K (KJ/mol)	552.096	59.201	56.136	-302.071	-168.782	-53.799	52.950
Entropy at 2000K (KJ/mol-K)	1.171	0.269	0.252	0.309	0.265	0.259	0.188

Part II - Complete combustion

1. Global reaction equations

At stoichiometric($\Phi = 1$)

$$C_8H_{18} + 12.5(O_2 + N_2) \rightarrow CO_2 + H_2 + 47N_2$$

Fuel lean($\Phi < 1$):

$$\Phi C_8H_{18} + 12.5(O_2 + 3.76N_2) \rightarrow 8\Phi CO_2 + 9\Phi H_2O + 47N_2 + (-12.5\Phi + 12.5)O_2$$

Fuel rich($\Phi > 1$):

$$\Phi C_8H_{18} + 12.5(O_2 + 3.76N_2) \rightarrow 0.8\Phi CO + 7.2\Phi CO_2 + (-15.2\Phi + 25)H_2O$$
$$+(24.2\Phi - 25)H_2 + 47N_2$$

2. LHV and HHV comparison

The lower heating value at 300K can be calculated as follows:

$$\widetilde{q_{LHV}} = -h(C_8H_{18}) - 12.5h(O_2) + 8h(CO_2) + 9h(H_2O_{(g)}) = -5100392.819 kJ/kmol$$

$$q_{LHV} = \widetilde{q_{LHV}}/114 = -44.7407 MJ/kg$$

The higher heating value at 300K can be calculated as follow:

$$\widetilde{q_{HHV}} = -h(C_8H_{18}) - 12.5h(O_2) + 8h(CO_2) + 9h(H_2O_{(l)}) = -5496911.204 kJ/kmol$$

$$q_{\text{HHV}} = \widetilde{q_{\text{HHV}}}/114 = -48.219 Mj/kg$$

Comparing with literature value:

	Computed value (MJ/kg)	Course slide value (MJ/kg)	Internet researched value (MJ/kg)
LHV	-44.741	-44.430	-44.651
HHV	-48.219	-47.890	-48.119

- HHV is always higher than LHV since water exist latent heat for vaporization

Although there exists small gap between the computed value and course slide value, the computed values are highly aligned with the internet researched value from the book (S. McAllister et al., Fundamentals of Combustion Processes). In conclusion I think the difference is small and negligible.

3. Adiabatic flame temperature estimation with constant C_p:

Phi	Tad_estimation (K)	Phi	Tad_estimation (K)
0.5	1717.342545	1.05	2957.496077
0.55	1853.594189	1.1	2897.512477
0.6	1988.86009	1.15	2839.06114
0.65	2123.150906	1.2	2782.084094
0.7	2256.477143	1.25	2726.526258
0.75	2388.849157	1.3	2672.335256
0.8	2520.277154	1.35	2619.461263
0.85	2650.771199	1.4	2567.856842
0.9	2780.341209	1.45	2517.476812
0.95	2908.996967	1.5	2468.278106
1	3019.072992		

T_ad_estimation_max (K)	@ Phi
3019.072992	1

4. Adiabatic flame temperature estimation with integrated C_p:

Phi	Tad_integration (K)	Phi	Tad_integration (K)
0.5	1511.9443	1.05	2357.1678
0.55	1611.50358	1.1	2319.96217
0.6	1708.35635	1.15	2283.38067
0.65	1802.67053	1.2	2247.4029
0.7	1894.58947	1.25	2212.01499
0.75	1984.24193	1.3	2177.20214
0.8	2071.74254	1.35	2142.95009

0.85	2157.1948	1.4	2109.24511
0.9	2240.69285	1.45	2076.07393
0.95	2322.32287	1.5	2043.42374
1	2395.00973		

T_ad_integration_max (K)	@ Phi
2395.00973	1

5. Plot of T_ad against Φ :
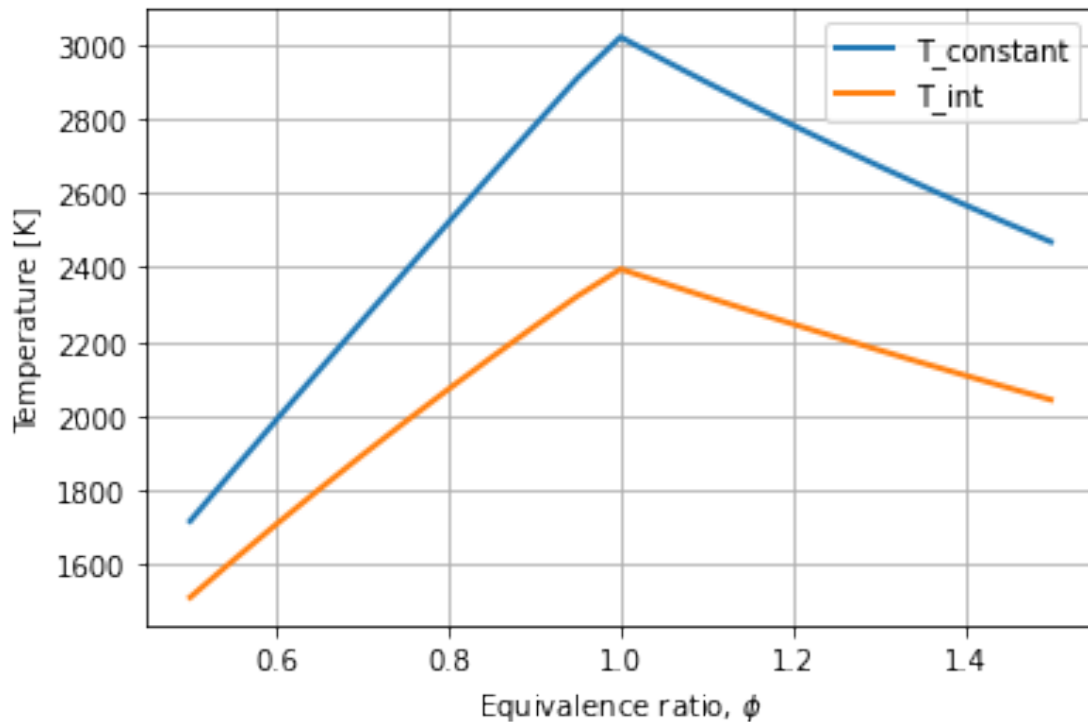
The adiabatic flame temperature (y-axis) against Φ (x-axis)

Note that the T_constant in above figure stand for T_ad_estimation (constant Cp) and T_int stand for T_ad_integration.

- Both plots have the same trend, peaked at Φ = 1 since theoretically, fuel is fully oxidized to produce maximum heat output and no excessive product is formed to be heated by the heat released.
- The adiabatic flame temperature obtained from integrated Cp is much smaller than that from assuming the constant Cp, since Cp value is increasing as temperature increases. Therefore, the result is expected.

Part III – Calculation through Cantera:
1. The result and plot

The following result and plot are obtained at T=300K and 1 atm.

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phi	T_ad_equi (K)	phi	T_ad_equi (K)
0.5	1511.33968	1.3	2132.87418
0.55	1609.68816	1.35	2093.79879
0.6	1704.82397	1.4	2055.06876
0.65	1796.71843	1.45	2016.83221
0.7	1885.16694	1.5	1979.14913
0.75	1969.67783	1.55	1942.03744
0.8	2049.3145	1.6	1905.49465
0.85	2122.50123	1.65	1869.50852
0.9	2186.81929	1.7	1834.06254
0.95	2238.78257	1.75	1799.1386
1	2273.55994	1.8	1764.71841
1.05	2285.63329	1.85	1730.78407
1.1	2273.84853	1.9	1697.31833
1.15	2245.77256	1.95	1664.30462
1.2	2210.23615	2	1631.72697
1.25	2171.95305		
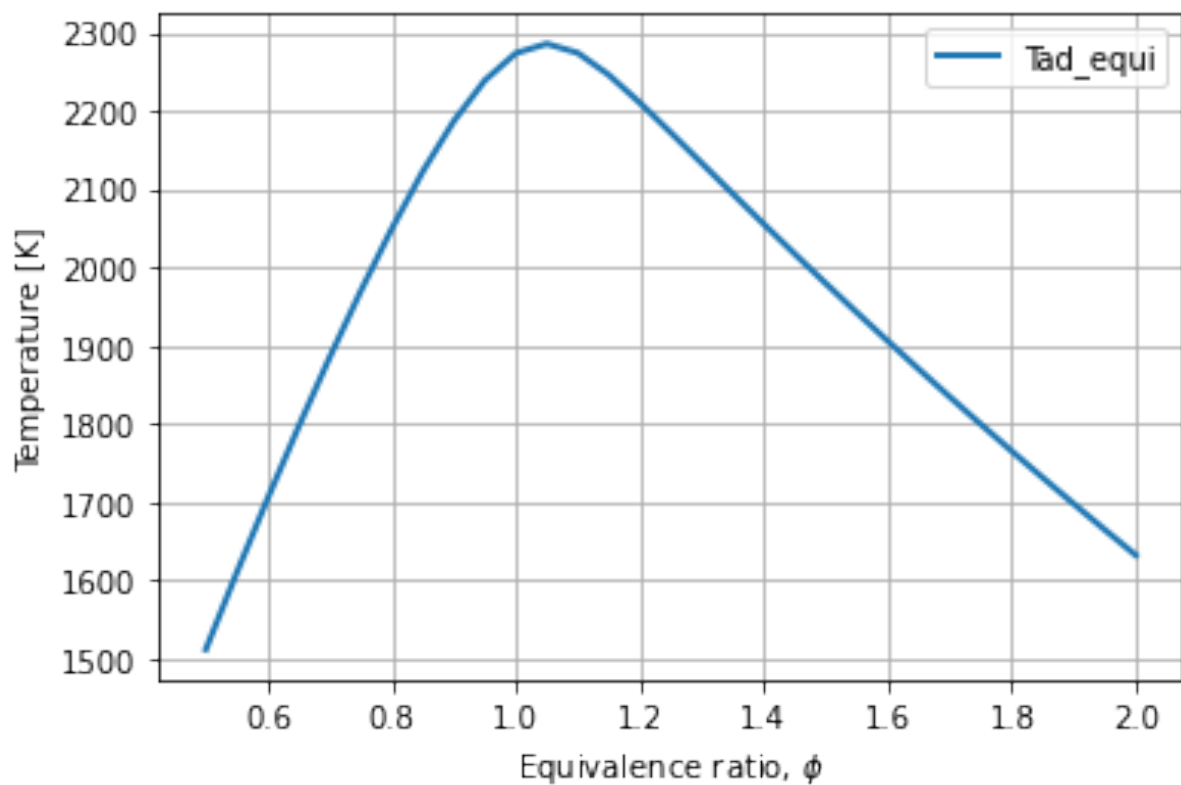
Adiabatic flame temperature vs Φ using cantera

2. Maximum flame temperature

| T_ad_equilibrium_max (K)	@ Phi
2285.63329	1.05

- The maximum adiabatic flame temperature occurred as slightly over stoichiometric equivalence ratio since the little added fuel in the reactant have promoted the combustion process
- The reaction could never make the isoocatane in the product to be zero, in the other word, there is always not-reacted isooctane left as product in the reaction, unless the pressure of the reaction approaches to infinite. Therefore, the C8H18 at stoichiometric ratio cannot have a complete combustion.
- CO2 formed in the product will dissociate into CO (H2O dissociate to H2 as well). Slightly more fuel in the reactant could also promote the reaction with CO formed in the reactant to contribute to full combustion.

3. Results comparison with Cantera and estimations
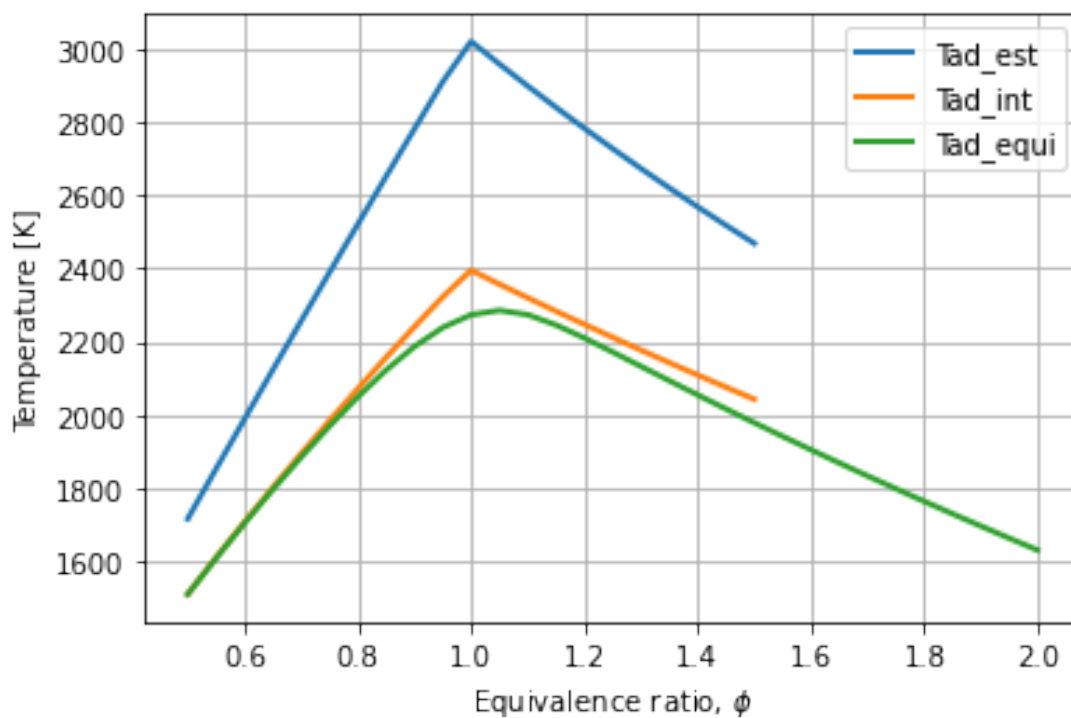
- The adiabatic flame temperature formed from using the integration Cp method is somewhat aligned with the result from Cantera.
- The plot from the integration method can be seen as the combustion result under 'optimal' and 'idealized' conditions
- The plot of the equilibrium condition in Cantera has the lowest adiabatic flame temperature, due to the fact that Cantera considers a lot non-idealized product and energy were taken up by those product to heat them up to the flame temperature. Hence, its temperatures are the lowest.

4. Bonus I – H2 compare with C8H18
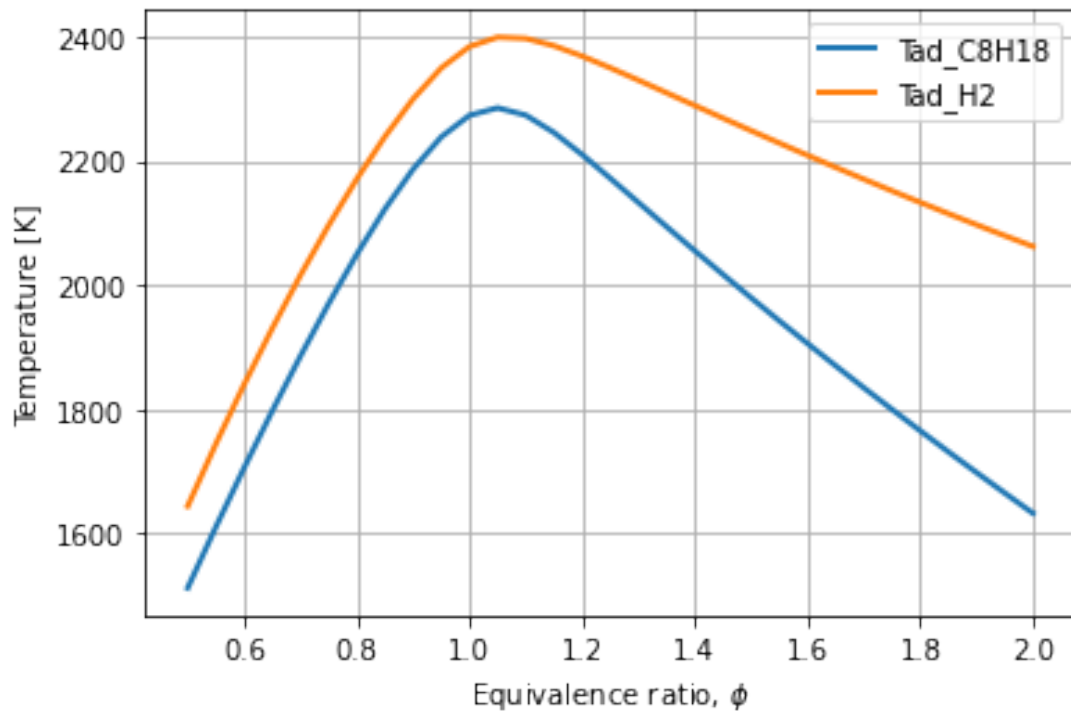
Adiabatic flame temperature of two substances vs equivalence ratio

- The adiabatic flame temperature of hydrogen is higher than that of the isooctane since hydrogen contains more energy per mole of mass.
- H2 needs less energy per mole to dissociate it compare to C8H18, that could be one of the reasons why it has an increased adiabatic flame temperature compared to C8H18.

Part IV – Parameters affecting T_ad:

1. Species concentrations at different equivalence ratios:

phi	T (K)	O	H	OH	H2	H2O	CO	CO2	NO
0.5	1511.34	1.53E-06	9.15E-04	9.15E-04	5.15E-07	7.50E-02	1.20E-06	6.67E-02	9.15E-04
0.55	1609.69	4.99E-06	1.35E-03	1.35E-03	2.02E-06	8.24E-02	5.44E-06	7.33E-02	1.35E-03
0.6	1704.82	1.36E-05	1.86E-03	1.86E-03	6.67E-06	8.97E-02	2.03E-05	7.98E-02	1.86E-03
0.65	1796.72	3.18E-05	2.41E-03	2.41E-03	1.92E-05	9.70E-02	6.45E-05	8.64E-02	2.41E-03
0.7	1885.17	6.54E-05	2.96E-03	2.96E-03	4.92E-05	1.04E-01	1.81E-04	9.28E-02	2.96E-03
0.75	1969.68	1.20E-04	3.45E-03	3.45E-03	1.15E-04	1.11E-01	4.56E-04	9.91E-02	3.45E-03
0.8	2049.31	1.96E-04	3.81E-03	3.81E-03	2.51E-04	1.18E-01	1.05E-03	1.05E-01	3.81E-03
0.85	2122.50	2.84E-04	3.97E-03	3.97E-03	5.11E-04	1.25E-01	2.24E-03	1.10E-01	3.97E-03
0.9	2186.82	3.63E-04	3.85E-03	3.85E-03	9.84E-04	1.32E-01	4.45E-03	1.15E-01	3.85E-03
0.95	2238.78	3.97E-04	3.40E-03	3.40E-03	1.81E-03	1.38E-01	8.27E-03	1.17E-01	3.40E-03
1	2273.56	3.55E-04	2.65E-03	2.65E-03	3.23E-03	1.44E-01	1.45E-02	1.18E-01	2.65E-03
1.05	2285.63	2.16E-04	1.53E-03	1.53E-03	4.86E-03	1.30E-01	2.07E-02	1.00E-01	1.53E-03
1.1	2273.85	1.16E-04	8.59E-04	8.59E-04	7.82E-03	1.31E-01	3.06E-02	9.36E-02	8.59E-04

1.15	2245.77	5.52E-05	4.51E-04	4.51E-04	1.17E-02	1.31E-01	4.15E-02	8.60E-02	4.51E-04
1.2	2210.24	2.52E-05	2.36E-04	2.36E-04	1.64E-02	1.30E-01	5.22E-02	7.86E-02	2.36E-04
1.25	2171.95	1.15E-05	1.25E-04	1.25E-04	2.16E-02	1.28E-01	6.19E-02	7.15E-02	1.25E-04
1.3	2132.87	6.66E-06	8.51E-05	8.51E-05	3.42E-02	1.58E-01	8.91E-02	8.20E-02	8.51E-05
1.35	2093.80	3.15E-06	4.77E-05	4.77E-05	4.25E-02	1.57E-01	1.01E-01	7.64E-02	4.77E-05
1.4	2055.07	1.50E-06	2.70E-05	2.70E-05	5.15E-02	1.55E-01	1.13E-01	7.14E-02	2.70E-05
1.45	2016.83	7.21E-07	1.54E-05	1.54E-05	6.11E-02	1.53E-01	1.23E-01	6.70E-02	1.54E-05
1.5	1979.15	3.46E-07	8.85E-06	8.85E-06	7.11E-02	1.50E-01	1.34E-01	6.31E-02	8.85E-06
1.55	1942.04	1.65E-07	5.10E-06	5.10E-06	8.16E-02	1.47E-01	1.44E-01	5.96E-02	5.10E-06
1.6	1905.49	7.89E-08	2.94E-06	2.94E-06	9.24E-02	1.43E-01	1.53E-01	5.65E-02	2.94E-06
1.65	1869.51	3.74E-08	1.69E-06	1.69E-06	1.03E-01	1.39E-01	1.62E-01	5.37E-02	1.69E-06
1.7	1834.06	1.76E-08	9.68E-07	9.68E-07	1.15E-01	1.35E-01	1.71E-01	5.12E-02	9.68E-07
1.75	1799.14	8.21E-09	5.53E-07	5.53E-07	1.26E-01	1.31E-01	1.80E-01	4.90E-02	5.53E-07
1.8	1764.72	3.78E-09	3.13E-07	3.13E-07	1.38E-01	1.26E-01	1.88E-01	4.69E-02	3.13E-07
1.85	1730.78	1.72E-09	1.77E-07	1.77E-07	1.50E-01	1.21E-01	1.96E-01	4.50E-02	1.77E-07
1.9	1697.32	7.72E-10	9.85E-08	9.85E-08	1.62E-01	1.16E-01	2.04E-01	4.33E-02	9.85E-08
1.95	1664.30	3.41E-10	5.45E-08	5.45E-08	1.74E-01	1.11E-01	2.12E-01	4.17E-02	5.45E-08
2	1631.73	1.48E-10	2.98E-08	2.98E-08	1.86E-01	1.06E-01	2.20E-01	4.02E-02	2.98E-08
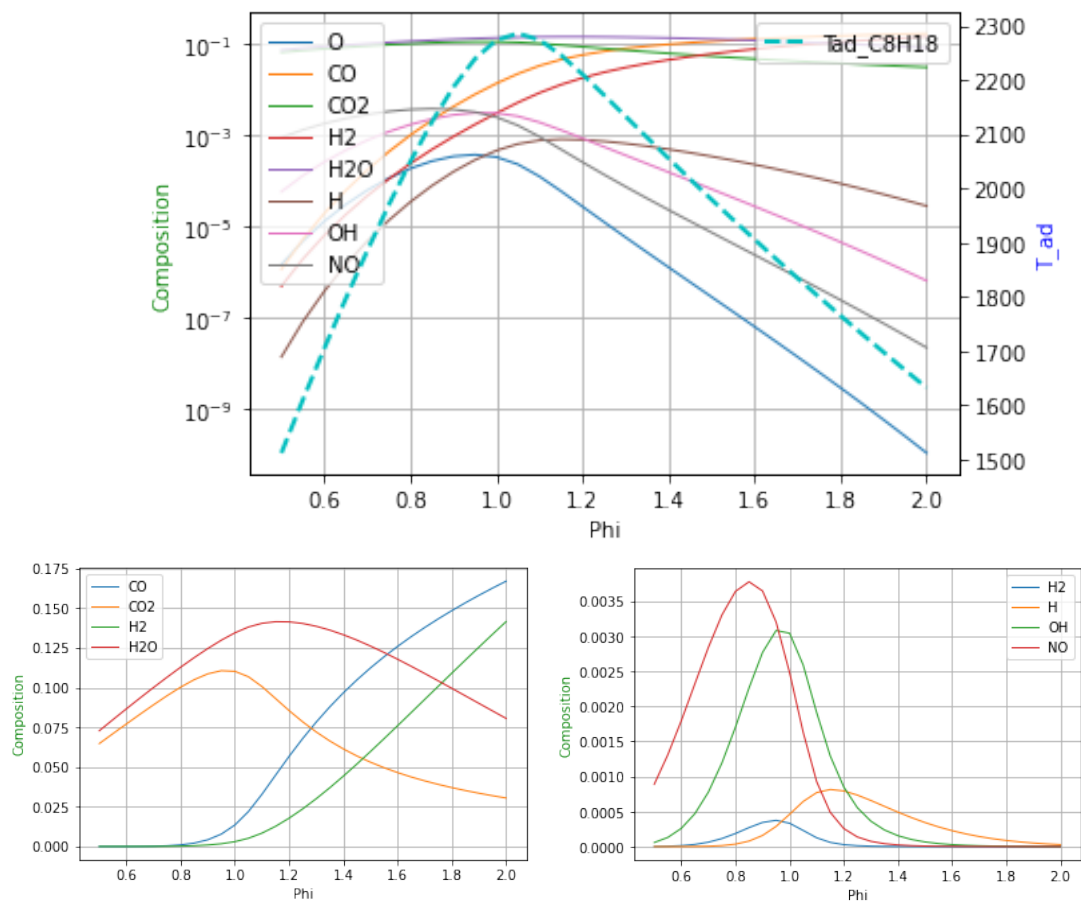
Top: Composition of all products in logarithm, Tad vs phi, bottom left: major species in linear vs phi, bottom right: minor species in linear vs phi

- Composition of CO and H2 have a significant increase as the equivalence ratio exceeds 1
- All other products have a favour of specific equivalence ratio to have a peak
- CO2 peaks at equivalence ratio = 1 since that's around the complete reaction, and no excess O2 are produced
- H2O peaks at equivalence ratio just passed 1, going onto the fuel rich side.
- The trend between CO2 and CO, H2O and H2 are very similar, CO2 and H2O both reach its peak right after the formation of CO and H2 starts.
- NO, O and OH peaks just before stoichiometric ratio, on fuel lean side.
- NO peaks since flame temperature at such equivalence ratio become high enough to oxidize the N2 in the product with O2 to form NO.
- The peak of O and OH are aligned since water will dissociate into O and OH together, hence they peaked at same ratio

2. Species concentrations at different pressures:

Pressure	T (K)	O	H2	H	OH	H2O	NO	CO	CO2
101325	2273.559937	3.55E-04	3.23E-03	4.92E-04	3.25E-03	1.44E-01	2.85E-17	1.45E-02	1.18E-01
607950	2316.116999	1.49E-04	2.12E-03	2.03E-04	2.19E-03	1.45E-01	6.35E-17	9.95E-03	1.22E-01

| 1114575	2327.919851	1.09E-04	1.82E-03	1.47E-04	1.89E-03	1.46E-01	7.94E-17	8.66E-03	1.24E-01
1621200	2334.583337	8.87E-05	1.65E-03	1.20E-04	1.72E-03	1.46E-01	9.03E-17	7.93E-03	1.24E-01
2127825	2339.125652	7.64E-05	1.54E-03	1.04E-04	1.60E-03	1.46E-01	9.86E-17	7.43E-03	1.25E-01
2634450	2342.524247	6.78E-05	1.45E-03	9.22E-05	1.51E-03	1.47E-01	1.05E-16	7.05E-03	1.25E-01
3141075	2345.214007	6.14E-05	1.39E-03	8.36E-05	1.44E-03	1.47E-01	1.11E-16	6.75E-03	1.25E-01
3647700	2347.424599	5.64E-05	1.33E-03	7.69E-05	1.39E-03	1.47E-01	1.16E-16	6.50E-03	1.26E-01
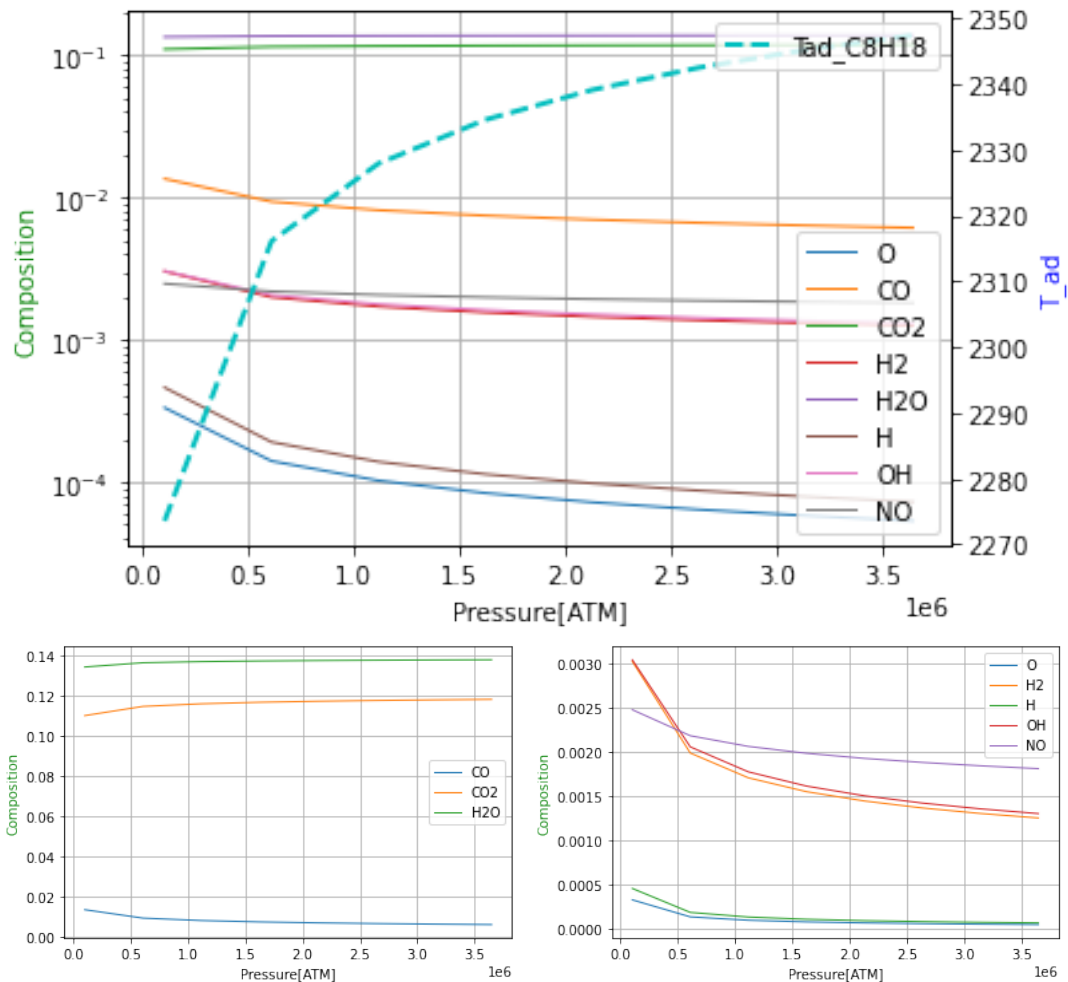
Top: Composition of all products in logarithm, Tad vs pressure, bottom left: major species in linear vs pressure, bottom right: minor species in linear vs pressure

- The molar fraction of CO_2, H_2O increases as pressure increases since they are the main product of the reaction.
- Molar fraction of all other minor species in the product decreases as the pressure increases.
- Both bullet points above have indicated a more complete combustion as pressure increases.
- A more complete combustion at higher pressure have made a higher adiabatic flame temperature. Therefore, the T_{ad} increases as pressure increases.

3. Species concentration at different temperatures:

T_in	T (K)	O	H2	H	OH	H2O	CO	N	NO
300	2273.559937	3.55E-04	3.23E-03	4.92E-04	3.25E-03	1.44E-01	1.45E-02	1.18E-01	2.65E-03
400	2319.446165	5.06E-04	3.83E-03	6.82E-04	4.01E-03	1.43E-01	1.73E-02	1.15E-01	3.17E-03
500	2364.538248	7.06E-04	4.51E-03	9.27E-04	4.88E-03	1.41E-01	2.05E-02	1.12E-01	3.76E-03
600	2408.752787	9.67E-04	5.26E-03	1.24E-03	5.86E-03	1.40E-01	2.39E-02	1.08E-01	4.40E-03
700	2452.094131	1.30E-03	6.08E-03	1.63E-03	6.97E-03	1.38E-01	2.75E-02	1.05E-01	5.10E-03
800	2494.584992	1.71E-03	6.97E-03	2.12E-03	8.18E-03	1.37E-01	3.14E-02	1.01E-01	5.86E-03
900	2536.214896	2.22E-03	7.94E-03	2.72E-03	9.51E-03	1.35E-01	3.55E-02	9.68E-02	6.66E-03
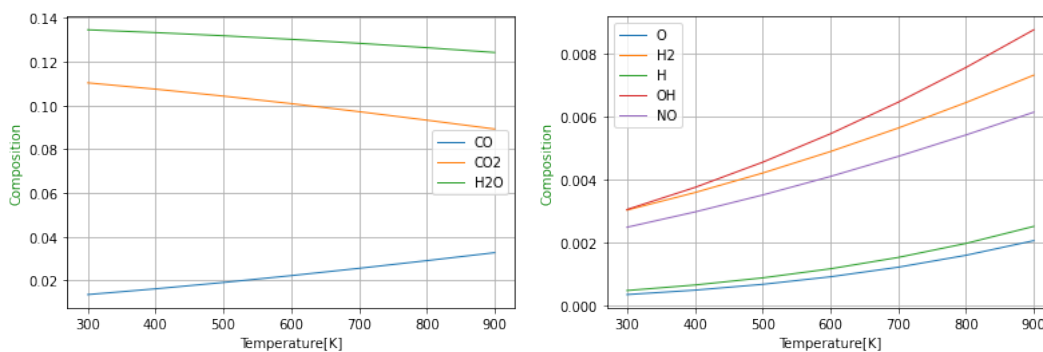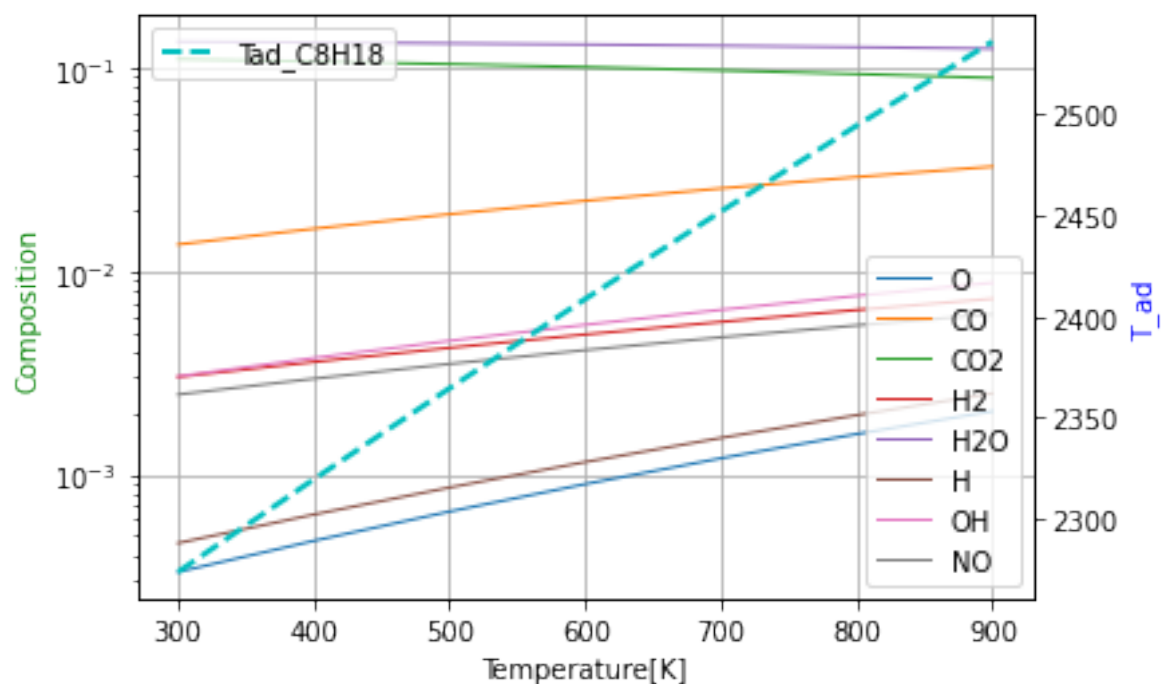
Top: Composition of all products in logarithm, Tad vs T_in, bottom left: major species in linear vs T_in, bottom right: minor species in linear vs T_in

- As initial temperature increases, less major products (CO_2 and H_2O) are formed.
- As initial temperature increases, more minor species in the products are formed.

- Above two bullet points have indicated a less complete combustion process.
- Although adiabatic flame temperature increases as initial temperature increases. It has increased for less 400 K while T_in has increased for 600 K. Overall, the adiabatic flame temperature showed a decreasing trend, which is aligned with the theory that a less complete combustion should have a lower T_ad as a result, since not all chemical potentials of the reactants are released.

Part V - Effect of dilution on T_ad:

1. Influence of CO2

Data was obtained using Cantera 2.6.0, csv files are not exportable in that version of Cantera for some reason, hence no table can be put out, please allow me to put a rough output result from jupyter, figures are exported using cached data. Instead of Gibbs solver, auto solver is selected to have a valid result for fraction over around 0,7.

```
At Fraction =          0, Tad =      2549  The fraction of: NO 0.0072504106 NO2 0.0000101136 CO 0.0066373070 CO2 0.1060543622
At Fraction =       0.05, Tad =      2450  The fraction of: NO 0.0058524608 NO2 0.0000089089 CO 0.0056135562 CO2 0.1492840903
At Fraction =        0.1, Tad =      2353  The fraction of: NO 0.0046303373 NO2 0.0000076814 CO 0.0042597865 CO2 0.1931432532
At Fraction =       0.15, Tad =      2256  The fraction of: NO 0.0035891511 NO2 0.0000065218 CO 0.0029462406 CO2 0.2372289154
At Fraction =        0.2, Tad =      2160  The fraction of: NO 0.0027227516 NO2 0.0000054712 CO 0.0018652808 CO2 0.2813146051
At Fraction =       0.25, Tad =      2064  The fraction of: NO 0.0020183140 NO2 0.0000045406 CO 0.0010821848 CO2 0.3253084420
At Fraction =        0.3, Tad =      1968  The fraction of: NO 0.0014590244 NO2 0.0000037249 CO 0.0005757800 CO2 0.3692175005
At Fraction =       0.35, Tad =      1873  The fraction of: NO 0.0010260235 NO2 0.0000030140 CO 0.0002810778 CO2 0.4131047881
At Fraction =        0.4, Tad =      1779  The fraction of: NO 0.0006998171 NO2 0.0000023981 CO 0.0001258032 CO2 0.4570484069
At Fraction =       0.45, Tad =      1688  The fraction of: NO 0.0004613081 NO2 0.0000018700 CO 0.0000514684 CO2 0.5011155331
At Fraction =        0.5, Tad =      1598  The fraction of: NO 0.0002925975 NO2 0.0000014239 CO 0.0000191341 CO2 0.5453533575
At Fraction =       0.55, Tad =      1511  The fraction of: NO 0.0001775985 NO2 0.0000010543 CO 0.0000064058 CO2 0.5897907743
At Fraction =        0.6, Tad =      1425  The fraction of: NO 0.0001024385 NO2 0.0000007552 CO 0.0000019076 CO2 0.6344438655
At Fraction =       0.65, Tad =      1342  The fraction of: NO 0.0000556426 NO2 0.0000005196 CO 0.0000004974 CO2 0.6793211529
At Fraction =        0.7, Tad =      1260  The fraction of: NO 0.0000281220 NO2 0.0000003402 CO 0.0000001113 CO2 0.7244272681
At Fraction =       0.75, Tad =      1180  The fraction of: NO 0.0000130072 NO2 0.0000002089 CO 0.0000000209 CO2 0.7697650789
At Fraction =        0.8, Tad =      1101  The fraction of: NO 0.0000053746 NO2 0.0000001175 CO 0.0000000032 CO2 0.8153367526
At Fraction =       0.85, Tad =      1024  The fraction of: NO 0.0000019090 NO2 0.0000000582 CO 0.0000000004 CO2 0.8611442170
At Fraction =        0.9, Tad =     948.7  The fraction of: NO 0.0000005420 NO2 0.0000000233 CO 0.0000000000 CO2 0.9071893373
At Fraction =       0.95, Tad =       874  The fraction of: NO 0.0000001010 NO2 0.0000000058 CO 0.0000000000 CO2 0.9534739737
```
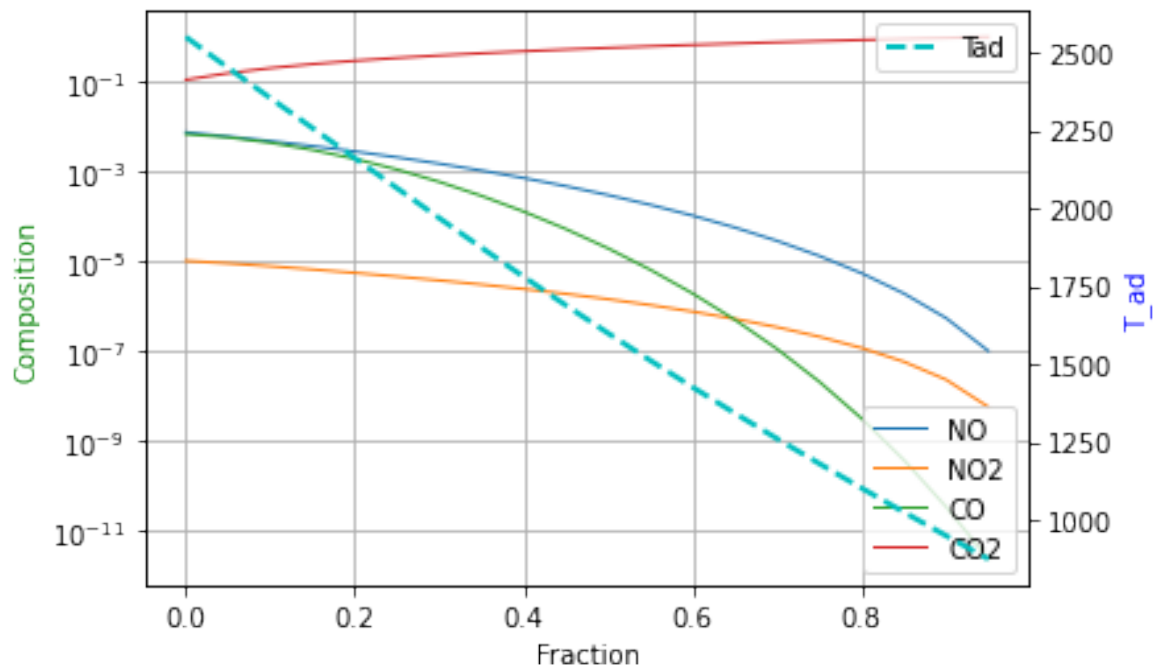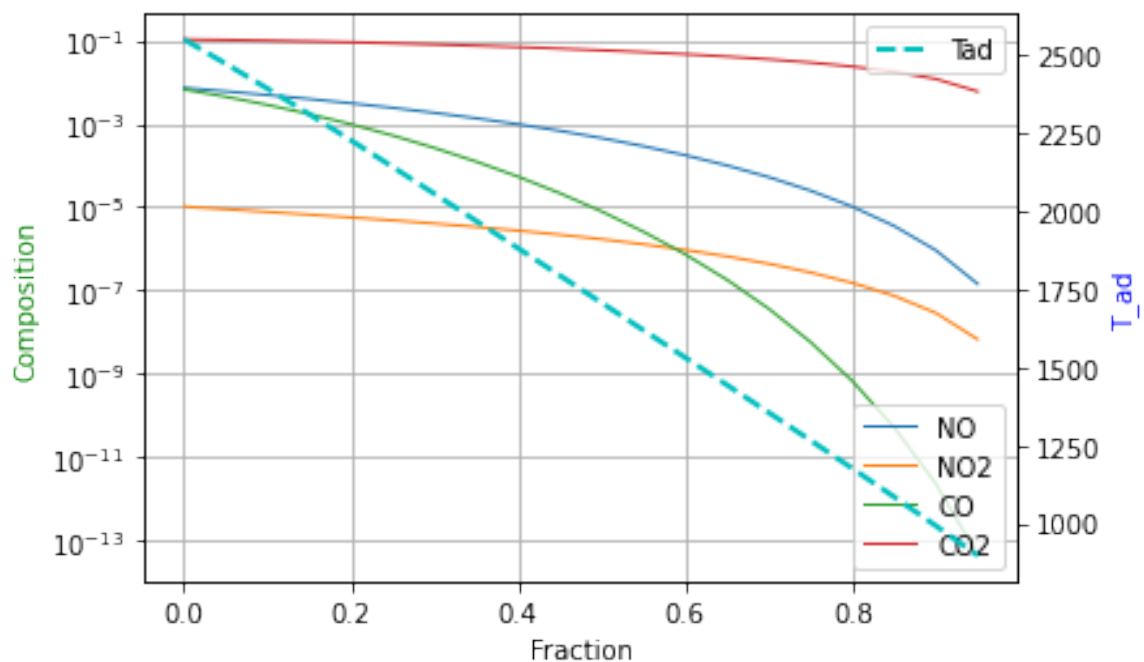

Molar fraction of 4 products in log and adiabatic flame temperature vs fraction of CO2 diluted

- As more fraction of CO2 gas is recirculated to dilute the reaction, less minor species, toxic gas, and pollutants are formed.

- Adiabatic flame temperature decreases as the fraction of CO2 increases since they do not participate in the reaction in theory and energy is required to heat up those molecules.
- The formation of NO decreases since the adiabatic flame temperature decreases.
- As the fraction increases, the reaction rate decreases. When fraction reaches 1, the reaction will be stopped in my prediction or at a very slow rate.

2. Influence of H2O

```
At Fraction =          0, Tad =       2549  The fraction of: NO 0.0072504106 NO2 0.0000101136 CO 0.0066373070 CO2 0.1060543622
At Fraction =       0.05, Tad =       2471  The fraction of: NO 0.0059780178 NO2 0.0000087362 CO 0.0044337945 CO2 0.1030362231
At Fraction =        0.1, Tad =       2391  The fraction of: NO 0.0048703967 NO2 0.0000075347 CO 0.0028201288 CO2 0.0993620094
At Fraction =       0.15, Tad =       2309  The fraction of: NO 0.0039123257 NO2 0.0000064797 CO 0.0016995438 CO2 0.0951319869
At Fraction =        0.2, Tad =       2226  The fraction of: NO 0.0030914035 NO2 0.0000055455 CO 0.0009667318 CO2 0.0904570183
At Fraction =       0.25, Tad =       2140  The fraction of: NO 0.0023966212 NO2 0.0000047105 CO 0.0005173985 CO2 0.0854477528
At Fraction =        0.3, Tad =       2054  The fraction of: NO 0.0018176454 NO2 0.0000039591 CO 0.0002597030 CO2 0.0802021086
At Fraction =       0.35, Tad =       1967  The fraction of: NO 0.0013442433 NO2 0.0000032816 CO 0.0001217310 CO2 0.0747970915
At Fraction =        0.4, Tad =       1880  The fraction of: NO 0.0009658290 NO2 0.0000026734 CO 0.0000529587 CO2 0.0692870673
At Fraction =       0.45, Tad =       1793  The fraction of: NO 0.0006712553 NO2 0.0000021333 CO 0.0000212001 CO2 0.0637068812
At Fraction =        0.5, Tad =       1706  The fraction of: NO 0.0004488931 NO2 0.0000016609 CO 0.0000077180 CO2 0.0580769753
At Fraction =       0.55, Tad =       1618  The fraction of: NO 0.0002869347 NO2 0.0000012560 CO 0.0000025158 CO2 0.0524083531
At Fraction =        0.6, Tad =       1531  The fraction of: NO 0.0001738165 NO2 0.0000009173 CO 0.0000007194 CO2 0.0467064174
At Fraction =       0.65, Tad =       1443  The fraction of: NO 0.0000986612 NO2 0.0000006420 CO 0.0000001757 CO2 0.0409735377
At Fraction =        0.7, Tad =       1354  The fraction of: NO 0.0000516712 NO2 0.0000004259 CO 0.0000000353 CO2 0.0352105833
At Fraction =       0.75, Tad =       1266  The fraction of: NO 0.0000244311 NO2 0.0000002635 CO 0.0000000056 CO2 0.0294177478
At Fraction =        0.8, Tad =       1176  The fraction of: NO 0.0000100977 NO2 0.0000001482 CO 0.0000000006 CO2 0.0235949489
At Fraction =       0.85, Tad =       1085  The fraction of: NO 0.0000034653 NO2 0.0000000724 CO 0.0000000000 CO2 0.0177420014
At Fraction =        0.9, Tad =      992.1  The fraction of: NO 0.0000008990 NO2 0.0000000280 CO 0.0000000000 CO2 0.0118586841
At Fraction =       0.95, Tad =      897.3  The fraction of: NO 0.0000001398 NO2 0.0000000065 CO 0.0000000000 CO2 0.0059447633
```
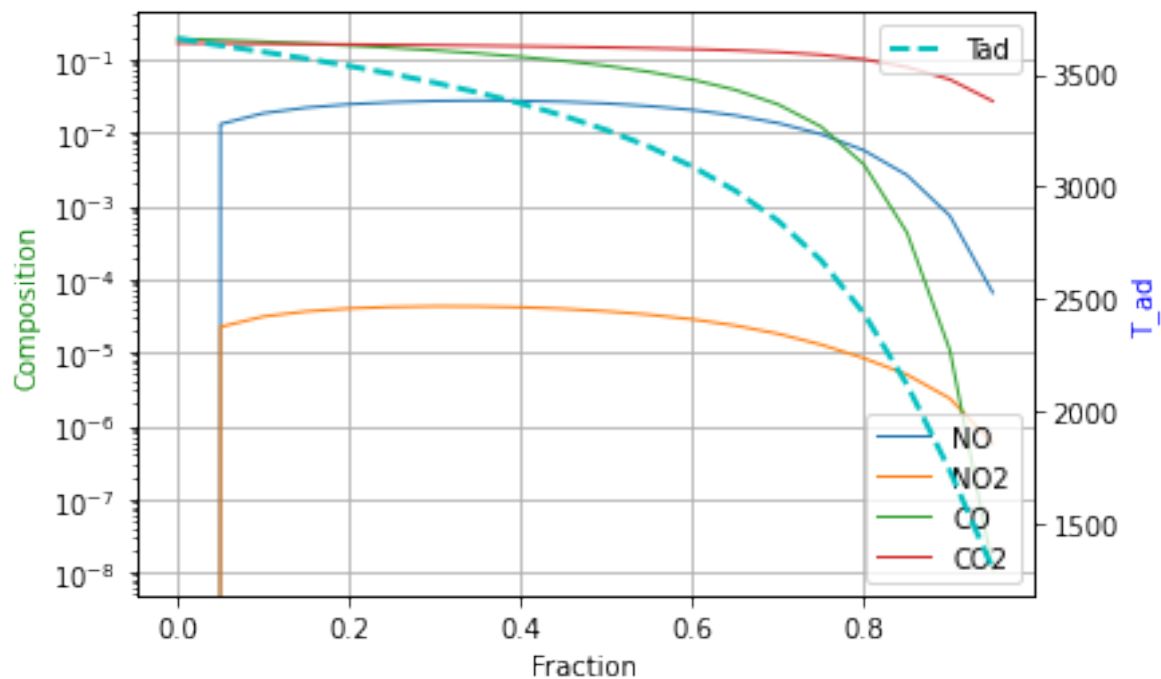

Molar fraction of 4 products in log and adiabatic flame temperature
vs fraction of H2O diluted

- The general trend of H2O as dilutant is very similar to that of CO2.
- Amount of NO and NO2 pollutant produced is very similar to the result using CO2 as dilutant, with slightly more NO and NO2 produced at higher molar fractions.
- The reaction rate should be faster and at higher fractions, the reaction is more thorough compared to CO2 since more pollutant are formed.
- More CO is formed compared to CO2 at higher fraction.
- The adiabatic flame temperature is highly aligned with that of CO2 since the Cp value of H2O and CO2 are similar.

3. No Nitrogen

```
At Fraction =        0, Tad =        3658  The fraction of: NO 0.0000000000 NO2 0.0000000000 CO 0.1893177447 CO2 0.1642060793
At Fraction =     0.05, Tad =        3628  The fraction of: NO 0.0129182979 NO2 0.0000222679 CO 0.1809307463 CO2 0.1628400022
At Fraction =      0.1, Tad =        3599  The fraction of: NO 0.0181621993 NO2 0.0000308010 CO 0.1719117145 CO2 0.1612626356
At Fraction =     0.15, Tad =        3569  The fraction of: NO 0.0216524344 NO2 0.0000361554 CO 0.1623926181 CO2 0.1595686310
At Fraction =      0.2, Tad =        3536  The fraction of: NO 0.0240924149 NO2 0.0000396086 CO 0.1523665720 CO2 0.1577602080
At Fraction =     0.25, Tad =        3501  The fraction of: NO 0.0257430351 NO2 0.0000416493 CO 0.1418138219 CO2 0.1558290052
At Fraction =      0.3, Tad =        3462  The fraction of: NO 0.0267245471 NO2 0.0000425179 CO 0.1307112088 CO2 0.1537598868
At Fraction =     0.35, Tad =        3419  The fraction of: NO 0.0270947335 NO2 0.0000423482 CO 0.1190363763 CO2 0.1515299901
At Fraction =      0.4, Tad =        3370  The fraction of: NO 0.0268780818 NO2 0.0000412211 CO 0.1067721153 CO2 0.1491053966
At Fraction =     0.45, Tad =        3315  The fraction of: NO 0.0260796191 NO2 0.0000391913 CO 0.0939129770 CO2 0.1464348247
At Fraction =      0.5, Tad =        3251  The fraction of: NO 0.0246934944 NO2 0.0000363051 CO 0.0804767120 CO2 0.1434382554
At Fraction =     0.55, Tad =        3177  The fraction of: NO 0.0227108063 NO2 0.0000326166 CO 0.0665251321 CO2 0.1399861189
At Fraction =      0.6, Tad =        3089  The fraction of: NO 0.0201302671 NO2 0.0000282086 CO 0.0522035619 CO2 0.1358600647
At Fraction =     0.65, Tad =        2982  The fraction of: NO 0.0169767820 NO2 0.0000232247 CO 0.0378177873 CO2 0.1306767438
At Fraction =      0.7, Tad =        2848  The fraction of: NO 0.0133369254 NO2 0.0000179207 CO 0.0239860846 CO2 0.1237380290
At Fraction =     0.75, Tad =        2673  The fraction of: NO 0.0094240864 NO2 0.0000127388 CO 0.0119162918 CO2 0.1137622154
At Fraction =      0.8, Tad =        2436  The fraction of: NO 0.0056585843 NO2 0.0000083116 CO 0.0036230805 CO2 0.0987045485
At Fraction =     0.85, Tad =        2121  The fraction of: NO 0.0026071366 NO2 0.0000049774 CO 0.0004293884 CO2 0.0773876473
At Fraction =      0.9, Tad =        1738  The fraction of: NO 0.0007272283 NO2 0.0000023548 CO 0.0000106951 CO2 0.0524853747
At Fraction =     0.95, Tad =        1302  The fraction of: NO 0.0000651540 NO2 0.0000005726 CO 0.0000000112 CO2 0.0265535578
```
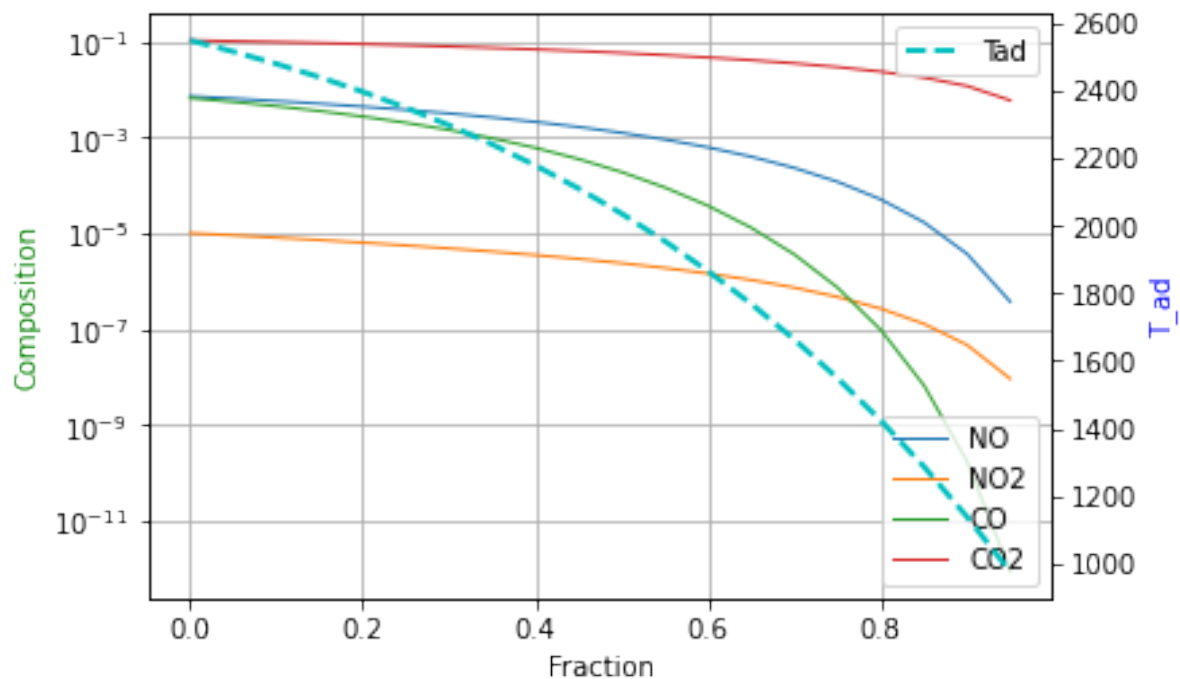

Molar fraction of 4 products in log and adiabatic flame temperature
vs fraction of N2 in (diluted) the air

- It seems that when no nitrogen is added, Cantera cannot compute successfully using the auto solver, gibbs solver is used to obtain the above data and plots.
- The adiabatic flame temperature become much higher compare to N2 is included, it decreases as the fraction of N2 increases.
- Since no energy is needed to heat up the nitrogen gas.
- As N2 in the reaction increases, the pollutant first increases then decreases. And Nitrous pollutant are not formed when fraction is zero since no N atom can be reached.
- Pollutants concentration at high N2 concentration is lower than atmospheric air
- What I did not expect is that the pollutant concentration, especially nitrous (NO.NO2) pollutants are higher than the values obtained in the atmospheric conditions.

4. Bonus – Ar for dilution

```
At Fraction =            0, Tad =      2549  The fraction of: NO 0.0072504106 NO2 0.0000101136 CO 0.0066373070 CO2 0.1060543622
At Fraction =         0.05, Tad =      2516  The fraction of: NO 0.0064998722 NO2 0.0000091159 CO 0.0055251218 CO2 0.1018904438
At Fraction =          0.1, Tad =      2479  The fraction of: NO 0.0057735028 NO2 0.0000081655 CO 0.0044978581 CO2 0.0975990820
At Fraction =         0.15, Tad =      2440  The fraction of: NO 0.0050744272 NO2 0.0000072645 CO 0.0035662328 CO2 0.0931696093
At Fraction =          0.2, Tad =      2397  The fraction of: NO 0.0044060217 NO2 0.0000064145 CO 0.0027403744 CO2 0.0885921504
At Fraction =         0.25, Tad =      2349  The fraction of: NO 0.0037718954 NO2 0.0000056165 CO 0.0020287328 CO2 0.0838587638
At Fraction =          0.3, Tad =      2298  The fraction of: NO 0.0031758641 NO2 0.0000048708 CO 0.0014366733 CO2 0.0789648920
At Fraction =         0.35, Tad =      2241  The fraction of: NO 0.0026219150 NO2 0.0000041769 CO 0.0009649452 CO2 0.0739109139
At Fraction =          0.4, Tad =      2179  The fraction of: NO 0.0021141547 NO2 0.0000035339 CO 0.0006084233 CO2 0.0687033819
At Fraction =         0.45, Tad =      2110  The fraction of: NO 0.0016567114 NO2 0.0000029406 CO 0.0003556705 CO2 0.0633553759
At Fraction =          0.5, Tad =      2036  The fraction of: NO 0.0012535405 NO2 0.0000023965 CO 0.0001897872 CO2 0.0578855126
At Fraction =         0.55, Tad =      1954  The fraction of: NO 0.0009080722 NO2 0.0000019019 CO 0.0000906008 CO2 0.0523155819
At Fraction =          0.6, Tad =      1866  The fraction of: NO 0.0006226647 NO2 0.0000014587 CO 0.0000376642 CO2 0.0466673877
At Fraction =         0.65, Tad =      1769  The fraction of: NO 0.0003978896 NO2 0.0000010702 CO 0.0000131327 CO2 0.0409597711
At Fraction =          0.7, Tad =      1663  The fraction of: NO 0.0002317593 NO2 0.0000007405 CO 0.0000036388 CO2 0.0352067147
At Fraction =         0.75, Tad =      1549  The fraction of: NO 0.0001190947 NO2 0.0000004733 CO 0.0000007393 CO2 0.0294169451
At Fraction =          0.8, Tad =      1424  The fraction of: NO 0.0000513202 NO2 0.0000002703 CO 0.0000000973 CO2 0.0235948396
At Fraction =         0.85, Tad =      1287  The fraction of: NO 0.0000170428 NO2 0.0000001303 CO 0.0000000068 CO2 0.0177419935
At Fraction =          0.9, Tad =      1138  The fraction of: NO 0.0000037307 NO2 0.0000000472 CO 0.0000000002 CO2 0.0118586839
At Fraction =         0.95, Tad =     976.1  The fraction of: NO 0.0000003760 NO2 0.0000000093 CO 0.0000000000 CO2 0.0059447633
```


Molar fraction of 4 products in log and adiabatic flame temperature
vs fraction of diluted Ar added

- Adiabatic flame temperature curve is no longer a straight line, but more curved, since the Cp value of Ar does not vary too much with temperature
- By looking very closely to the figure (since I did not plot them on one single figure, or they are too overlapped), I found that the pollutant fraction with Ar as dilutant is actually higher than using H2O, CO2. CO has a more significant impact.
- Since dissociation of CO2 to CO require participation of H2O, a theoretical guess would be that the concentration of CO is much higher compare to use CO2 and H2O as dilutant is due to the fact that lack of these two items have promoted the reaction equilibrium to the pollutant side, hence more CO is formed.

Part IV:

1. The chemical model you will need to use Cantera

- Chemical kinetics models describing nitrogen oxydation in combustion have been originally used to model thermal NO formation, such as the Konnov [1] mechanism.

- More recent models derived from older models are more suited to $NH3$ combustion modelling, such as the model from Xiao [2] wich will be used in our project.

- The Xiao combustion kinetics model contains 52 species and 272 reactions and was validated using experimental data in the 1-30 atm pressure range.

- The relatively high number of species and reactions for a $NH3$ oxydation mechanism should make it more accurate compared to the SanDiego [3] or the Jiang [4] mechanisms.

References:

1. KONNOV, A. A., & RUYCK, J. D. (1999). Kinetic Modeling of Nitrogen Oxides Decomposition at Flame Temperatures. Combustion Science and Technology, 149(1-6), 53-78. https://doi.org/10.1080/00102209908952099

2. Xiao, H., Valera-Medina, A., & Bowen, P. J. (2017). Modeling Combustion of Ammonia/Hydrogen Fuel Blends under Gas Turbine Conditions. Energy & Fuels, 31(8), 8631-8642. https://doi.org/10.1021/acs.energyfuels.7b00709

3. University of California at San Diego. (2020). Chemical-Kinetic Mechanisms for Combustion Applications. San Diego Mechanism web page. Repéré à https://web.eng.ucsd.edu/mae/groups/combustion/mechanism.html

4. Jiang, Y., Gruber, A., Seshadri, K., & Williams, F. (2020). An updated short chemical-kinetic nitrogen mechanism for carbon-free combustion applications. International Journal of Energy Research, 44(2), 795-810. https://doi.org/10.1002/er.4891

2. The global $NH3+H2+N2$ combustion reaction

- For $X_{NH3} = X_{H2}$ which is a plausible case

$$(NH_3 + H_2 + 0.33 N_2) + 1.25 (O_2 + 3.76 N_2) \rightarrow 0.5 N_2 + 2.5 H_2O + 5.03 N_2$$

3. The adiabatic temperature with varying equivalence ratio, initial temperature, and pressure.
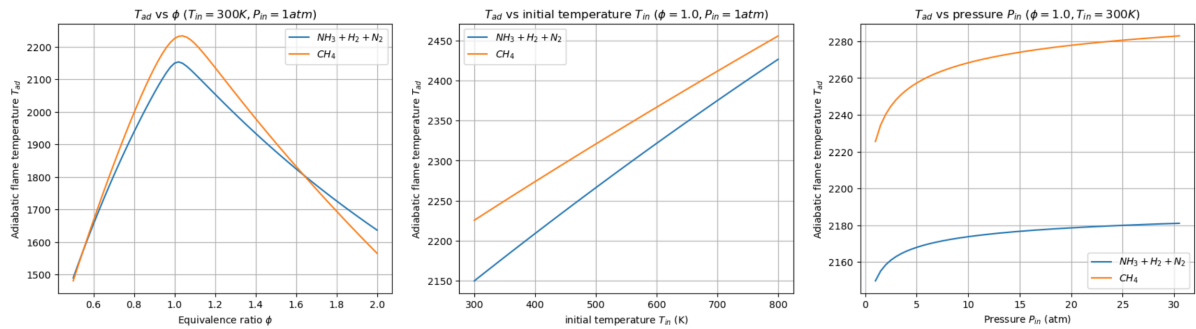
4. The concentration of the main pollutants after equilibrium