PROJECT ASSIGNMENT #1:   
COMBUSTION THERMODYNAMICS



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Submitted to:

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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

## Global reaction equations

### At stoichiometric( )

### Fuel lean( ):

### Fuel rich( ):

## LHV and HHV comparison

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

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

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.

## 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 |

### 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 |

## Plot of T\_ad against :

Chart, line chart

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The adiabatic flame temperature (y-axis) against (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 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:

## The result and plot

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

|  |  |  |  |
| --- | --- | --- | --- |
| 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 |  |  |

Chart, line chart

Description automatically generated

Adiabatic flame temperature vs using cantera

## 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.

## Results comparison with Cantera and estimations

Chart, line chart

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* 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.

## Bonus I – H2 compare with C8H18

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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:

## 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 |

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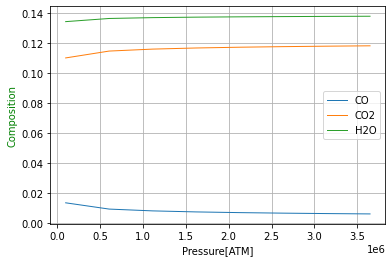
Top: Composition of all products in logarithm, Tad vs phi, bottom left: major species in linear vs phi, bottom right: minor species in linear vs phi

* 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

## 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 |

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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 CO2, H2O 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.

## 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 |

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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 (CO2 and H2O) 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:

## 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.*

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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.

## Influence of H2O

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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.

## No Nitrogen

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Chart

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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.

## Bonus – Ar for dilution

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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:

## 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>

## The global 𝑁𝐻3+𝐻2+𝑁2 combustion reaction

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

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## The concentration of the main pollutants after equilibrium

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