# Exercise 4 - Adiabatic Flame Temperature for Methane

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1. Problem 1.a - Combustion in Air

To calculate the temperature of the adiabatic flame (AFT) without using Cantera, we first define the combustion reaction of methane with air based on the global reaction and distinguish between lean-fuel ($\varphi \leq 1$) and rich-fuel ($\varphi > 1$) mixtures by using the equivalence ratio (φ). This allows us to identify the products and their amounts present after the combustion depending on the amount of oxygen reacted in the combustion.

The global reaction for the combustion is:

$$C_xH_y + a(O_2 + 3.76\,N_2) \longrightarrow bCO_2 + cCO + dH_2O + eH_2 + fO_2 + 3.76\,aN_2$$
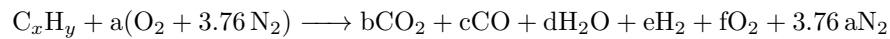
For lean mixtures, we assume that not all oxygen has reacted, and thus the global reaction changes to have spare oxygen:

$$C_xH_y + a(O_2 + 3.76\,N_2) \longrightarrow bCO_2 + dH_2O + fO_2 + 3.76\,aN_2$$
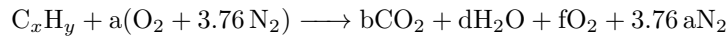
For the rich mixtures, we assume incomplete combustion. Due to the abundance in fuel, we get the following global reaction:

$$C_xH_y + a(O_2 + 3.76\,N_2) \longrightarrow bCO_2 + cCO + dH_2O + eH_2 + 3.76\,aN_2$$
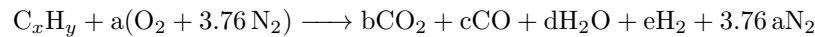
To compute the AFT, we apply the first law of thermodynamics for a steady-flow adiabatic system at constant pressure. This means the total enthalpy of reactants must equal the total enthalpy of products. The enthalpy of each species is calculated using its standard formation enthalpy at 298 K and then adjusted for temperature using temperature-dependent heat capacities ($C_p(T)$).

Because the product temperature (AFT) is unknown and appears inside integrals of $C_p(T)$, we use an iterative numerical approach. An initial temperature guess is refined until the enthalpy balance between reactants and products is satisfied within a small tolerance. This process is repeated across a range of equivalence ratios ($\varphi = 0.1$ to 2) to generate a curve of AFT versus φ. Figure 1 shows the results from the code run for combustion both in air and in pure oxygen for methane.
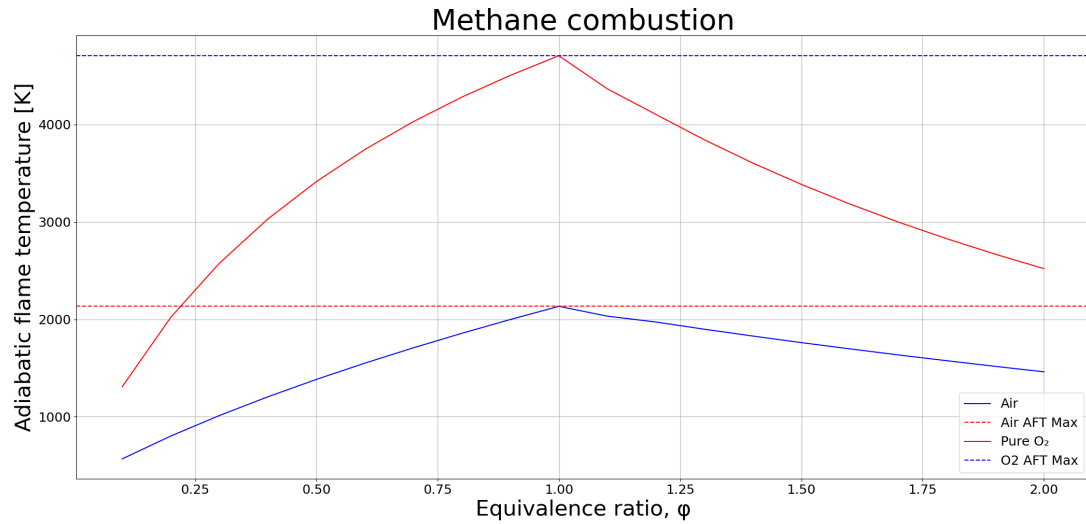
Figure 1: Adiabatic flame temperature vs. equivalence ratio for methane combustion in air and pure oxygen. Maximum AFT with air: 2134.08 K at $\phi = 1.00$. Maximum AFT with pure O_2: 4707.12 K at $\phi = 1.00$.

2. Problem 1.b - Combustion in pure oxygen

As we can see in the figure 1, the AFT for combustion in pure oxygen is significantly higher than combustion in air. This result was to be expected when looking at the global reaction. Nitrogen and oxygen have no enthalpy of formation when calculating the enthalpy of the reactants. So the overall energy in the combustion is still the same if the fuel is not changed. What is affected is the calculation for the enthalpy of the products, where one molecule, nitrogen, is removed from the equation. With nitrogen gone from the combustion, more of the energy goes to the molecules left and thus the AFT in the system becomes higher for combustion in pure oxygen than in air.
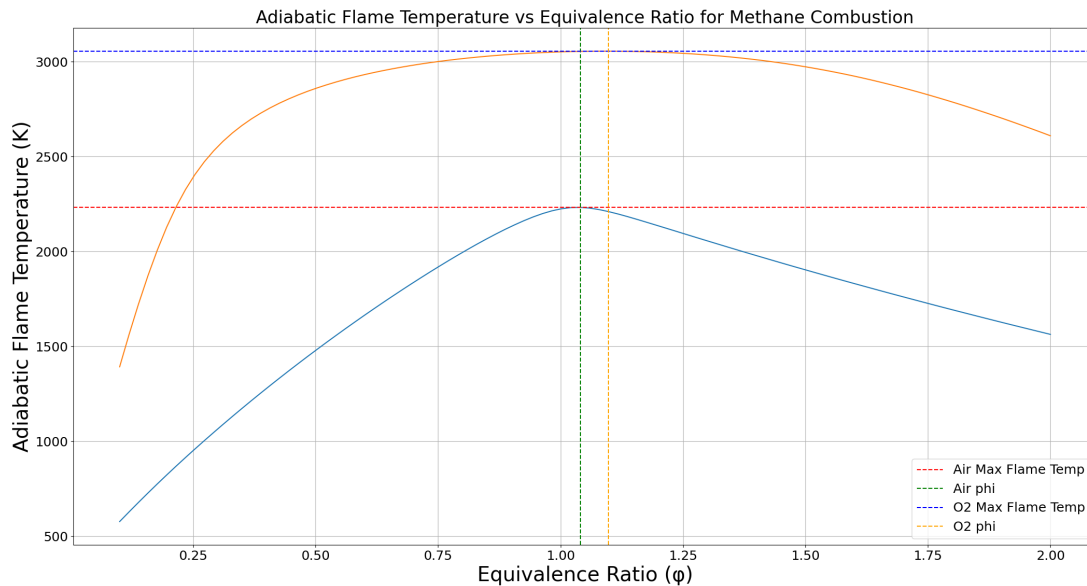
3. Problem 2 - Cantera Calculations

Figure 2: Max Adiabatic Flame Temperature with Air: 2232.66 K at Equivalence Ratio: 1.04,
Max Adiabatic Flame Temperature with pure O2: 3055.85 K at Equivalence Ratio: 1.10,

When comparing the results from problem 1 with canteras calculation of the methane combustion we see differences at the AFT and φ values.

Table 1: Comparison of AFT results between Python and Cantera methods

Method	Case	AFT	φ
Python	Air	2134.08 K	1.00
Python	Oxygen	4707.12 K	1.00
Cantera	Air	2232.66 K	1.04
Cantera	Oxygen	3055.85 K	1.10

Canteras values for AFT are slightly lower in air combustion but greatly lower in oxygen combustion in comparison to problem 1. The equivalence ratio from problem 1 is also always one and the value from cantera are both slightly higher than one.

The reasoning for these differences comes down to several factors.

First the Dissociation effects

Dissociation effects refers to the breakdown of combustion products such as CO_2 and H_2O into their constituent atoms or molecules when exposed to high temperatures which may be reached during combustions. These reactions often require energy to break the molecular bonds, which otherwise would have gone to increasing the temperature in the combustion and thus resulted in a higher AFT.

In problem 1, these dissociation effects are ignored and only focuses on the global reactions products such as H_2O, CO_2 and in cases of rich mixtures, H_2 and CO.

Cantera's gri30.yaml file which has over 300 reactions covers several different reactions between all present molecules in the global reaction setup, where some reactions present the dissociation effects.

Difference in the amount of Thermodynamic Data available

In problem 1, the data present is Standard enthalpy of formation, $C_{p,i}$ at 1200 kelvin, Water-gas equilibrium and the coefficients for calculating C_p in the interval between 1000-5000 kelvin. Gri30.yaml itself consists of 1778 lines of code, where a large part is just thermodynamic data. For example, Cantera has data to accurately calculate the C_p-value for all 53 species present in gri30 with temperatures interval between 200-1000K and 1000-3500K or 200-1000K and 1000-6000K.

Simplified Reactions

Problem 1 only assumes the global reaction takes place, with the expectation of Water-Gas equilibrium reaction CO + $H_2O \longleftrightarrow CO_2 + H_2$ in fuel rich mixtures. The global reaction is also not a reversible reaction due to its simplicity and how unlikely the reaction is to occur backwards.

Cantera on the other hand handles several more reactions, which is also reversible due to being single step elementary reactions. For example Reaction 11 which shows that methane could react with oxygen at the start of the combustion.

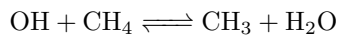$$O + CH_4 \rightleftharpoons OH + CH_3$$
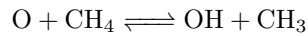
(Reaction 11)

We could also look at reaction 53 and 98 to see how methane reacts with potential bi-products from the combustion after initialization.

$$H + CH_4 \rightleftharpoons CH_3 + H_2$$

(Reaction 53)

$$OH + CH_4 \rightleftharpoons CH_3 + H_2O$$
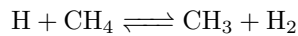
(Reaction 98)

So to summarize, Cantera shows different AFT-values than problem 1 due to cantera calculating the elementary reactions that take place instead of just the global reaction that problem 1 handles. This is also the reason why φ is one in problem 1 and slightly higher in cantera. Problem 1 calculation is the stoichiometric peak which occurs when $\varphi = 1$. Cantera requires a slightly higher φ value to ensure the fuel is fully combusted and the maximum of energy released.