Warsaw University of Technology

FACULTY OF
POWER AND AERONAUTICAL ENGINEERING

# Cloud Computing

# Influence of the Equivalence Ratio, Pressure and Preheat on Adiabatic Flame Temperature

Maciej Janus

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# Contents

# 1 Introduction

The goal of this paper is to investigate the relation between the adiabatic flame temperature and initial conditions such as equivalence ratio, pressure and temperature of propane - air mixture.

The constant pressure adiabatic flame temperature is the temperature that results from a complete combustion process that occurs without any heat loss in it.

All calculation will be conducted using AWS parallel clusters and the Python environment.

# 2 Theoretical background

## 2.1 Chemistry

Below there is presented the equation of complete combustion of propane in the air:

$$C_3H_8 + 5(O_2 + 3.78N_2) \longrightarrow 3CO_2 + 4H_2O + 18.9N_2$$

Above equation represents the stoichiometric reaction so basing on it we can calculate the stoichiometric air-to-fuel ratio which is given by the formula:

$$AFR_{st} = \frac{m^{st}_{air}}{m^{st}_{fuel}}$$

where $m$ represents the mass, suffix st stands for stoichiometric conditions.

The reciprocal of the stoichiometric air-to-fuel ratio is the stoichiometric fuel-to-air ratio and is given by the formula:

$$FAR_{st} = \frac{1}{AFR_{st}}$$

Now if we change the initial conditions the reaction will not be stoichiometric any more and the fuel-to-air ratio will change. Proportion of the new fuel-to-air ratio to stoichiometric fuel-to-air ratio is called the equivalence ratio. It is given by the relation:

$$\Phi = \frac{FAR}{FAR_{st}} = \frac{m_{fuel}/m_{air}}{(m_{fuel}/m_{air})_{st}} = \frac{n_{fuel}/n_{air}}{(n_{fuel}/n_{air})_{st}}$$

where $n$ represents number of moles, suffix st stands for stoichiometric conditions.

It appears form the relation above that equivalence ratios greater than one always mean there is more fuel in the fuel-air mixture than required for complete combustion (stoichiometric reaction), irrespective of the fuel and oxidizer being used.

## 2.2 Thermodynamics

In all below equations subscript $R$ stands for reactants and subscript $P$ stands for products.

Assume that the reacting system is closed. Thus from the first law of thermodynamics we have:

$$ {}_RQ_P - {}_R W_P = U_P - U_R \tag{1}$$

where:

- ${}_RQ_P$ is the heat transferred from the system to the surroundings during the process;
- ${}_RW_P$ is the work done by the system;
- $U_P$ is the internal energy of the products;
- $U_R$ is the internal energy of the reactants;

We usually assume that the combustion occur in the constant pressure which results in the following equation for the work:

$$ {}_RW_P = \int_R^P pdV = p(V_P - V_R) \tag{2}$$

The process is defined to be adiabatic thus there is no heat transfer. It means that:

$$ {}_RQ_P = 0 \tag{3}$$

Inserting (2) and (3) into equation (1) we get:

$$ -p(V_P - V_R) = U_P - U_R \Rightarrow U_P + pV_P = U_R + pV_R$$

Recalling the definition of enthalpy we recover that:

$$ H_P = H_R \tag{4}$$

The system is closed, so the mass of the products and reactants is constant and the first law of thermodynamics - equation (**??**) - can be written on a mass basis:

$$ H_P = H_R \Rightarrow m_P h_P = m_R h_R \Rightarrow h_P = h_R$$

When we make the assumption that combustion is complete, we can calculate the adiabatic flame temperature by hand. It is the result of the fact that then there are enough variables and molar equations to balance the left and right hand sides of any equation of complete combustion of any hydrocarbon.

If the equivalence ratio is different to 1, there are not enough variables. However, if we include the *Water gas shift reaction* and use the equilibrium constant for this reaction, we weil be able to complete all calculations.

# 3 Description of the code

The whole project was based on numerical calculations made in Python 3 environment with *Cantera* implemented to it.

*Cantera* is an open-source suite of tools for problems involving chemical kinetics, thermodynamics and transport processes.

Firs of all, it was investigated what is the influence of the equivalence ratio on the adiabatic flame temperature $T_a$. In order to declare the proper gas (propane) the *GRI-Mech 3.0* mechanism was used. Afterwards, for 50 different values of $\Phi$ in the range from $\Phi_{min} = 0.3$ to $\Phi_{max} = 3.5$, the equilibrium for the given reaction (subsection 2.1) was determined and the temperature was calculated. The initial pressure and temperature were constant ($T_0 = 300\ [K]$, $p_0 = 101325\ [Pa]$). Due to the fact that the reactants and products were in equilibrium state, the calculated temperature was the adiabatic flame temperature $T_a$. All results were presented on charts.

The next step was to examine the influence of the initial pressure on the adiabatic flame temperature $T_a$. Again, for 50 different values of $p$ in the range from $p_{min} = 0.1\ [atm]$ to $p_{max} = 5\ [atm]$, the equilibrium state was determined and the temperature was calculated. The initial temperature was constant - $T_0 = 300\ [K]$. Everything was repeated for four different values of equivalence ratio - $\Phi_1 = 0.5$, $\Phi_2 = 1$, $\Phi_3 = 2$, $\Phi_4 = 3$. Again, all results were presented on charts.

Additionally, the influence on the adiabatic flame temperature $T_a$ of the initial temperature was investigated. For 50 different values of $T$ in the range from $T_{min} = 273\ [K]$ to $T_{max} = 2000\ [K]$, the equilibrium temperature was calculated. In that case the initial pressure was constant - $p_0 = 101325\ [Pa]$. Again, everything was repeated for four different values of equivalence ratio - $\Phi_1 = 0.5$, $\Phi_2 = 1$, $\Phi_3 = 2$, $\Phi_4 = 3$. All results were also presented on charts.

Finally, based on calculations that had been conducted, 3D charts presenting the influence on the adiabatic flame temperature $T_a$ of both pressure and equivalence ratio, both temperature and equivalence ration, as well as both pressure and temperature were prepared.

In the table below the initial parameters of every examined case are shown.

| variable | initial values | | | | | |
|---|---|---|---|---|---|---|
| parameter | $T_0$ | $p_0$ | $\Phi_1$ | $\Phi_2$ | $\Phi_3$ | $\Phi_4$ |
| $\Phi$ | ✓ | ✓ | | | | |
| $p$ | ✓ | | ✓ | ✓ | ✓ | ✓ |
| $T$ | | ✓ | ✓ | ✓ | ✓ | ✓ |
| $p, \Phi$ | ✓ | | | | | |
| $T, \Phi$ | | ✓ | | | | |
| $p, T$ | | | ✓ | ✓ | ✓ | ✓ |

Table 1: Parameters of every examined case

# 4 Preparation of the computing environment

All calculations were conducted using the AWS infrastructure. The process of the preparation of the computing environment is presented below.

First of all, two *EC2 AMI* instances were launched. First of them was the master instance and the second was the slave instance. Both instances were *Ubuntu* instances. Additionally they were added two specially configured security group Communication with instances was conducted using the *ConEmu* terminal.While connecting with instances, two tunnels were established.

After connecting, with the master instance, *Ubuntu* was updated and upgraded. Additionally *Java*, *Scala*, and *Anaconda* were installed.

When everything was setup properly, *Apache Spark* was downloaded and installed. Thanks to this tool all calculations could be performed parallel on two separate instances.

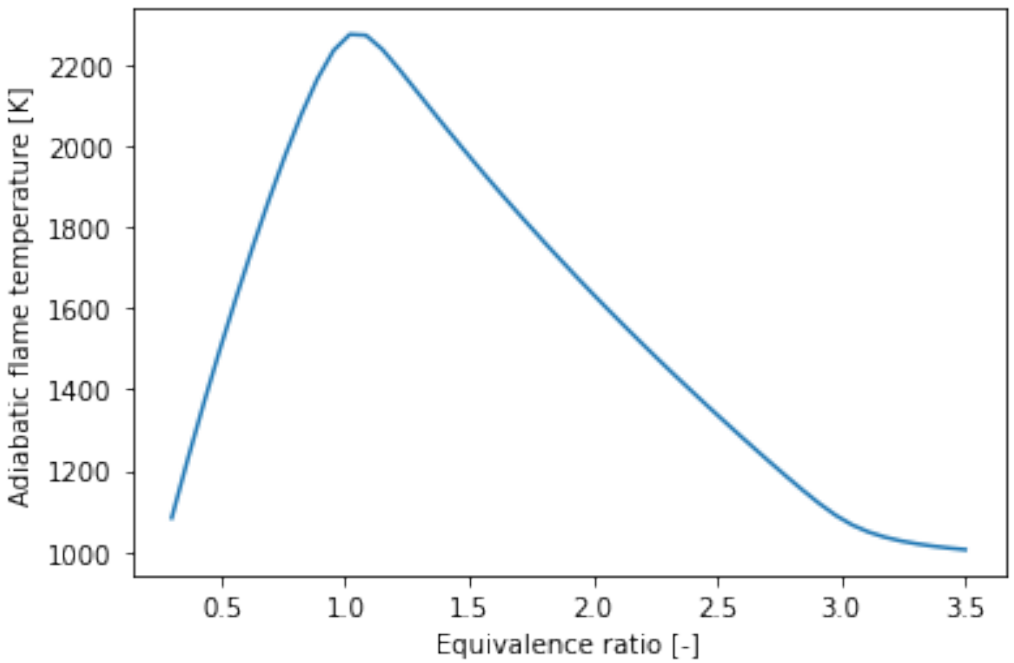
After setting up both computing nodes, *Jupyter notebook* was launched. Finally, calculations were run.

# 5 Results

## 5.1 Variable $\Phi$

Figure 1 presents the counted relation between the adiabatic flame temperature and the equivalence ratio of propane-air mixture. The initial values of pressure and temperature are $p_0 = 101325\ [Pa]$, $T_0 = 300\ [K]$.

Figure 1: $T_a(\Phi)$



## 5.2 Variable $p$

Figures 2-5 present the counted relation between the adiabatic flame temperature and the initial value of pressure for four different equivalence ratios of propane-air mixture. The initial temperature is $T_0 = 300\ [K]$.

Figure 2: $T_a(p)$ for $\Phi_1 = 0.5$

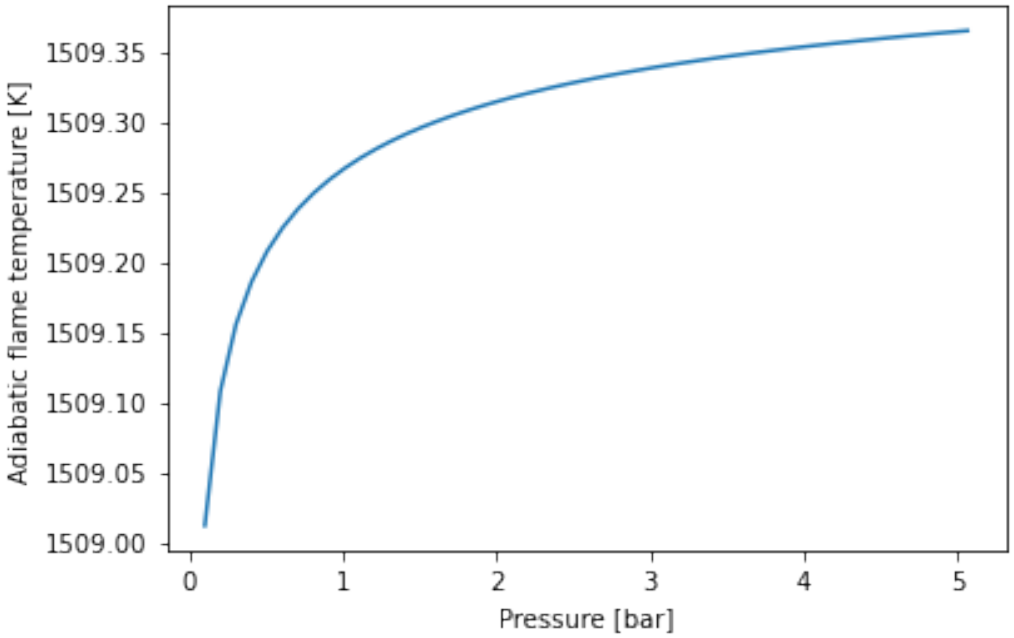



Figure 3: $T_a(p)$ for $\Phi_2 = 1$

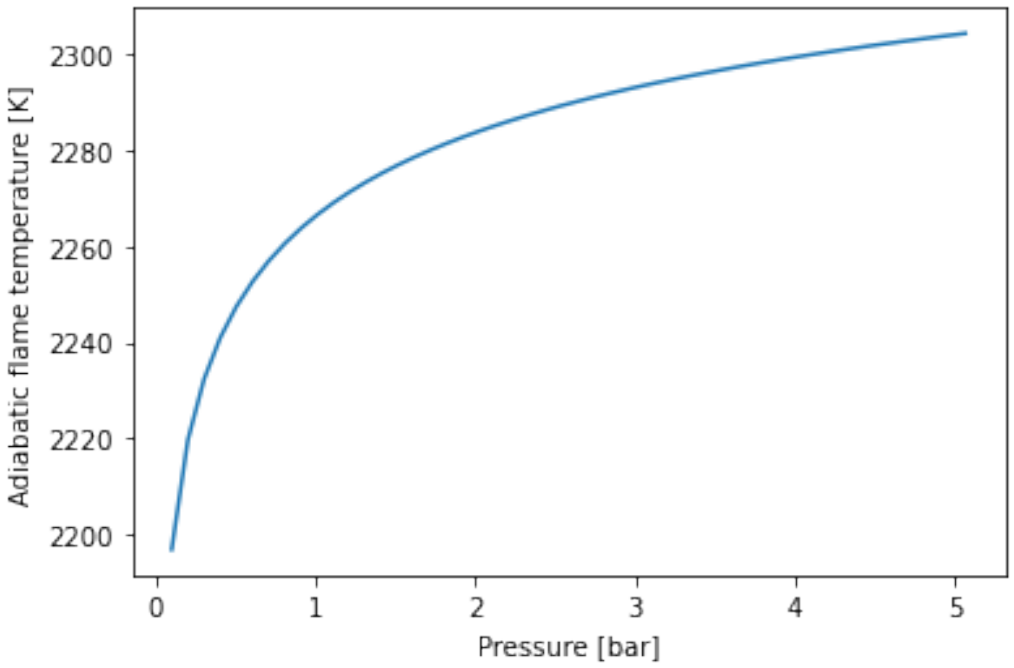


Figure 4: $T_a(p)$ for $\Phi_3 = 2$

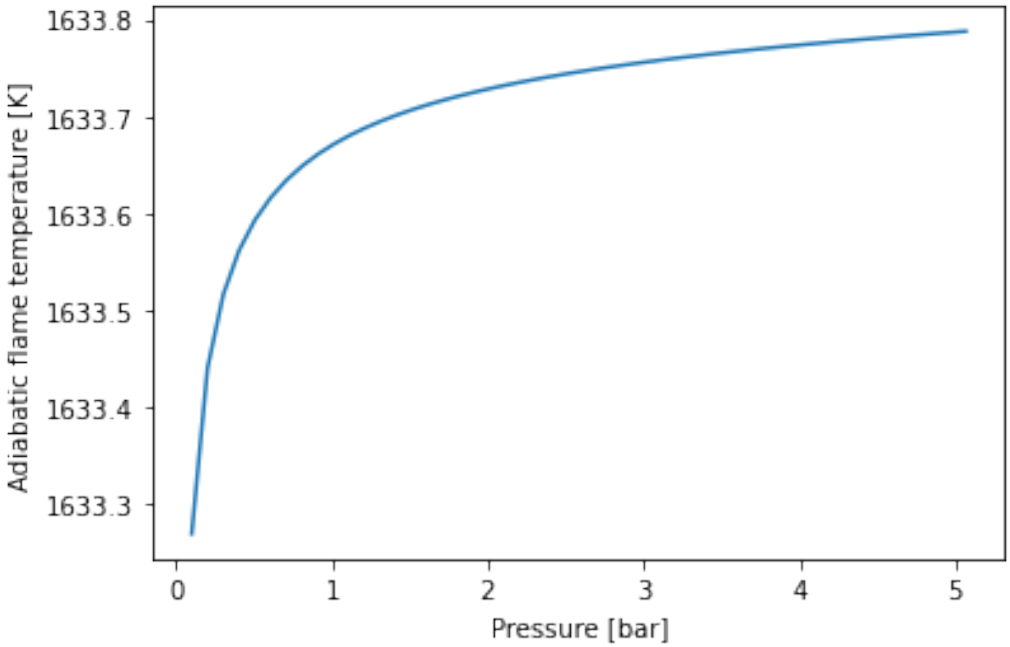
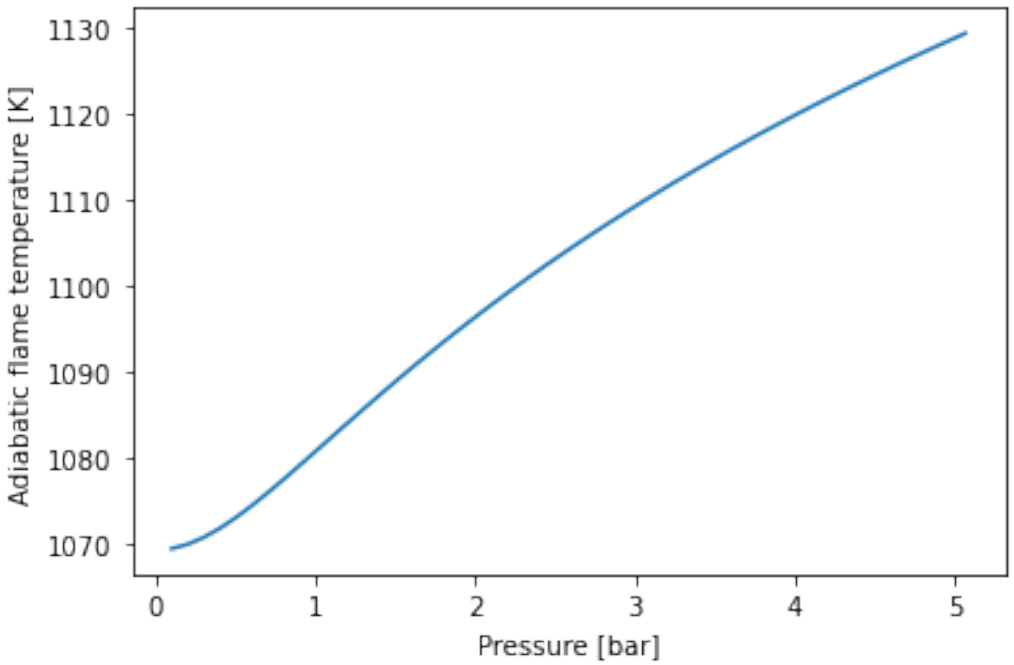
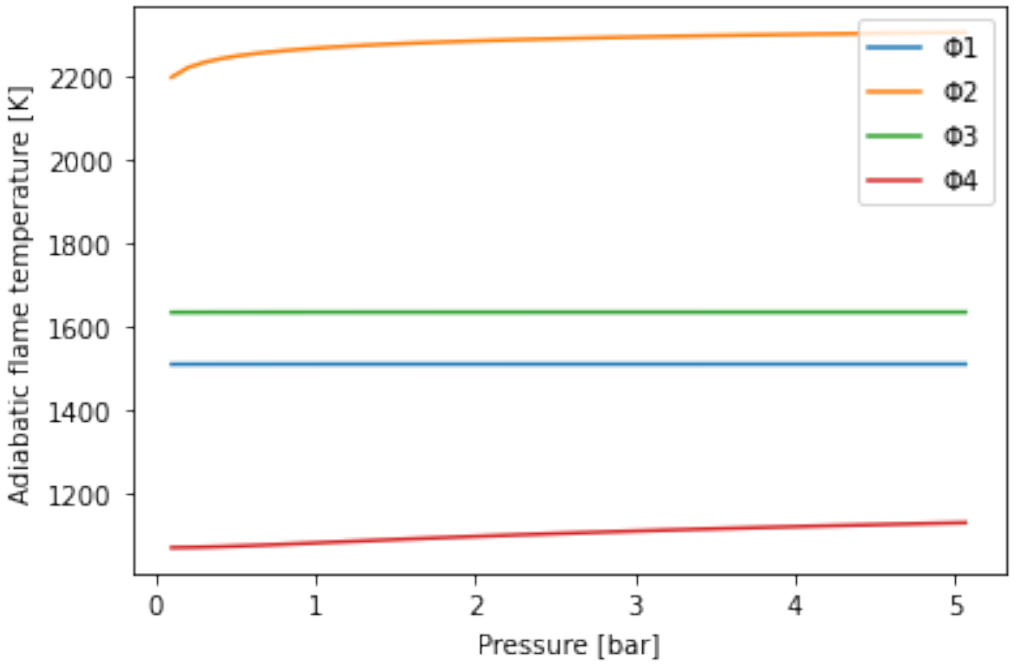



Figure 5: $T_a(p)$ for $\Phi_4 = 3$




In addition, a collective figure showing the change of temperature as a function of initial pressure for all four values of equivalence ratio is provided below.

Figure 6: $T_a(p)$ for all four values of $\Phi$




## 5.3 Variable $T$

Figures 7-10 present the counted relation between the adiabatic flame temperature and the initial value of temperature for 4 different equivalence ratios of propane-air mixture. The initial pressure for all four cases is $p_0 = 101325\ [Pa]$.

Figure 7: $T_a(T)$ for $\Phi_1 = 0.5$

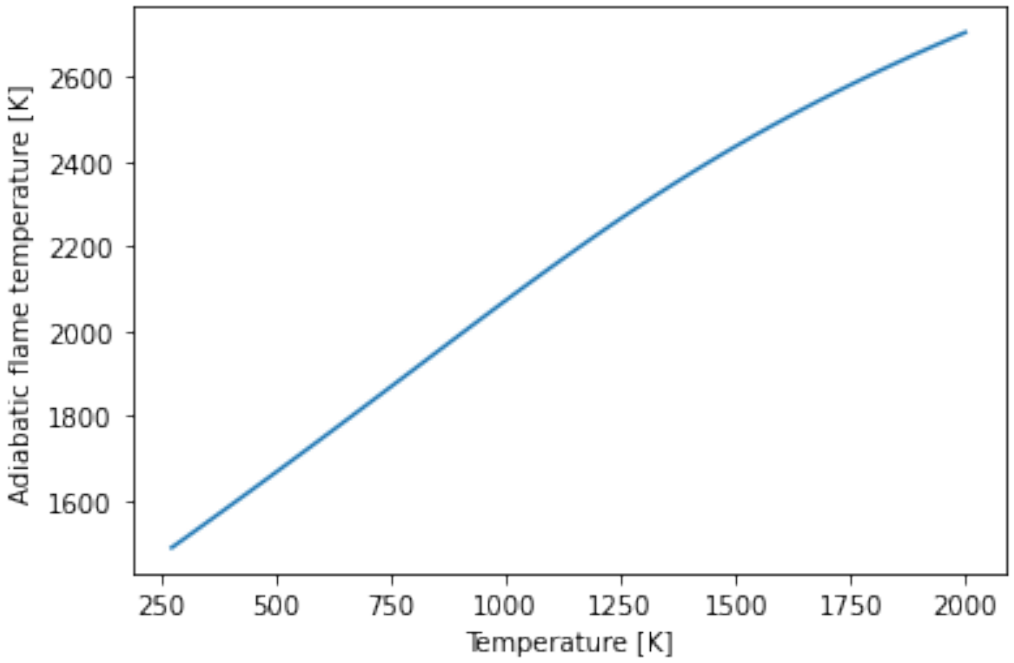


Figure 8: $T_a(T)$ for $\Phi_2 = 1$

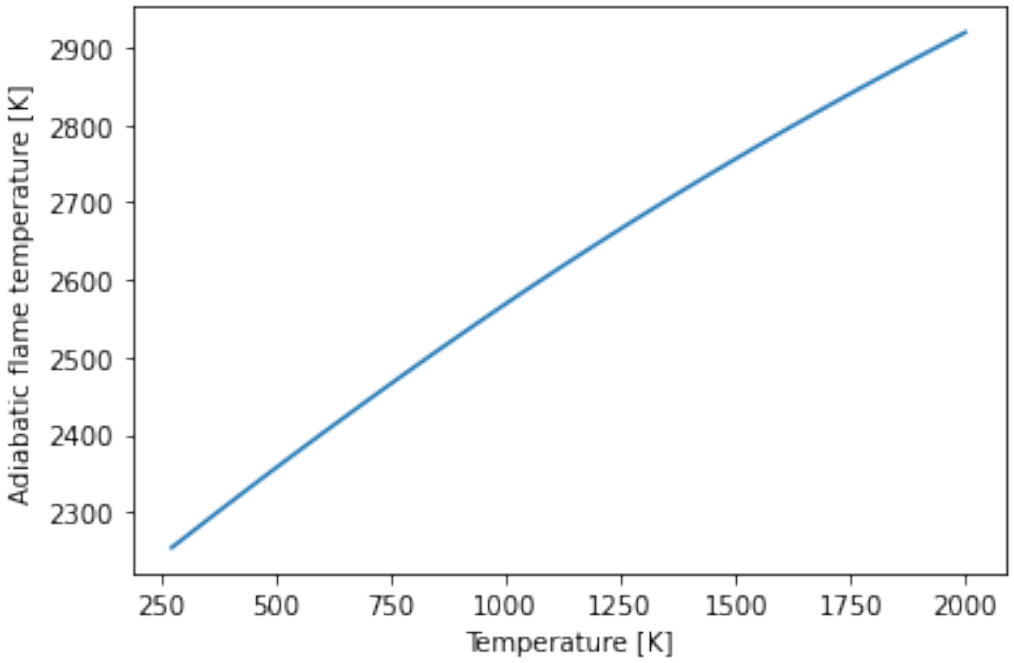



Figure 9: $T_a(T)$ for $\Phi_3 = 2$

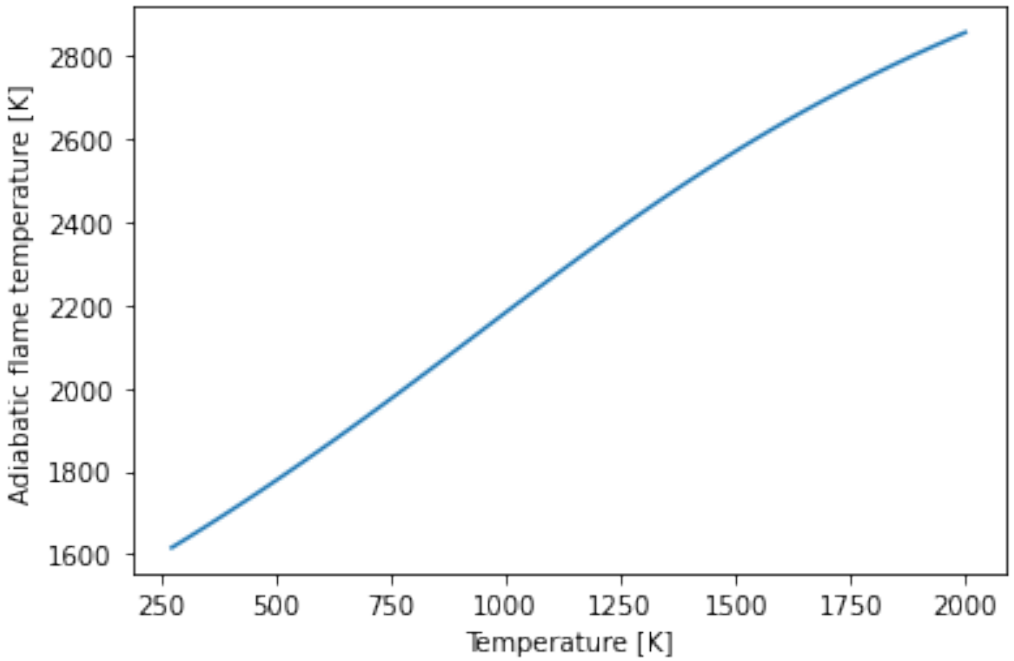
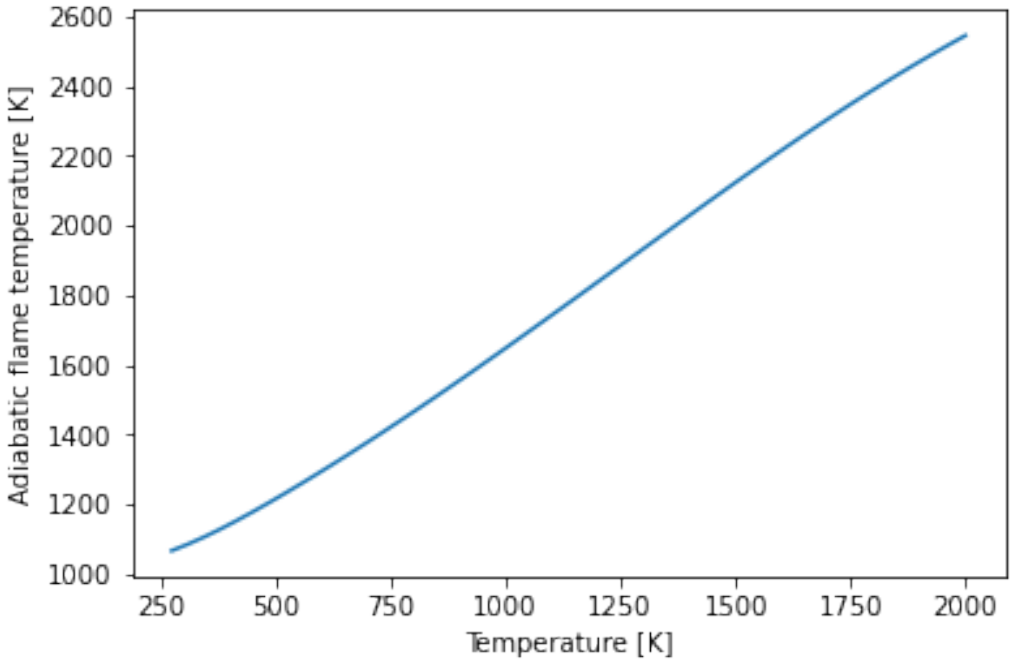
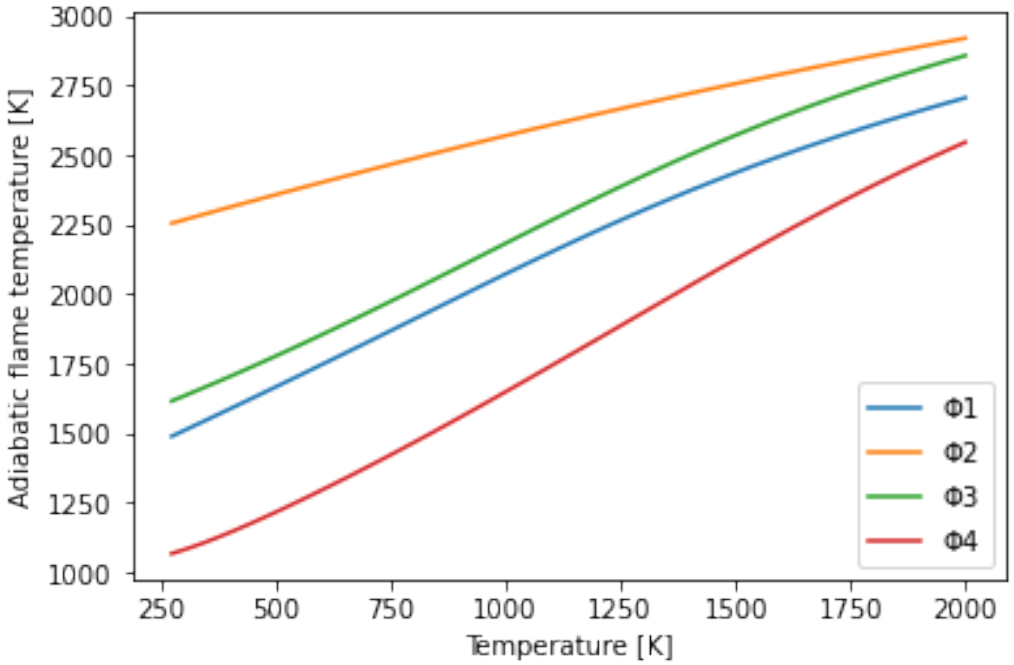


Figure 10: $T_a(T)$ for $\Phi_4 = 3$




Again, a collective figure showing the change of temperature as a function of initial temperature for all four values of equivalence ratio is provided below.

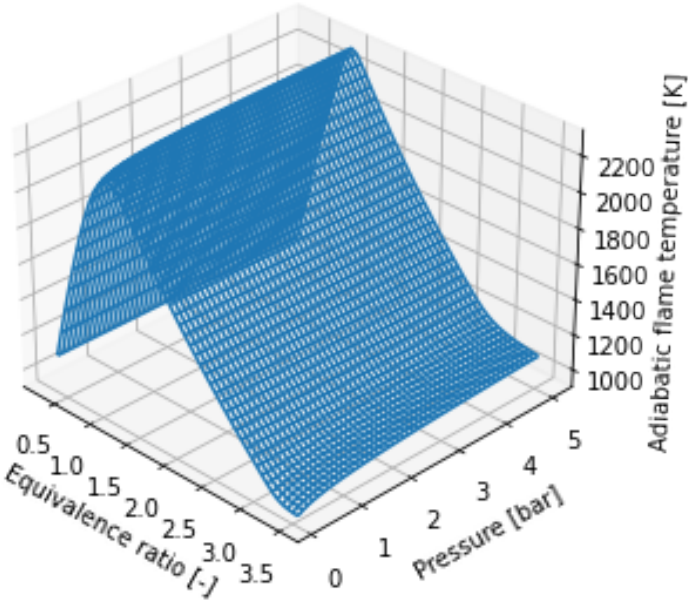
Figure 11: $T_a(T)$ for all four values of $\Phi$




## 5.4 Variables $p$ and $\Phi$

Figure 12 presents the counted relation between the adiabatic flame temperature and both the initial value of pressure and the initial equivalence ratio. The initial temperature is $T_0 = 300\ [K]$.

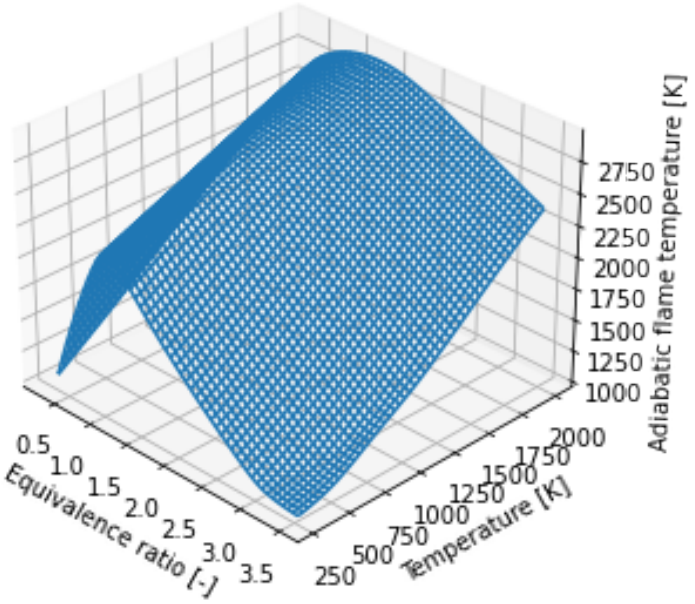
Figure 12: $T_a(p, \Phi)$




## 5.5 Variables $T$ and $\Phi$

Figure 13 presents the counted relation between the adiabatic flame temperature and both the initial value of temperature and the initial equivalence ratio. The initial pressure is $p_0 = 101325\ [Pa]$.

Figure 13: $T_a(T, \Phi)$



## 5.6 Variables $p$ and $T$

Figures 14-17 present the counted relation between the adiabatic flame temperature and both the initial value of pressure and the initial value of temperature for 4 different equivalence ratios of propane-air mixture.

Figure 14: $T_a(p, T)$ for $\Phi_1 = 0.5$

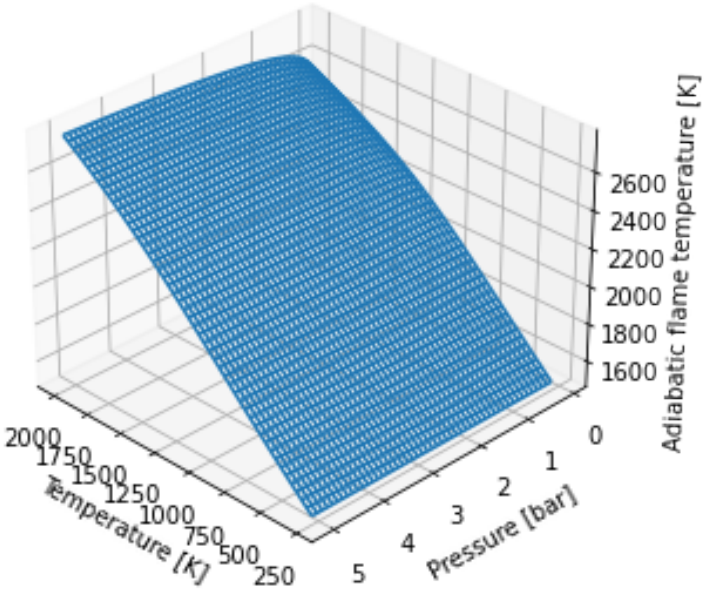



Figure 15: $T_a(p, T)$ for $\Phi_2 = 1$

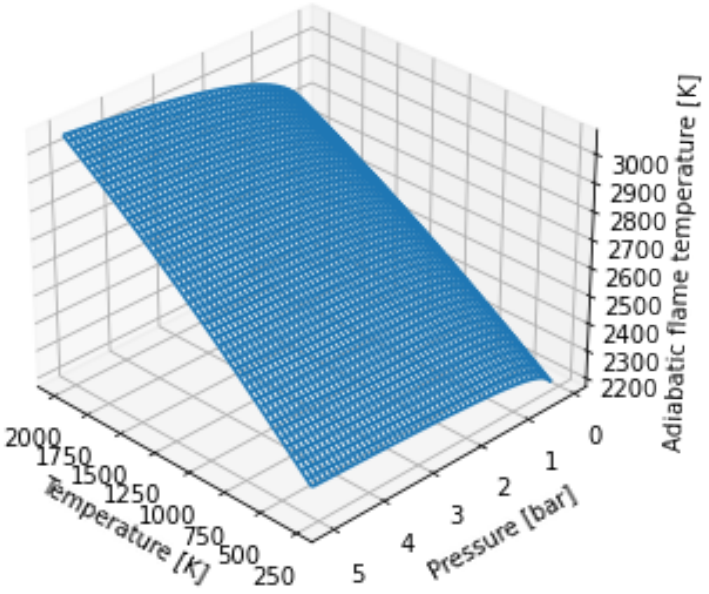


Figure 16: $T_a(p, T)$ for $\Phi_3 = 2$

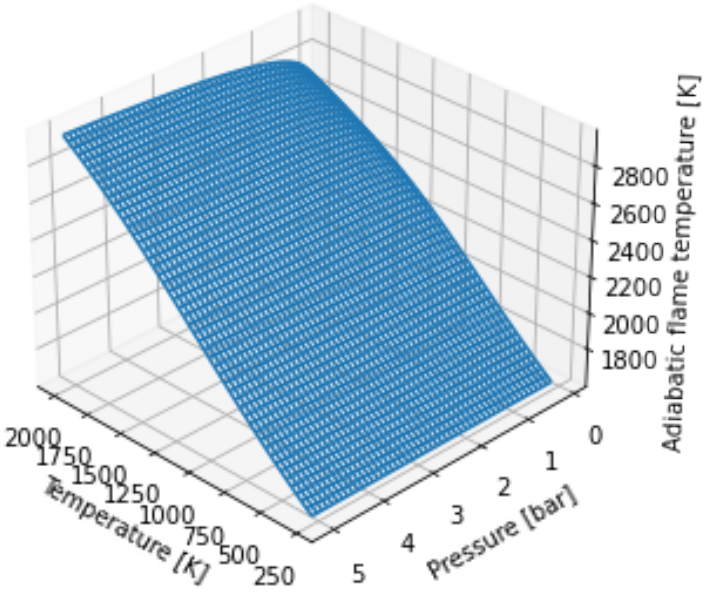
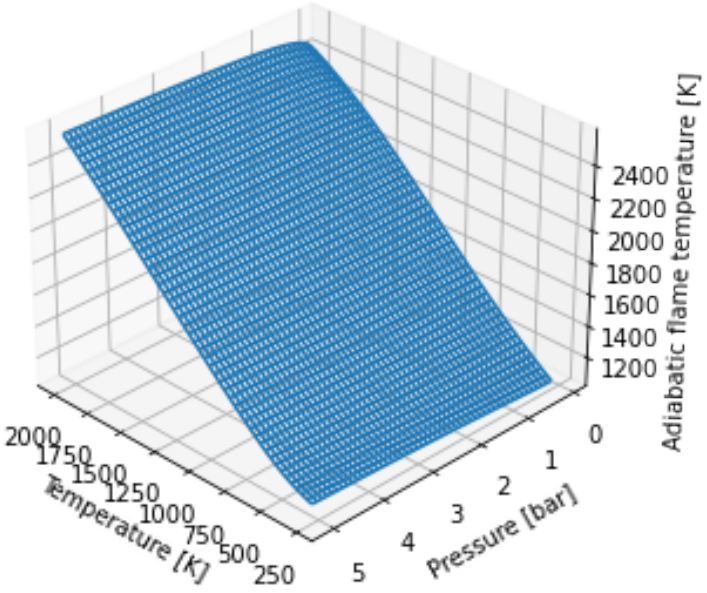



Figure 17: $T_a(p, T)$ for $\Phi_4 = 3$



# 6 Conclusions

For constant initial pressure and temperature the highest temperature of adiabatic flame is reached when the composition of the mixture is close to the stoichiometric composition - the equivalence ratio is equal to one.

When $T_0 = 300\ [K]$ and $p_0 = 101325[Pa]$ the maximum adiabatic flame temperature of propane-air mixture is higher than 2200 $[K]$.

It is also worth noticing that for very rich or very poor mixtures the adiabatic flame temperature is more than two times smaller than the maximum value which is reached for $\Phi = 1$.

Generally speaking, for every value of the equivalence ratio the adiabatic flame temperature grows with a pressure (for constant value of initial temperature $T_0 = 300\ [L]$). However, this increase is significant only in the case of stoichiometric mixture of propane and air. In other cases the growth of adiabatic flame temperature can be omitted. It can be seen very clearly in figure 6.

What is more, the figure 6 also shows that the highest temperature of adiabatic flame is reached for stoichiometric mixtures and the lowest is reached for very rich mixtures.

When the initial temperature increases, the adiabatic flame temperature also increases. The more the equivalence ratio deviates from 1, the greater that growth is. It is reflected in figure 11.

# References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