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Influence of the equivalence factor on pressure, temperature and selected undesirable combustion products for selected fuels

Computer methods in burning

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Contents

1 Introduction

The following report presents an analysis of the effect of the equivalence ratio on the maximum temperatures, pressures and undesirable combustion products obtained (in our study we included them as CO, N_2O, NO and NO_2). Equivalence ratio (ER) is the ratio of the oxygen content in the supplied oxidant to that required for complete stoichiometric combustion. This is probably the most important operational parameter for allothermic processes, as it strongly influences gas composition (including tar content) and its calorific value. Calculations were carried out for the combustion process of four types of mixtures: hydrogen - air, methane - air, ethane - air and propane - air. These fuels were chosen because methane, ethane and propane are the main components of natural gas, which is currently considered one of the most ecological fossil energy sources and is the most popular gas fuel. Hydrogen, on the other hand, is considered as an environmentally neutral fuel of the future, but in real combustion processes in the air it reacts with nitrogen. In the program, it is possible to use different initial values of temperature, pressure and equivalence ratio range in which we want to obtain data on the charts.

2 Description of the method

2.1 Calculation method

Calculations for each case were performed using the GRI-Mech 3.0 reaction mechanism in the Canter package for Python. Cantera is open source software developed at the Combustion Laboratory of the California Institute of Technology. It can be used to perform complex calculations of chemical equilibrium, thermodynamics and transport processes in all kinds of chemical systems. For the purposes of this project, the most valuable feature of the Canter package is the ability to carry out combustion reactions in a constant volume. The diagrams of the maximum obtained pressure and temperature determine the equivalence ratio for which we will be able to obtain the highest thermal and mechanical efficiency in engines or turbines. In addition, due to the fact that the program has the ability to change the temperature and pressure initiated for the purposes of ignition, we can more or less determine their minimum value for mixtures by analyzing the obtained graphs of maximum pressure and temperature. In order to increase the accuracy of the measurements, it was necessary to adjust the appropriate time for the end of the simulation for individual fuels (in our case, it was hydrogen - air (0.00135s), ethane - air (0.002), methane - air (0.0025) and propane - air (0.0025 s) .0027)), for the purposes of this report it was done approximately by analyzing the obtained temperature and pressure graphs so as to obtain a point approximation as close as possible to a differentiable function. Our program also calculates the proportion of undesirable combustion products in the exhaust gas, such as the main greenhouse gas (N_2O), poisonous gases (CO and NO_2) and the unstable and highly reactive (NO), which spontaneously reacts with oxygen in the air to form poisonous nitrogen dioxide (NO_2). Thanks to this, we will be able to determine the most ecological equivalence ratio of our fuels.

2.2 Initial conditions

Temperature $T = 1200K$ and pressure $P = 1atm$ were assumed as initial conditions. Combustion equations on which calculations are based (stoichiometric mixture):

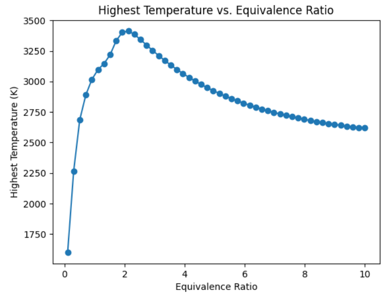
1. Hydrogen with air: $2\mathrm{H_2} + \frac{1}{2}(\mathrm{O_2} + 3.76\mathrm{N_2}) \rightarrow 2\mathrm{H_2O} + 1.88\mathrm{N_2}$
2. $\mathrm{CH_3}$ with air: $\mathrm{CH_3} + \frac{3}{2}(\mathrm{O_2} + 3.76\mathrm{N_2}) \rightarrow \mathrm{CO_2} + 2\mathrm{H_2O} + 5.64\mathrm{N_2}$
3. $\mathrm{CH_4}$ with air: $\mathrm{CH_4} + (\mathrm{O_2} + 3.76\mathrm{N_2}) \rightarrow \mathrm{CO_2} + 2\mathrm{H_2O} + 3.76\mathrm{N_2}$
4. $\mathrm{C_2H_6}$ with air: $2\mathrm{C_2H_6} + 7(\mathrm{O_2} + 3.76\mathrm{N_2}) \rightarrow 4\mathrm{CO_2} + 6\mathrm{H_2O} + 26.32\mathrm{N_2}$

2.3 Code

The code used to calculate these cases was written in Python 3.9 using the Canter package. The code can be found in the repository: https://github.com/KamlotPol45/MKWS.git.

3 Results

3.1 Results for propane (CH_3)



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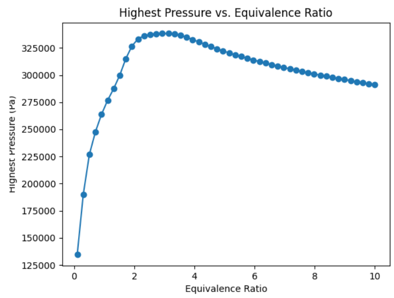

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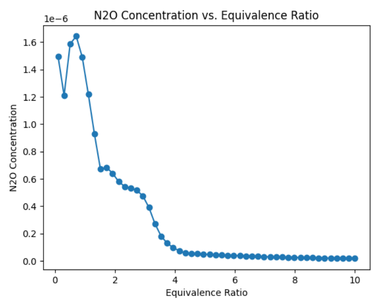

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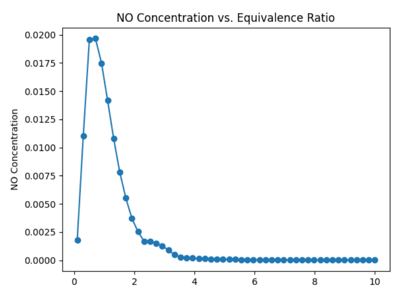

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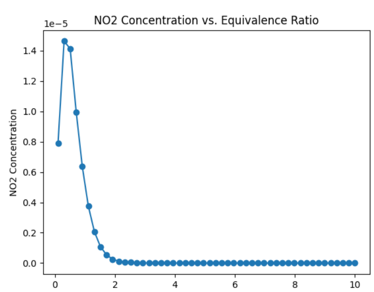
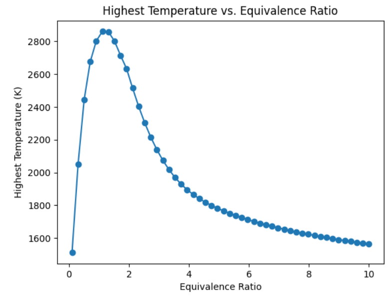


[5]

[1] Maximum temperature
[2] Maximum pressure
[3] Concentration of N_2O
[4] Concentration of NO
[5] Concentration of NO_2

3.2 Results for methane (CH_4)



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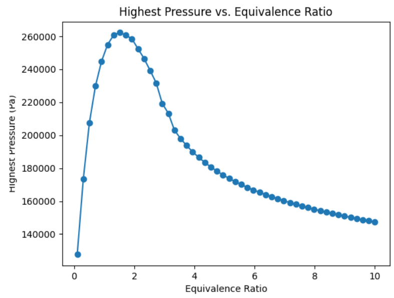

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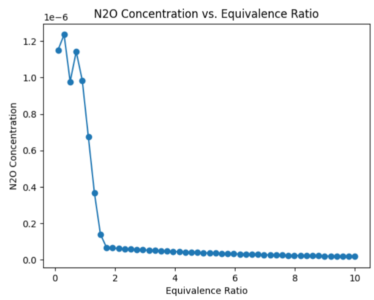

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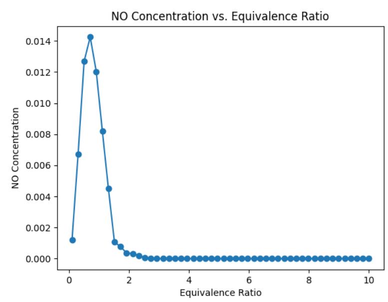

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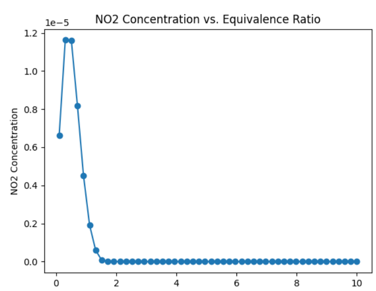
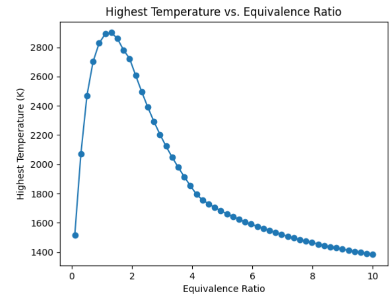


[10]

[6] Maximum temperature
[7] Maximum pressure
[8] Concentration of N_2O
[9] Concentration of NO
[10] Concentration of NO_2

3.3 Results for ethane (C_2H_6)



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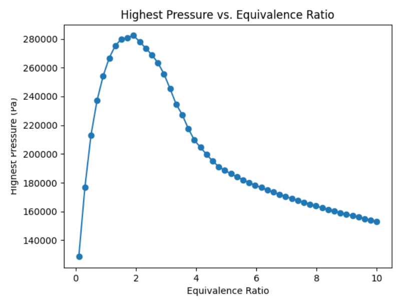

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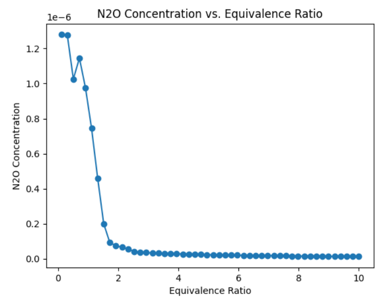

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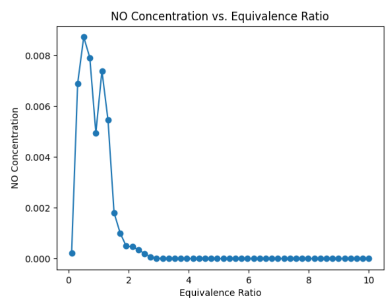

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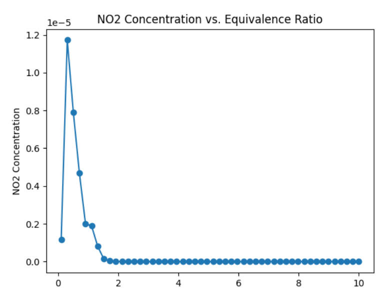
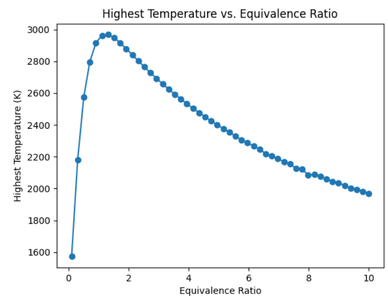


[15]

[11] Maximum temperature
[12] Maximum pressure
[13] Concentration of N_2O
[14] Concentration of NO
[15] Concentration of NO_2

3.4 Results for hydrogen (H_2)



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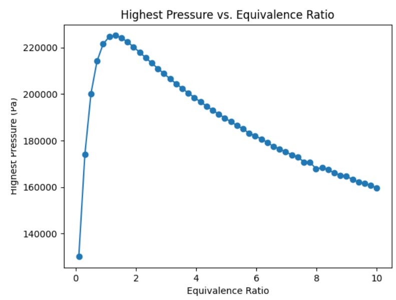

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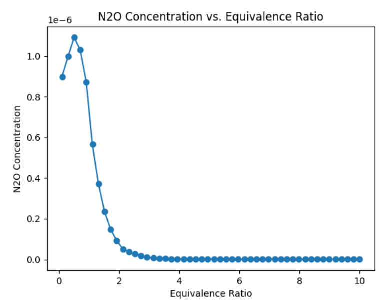

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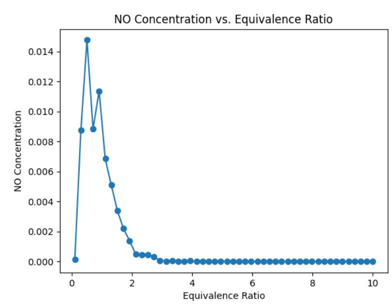

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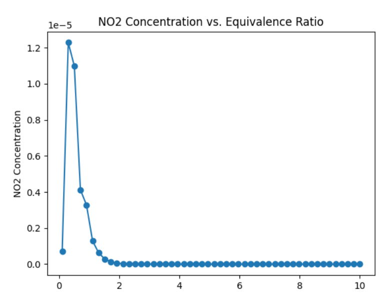
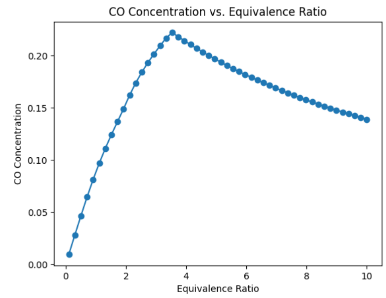


[20]

[16]Maximum temperature
[17]Maximum pressure
[18]Concentration of N_2O
[19]Concentration of NO
[20]Concentration of NO_2

3.5 Results for carbon monoxide (CO)



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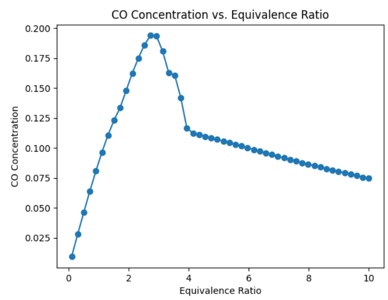

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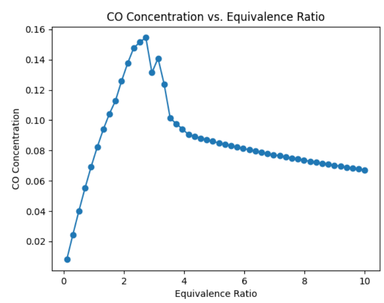

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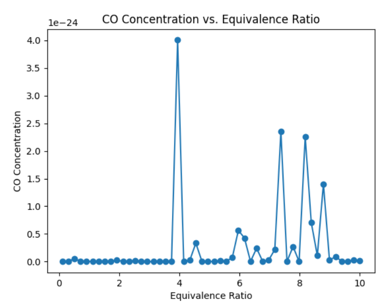

[24]

[21] Concentration of CO for CH_3
[22] Concentration of CO for CH_4
[23] Concentration of CO for C_2H_6
[24] Concentration of CO for H_2

4 Conclusions

From the graphs, we can conclude that the most favorable combustion is combustion with a large equivalence ratio. Then, the share of undesirable gases in the combustion products decreases and the maximum temperature and pressure decrease slightly, which can also be considered an advantage in the case of turbine engines, because then the thermal load on the turbine blades is lower. The share of NOx in the combustion products for hydrocarbons is very similar to the share for hydrogen. However, we can see the difference in the share of CO, where for hydrogen it is zero, which is in line with the predictions (the graph shows sharp peaks, which may suggest errors in the adopted models)