Faculty of Power and Aeronautical Engineering

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Examination of NO_x concentration in hydrogen-air mixtures combustion products

Computational methods in combustion

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1 Introduction

In the last decade an ongoing trend of creating eco-friendly internal combustion engines can be observed; amongst them - hydrogen internal combustion engine. Though up to this day it's idea was mainly considered in regards to vehicles, in recent years Airbus announced that they are working on a hydrogen powered jet engine and one of the considered application of hydrogen in it is hydrogen combustion [1]. Popular media often refers to engines such as the one described above as 'non-emission engines' due to lack of CO_2 particles in the combustion products, however this does not present the full picture of the situation since there are NO_x particles (which according to Euro Emissions Standard are emissions) present in hydrogen combustion products. This work will focus on examining how the concentration of NO_x particles will change in different conditions of a hypothetical hydrogen-burning jet engine.

2 Computational method

2.1 Brayton cycle

Brayton cycle is a type of thermodynamic cycle generally used to approximate the work of a gas turbine. The p-V graph showing the idealized processes during the cycle is shown below:

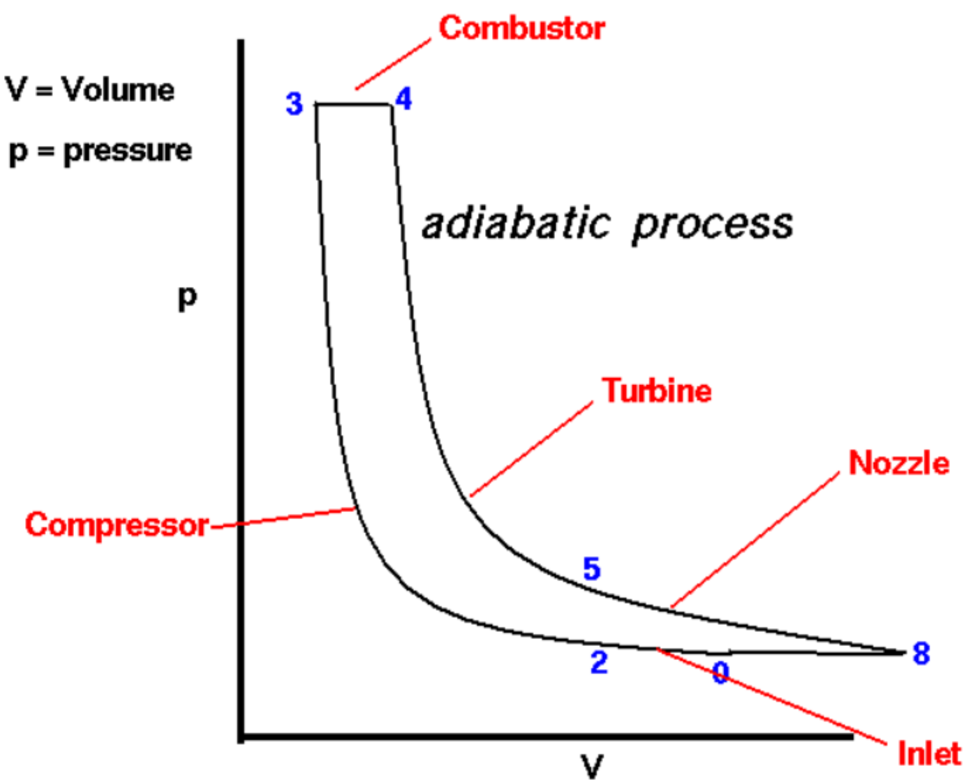

Figure 1: Brayton cycle in p-V coordinates [2]

The processes above are:

- 0-2 - isentropic compression of air in the inlet,
- 2-3 - isentropic compression of air in the compressor,
- 3-4 - isobaric addition of heat to the system,
- 4-5 - isentropic decompression of combustion products on the turbine,

- 5-8 - isentropic decompression of combustion products in the nozzle,

In this work the focus will be put on the process 3-4 since in jet engines during that phase the combustion occurs and emissions are generated.

2.2 Cantera package

Cantera is an 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 purpose of this project the most valuable feature of the Cantera package is the option of performing combustion reaction in constant pressure.

2.3 Equivalence ratio

The simulation of combustion process will be performed for a range of equivalence ratios. The equivalence ratio is defined as:

$$\Phi = \frac{(\frac{A}{F})_{stoich}}{\frac{A}{F}} \tag{1}$$

For hydrogen combustion:

$$\frac{A}{F} = \frac{a \cdot 4,76}{b} \cdot \frac{\mu_{air}}{\mu_{hydrogen}} \tag{2}$$

Where a and b are:

$$bH_2 + a(O_2 + 3,76N_2) -> H_2O + a3,76N_2$$

For stoichiometric reaction a=0.5 and b=1. Considering that the molar mass of air equals to 28,96 $\frac{g}{mol}$ and molar mass of molecular hydrogen is 2 $\frac{g}{mol}$, the stoichiometric air-to-fuel ratio for hydrogen combustion equals to approx. 34.

2.4 Cases analyzed

For the purposes of this project 3 different cases where analyzed:

- Case 1 - parameters corresponding to the technology of engines made between 1980 and 1990. (mean burning chamber temperature = 1500K, burning chamber pressure = 1 MPa)
- Case 2 - parameters corresponding to the technology of engines made nowadays (mean burning chamber temperature = 1700K, burning chamber pressure = 3,5 MPa)
- Case 3 - parameters corresponding to the possible future technologies, taken from graphs presenting trends in jet propulsion technologies. (mean burning chamber temperature = 1900K, burning chamber pressure = 5 MPa)

The analysis will be made for a range of equivalence ratios beginning from 0.2 and ending at 1.2

3 Code

The code used for calculating mentioned cases was written in Python 3.10 using Cantera package. The code can be found in the repository: https://github.com/Shyggy/Badanie-zawartosci-NOX-w-spalinach-mieszanin-wodorowo-powietrznych.

4 Results

Results of the performed analysis are presented below:

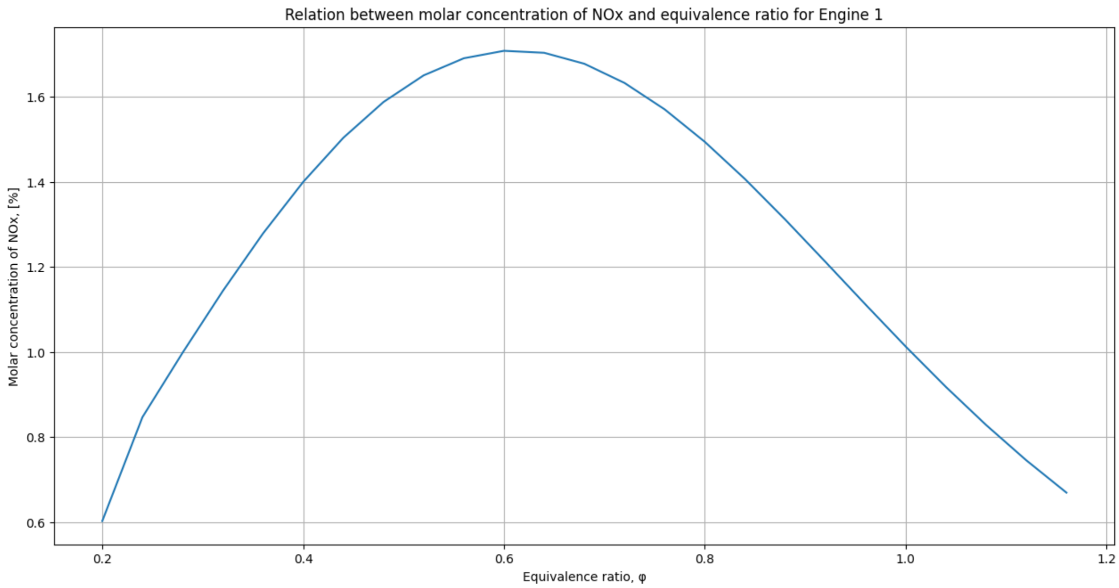

Figure 2: Concentration of NO_x in the engine from case 1

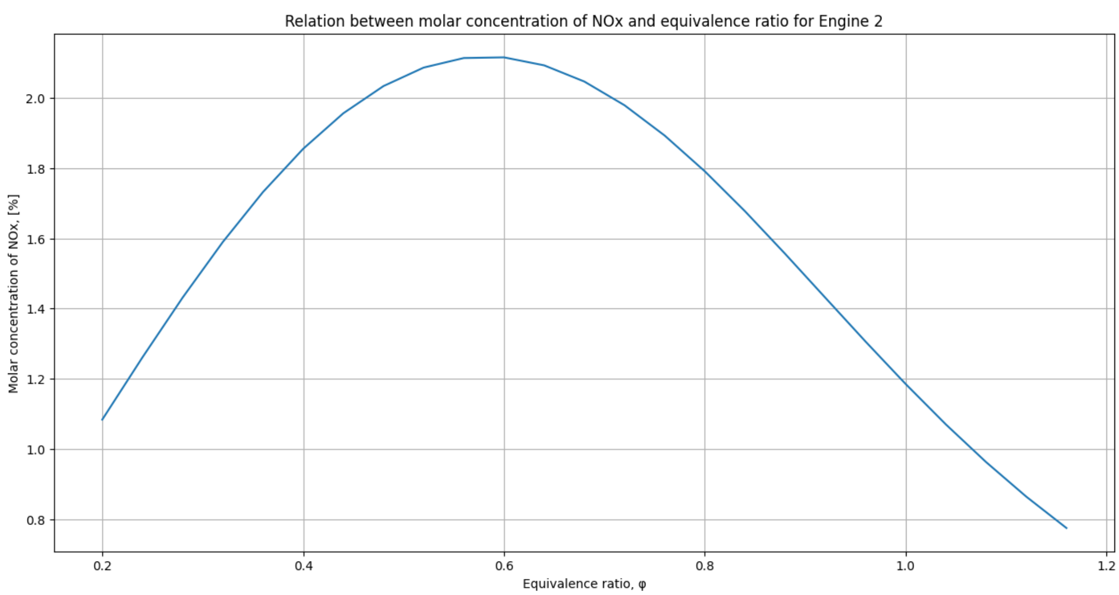

Figure 3: Concentration of NO_x in the engine from case 2

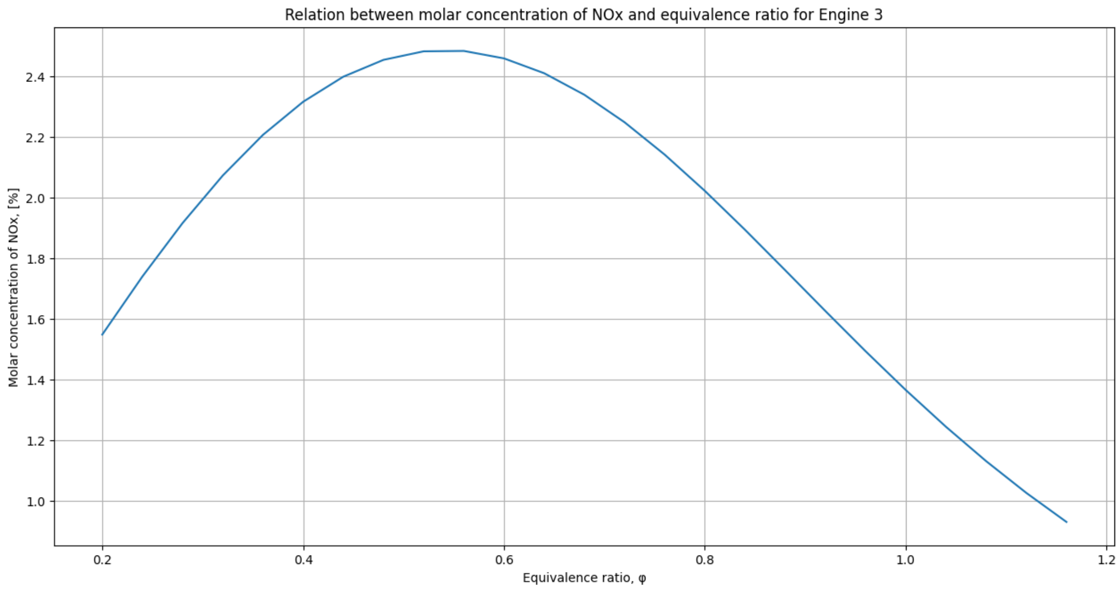

Figure 4: Concentration of NO_x in the engine from case 3

5 Conclusions

- Overall, the amount of NO_x generated in all cases is rather small, meaning that using some sort of catalytic converter can bring down the NO_x emissions to zero.
- The amount of NO_x particles rises with the rise of mean temperature in the burning chamber and pressure inside the burning chamber.
- Overall equivalence ratios between 0,55 and 0,65 should be omitted since at those equivalence ratios the concentration of NO_x particles are the greatest.
- Overall, considering low amount of NO_x particles generated hydrogen turbine engine could be defined as eco-friendly.

References

[1] `https://www.airbus.com/en/innovation/low-carbon-aviation/hydrogen`, access on day: 2023-05-28

[2] `https://www.grc.nasa.gov/www/k-12/airplane/brayton.html`, access on day: 2023-05-28

[3] `https://cantera.org`, access on day: 2023-05-08