Examination of NO_x concentration in propane-air and methane-air mixtures combustion products

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Computational methods in combustion

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0 Introduction

Combustion processes involving hydrocarbon fuels like propane and methane are fundamental to numerous industrial applications, including power generation, heating, and transportation. These processes, however, produce various pollutants, among which nitrogen oxides (NO_x) are of significant environmental concern due to their contribution to air pollution, acid rain, and the formation of ground-level ozone. Understanding the formation mechanisms and concentration levels of NO_x in combustion products is crucial for developing effective strategies to minimize emissions and meet regulatory standards.

Propane and methane, being widely used fuels, present distinct combustion characteristics that influence NO_x formation. Propane (C_3H_8) is a heavier hydrocarbon compared to methane (CH_4), leading to differences in flame temperature, combustion efficiency, and NO_x production. Methane, the primary component of natural gas, is known for its cleaner combustion properties but still poses challenges regarding NO_x emissions, especially under certain combustion conditions.

This study aims to examine the NO_x concentration in the combustion products of propane-air and methane-air mixtures. By comparing these two fuels, we seek to identify the key factors that influence NO_x formation and evaluate the effectiveness of various combustion strategies in reducing NO_x emissions. This research will contribute to a deeper understanding of combustion dynamics and support the development of cleaner and more efficient combustion technologies.

1 Computational model

1.1 Brayton cycle

When approximating the work of a gas turbine one normally uses Brayton cycle as an exact representation of idealized process. Below are inserted p-V and T-s graphs representing the cycle.

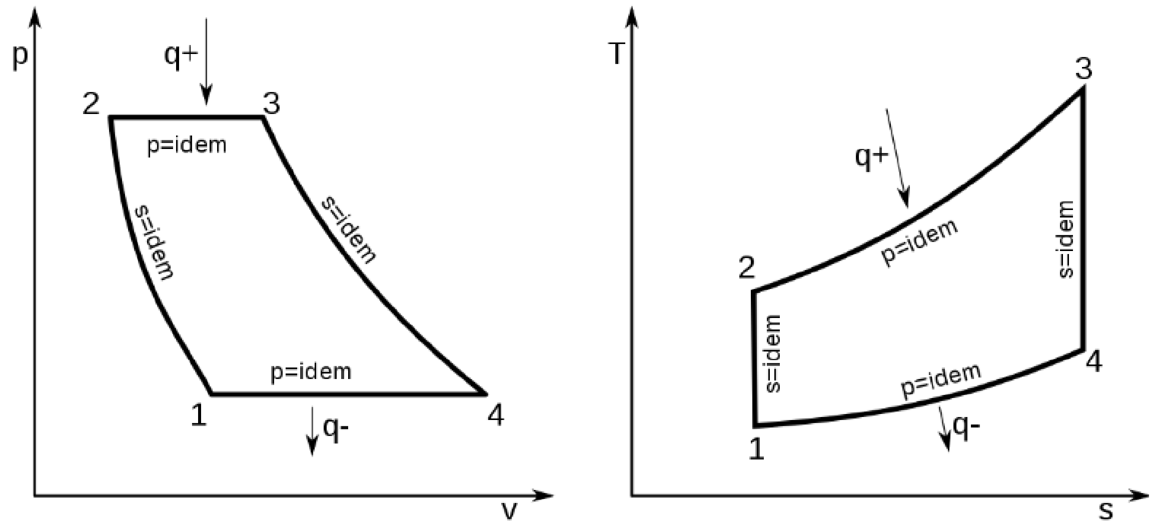

Figure 1: Brayton cycle in p-V and T-s coordinates

The processes presented above are as listed:

- 1-2 adiabatic process - compression
- 2-3 isobaric process - heat addition
- 3-4 adiabatic process - expansion
- 4-1 isobaric process - heat rejection

Because of the specific requirements of this article of examination of NO_x, only the 3-4 process will be discussed.

1.2 Cantera package

Cantera is an open-source suite of tools for problems involving chemical kinetics, thermodynamics, and transport processes. It is widely used in the fields of combustion, chemical engineering, and atmospheric sciences. The package provides a flexible and extensible platform for simulating and analyzing a wide range of chemically reacting systems. For this project option of performing combustion reactions under constant pressure is the most valuable feature of this program.

1.3 Equivalence ratio

To obtain the most diverse data possible, covering various initial conditions several simulations were 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 methane combustion:

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

For propane combustion:

$$\frac{A}{F} = \frac{a \cdot 4,76}{b} \cdot \frac{\mu_{air}}{\mu_{propane}} \tag{3}$$

Methane

$$bCH_4 + a(O_2 + 3,76N_2) \longrightarrow CO_2 + cH_2O + a \cdot 3,76N_2 \tag{4}$$

$$CH_4 + 2(O_2 + 3,76N_2) \longrightarrow CO_2 + 2H_2O + 7,52N_2 \tag{5}$$

$$a = 2; b = 1$$
$$\mu_{CH_4} = 16\frac{g}{mol}$$
$$\mu_{air} = 28,96\frac{g}{mol}$$

$$\frac{A}{F} = \frac{2 \cdot 4,76}{1} \cdot \frac{28,96}{16} = 17,23 \tag{6}$$

Propane

$$bC_3H_8 + a(O_2 + 3,76N_2) \longrightarrow CO_2 + cH_2O + a \cdot 3,76N_2 \tag{7}$$

$$C_3H_8 + 5(O_2 + 3,76N_2) \longrightarrow 3CO_2 + 4H_2O + 18,8N_2 \tag{8}$$

$$a = 5; b = 1$$
$$\mu_{C_3H_8} = 44\frac{g}{mol}$$
$$\mu_{air} = 28,96\frac{g}{mol}$$

$$\frac{A}{F} = \frac{5 \cdot 4,76}{1} \cdot \frac{28,96}{44} = 15,66 \tag{9}$$

1.4 Cases

For this project, 3 different cases of different temperatures were analyzed:
METHANE:

- Case 1 - $T_1 = 2100K; \Phi = 0,54; 2,701\%NO_X; p = 6MPa$
- Case 2 - $T_2 = 2400K; \Phi = 0,468; 3,311\%NO_X; p = 6MPa$
- Case 3 - $T_3 = 2700K; \Phi = 0,387; 3,942\%NO_X; p = 6MPa$

PROPANE:

- Case 1 - $T_1 = 2100K; \Phi = 0,553; 2,811\%NO_X; p = 6MPa$
- Case 2 - $T_2 = 2400K; \Phi = 0,479; 3,409\%NO_X; p = 6MPa$
- Case 3 - $T_3 = 2700K; \Phi = 0,394; 4,039\%NO_X; p = 6MPa$

2 Code

Code used for all the calculations was written in Python 3.19 using Cantera package. The code can be found in the repository: https://github.com/qeicam/Examination-of-NOX-concentration-in-propane-air-and-methane-air-mixtures-combustion-products.

3 Results

After running the simulations the results are presented below:

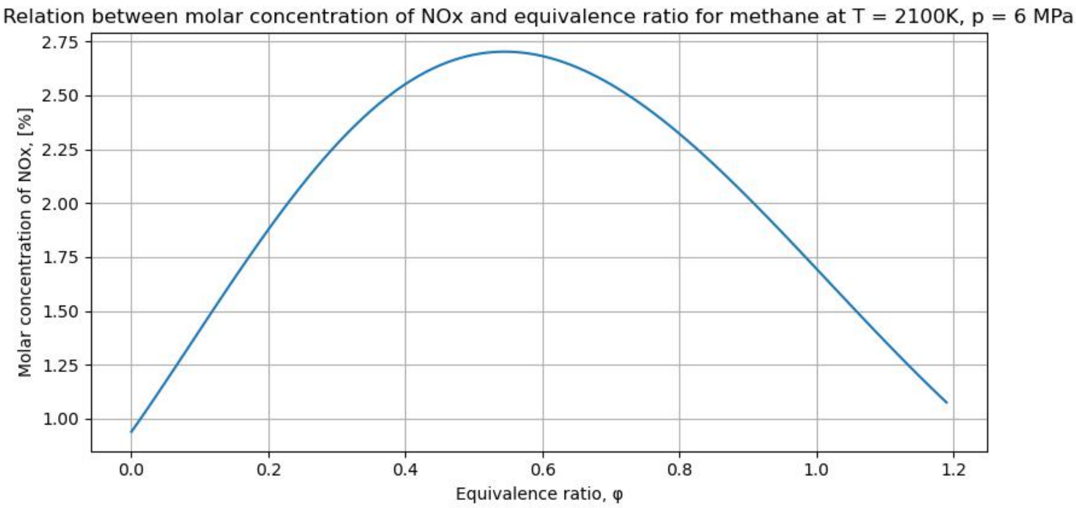

Figure 2: Concentration of NO_x in the engine from case 1 - METHANE

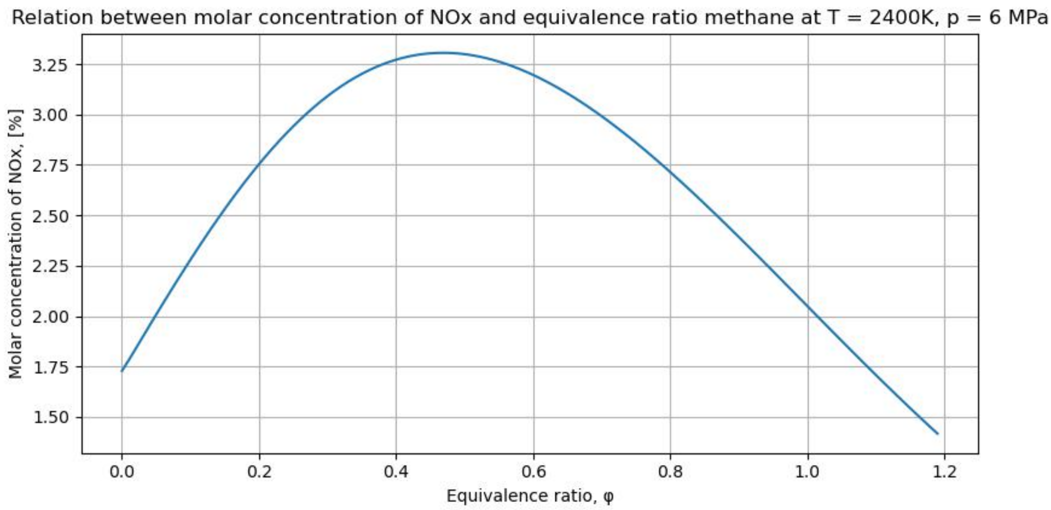

Figure 3: Concentration of NO_x in the engine from case 2 - METHANE

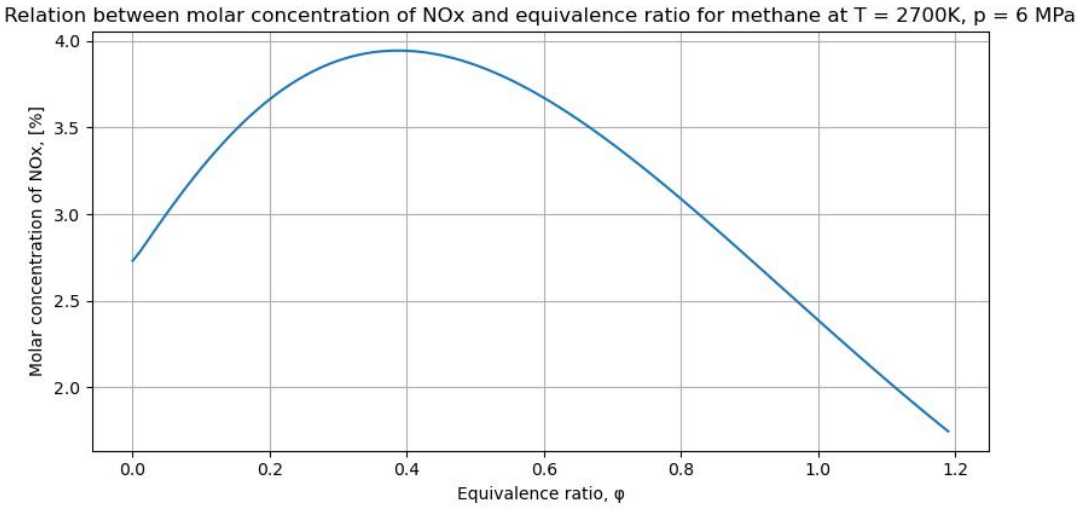

Figure 4: Concentration of NO_x in the engine from case 3 - METHANE

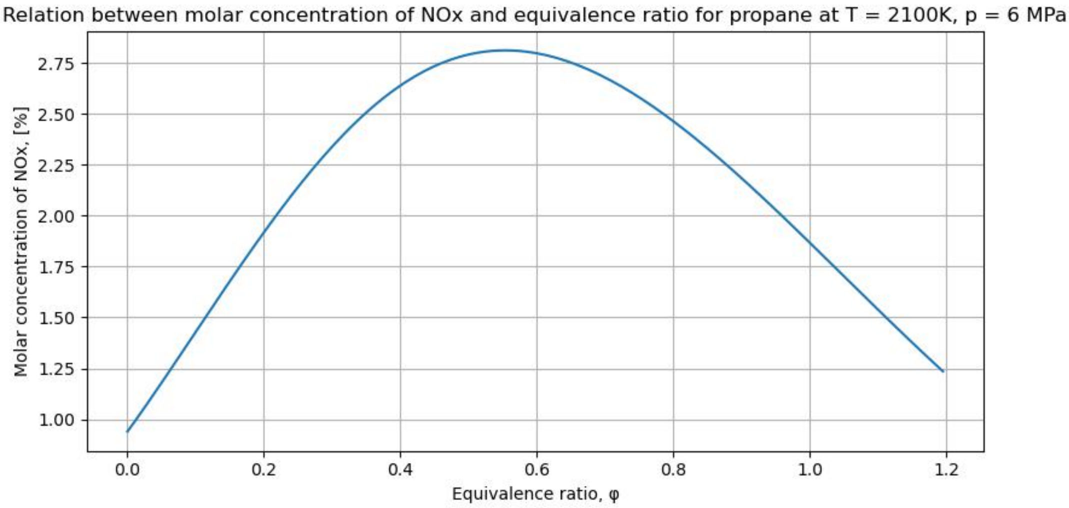

Figure 5: Concentration of NO_x in the engine from case 1 - PROPANE

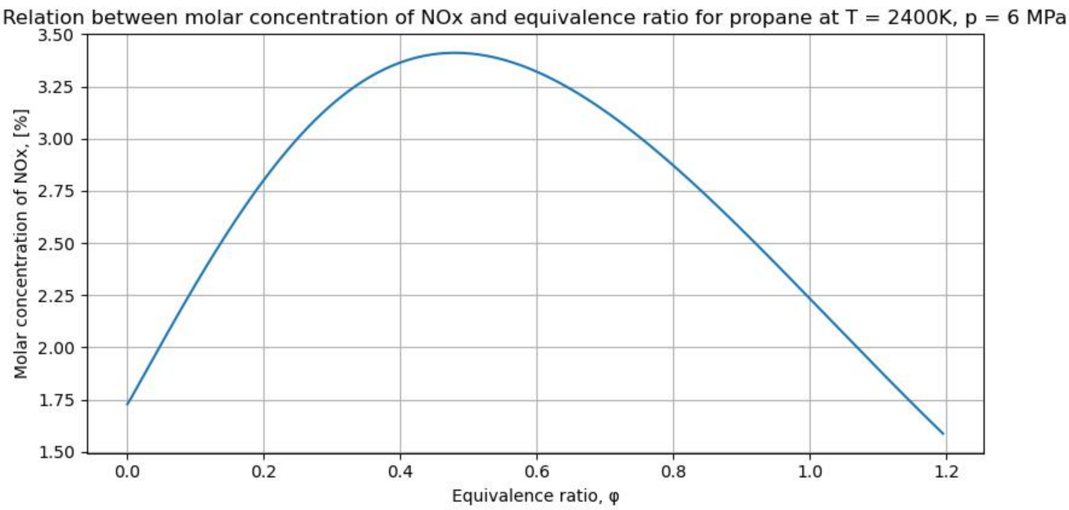

Figure 6: Concentration of NO_x in the engine from case 2 - PROPANE

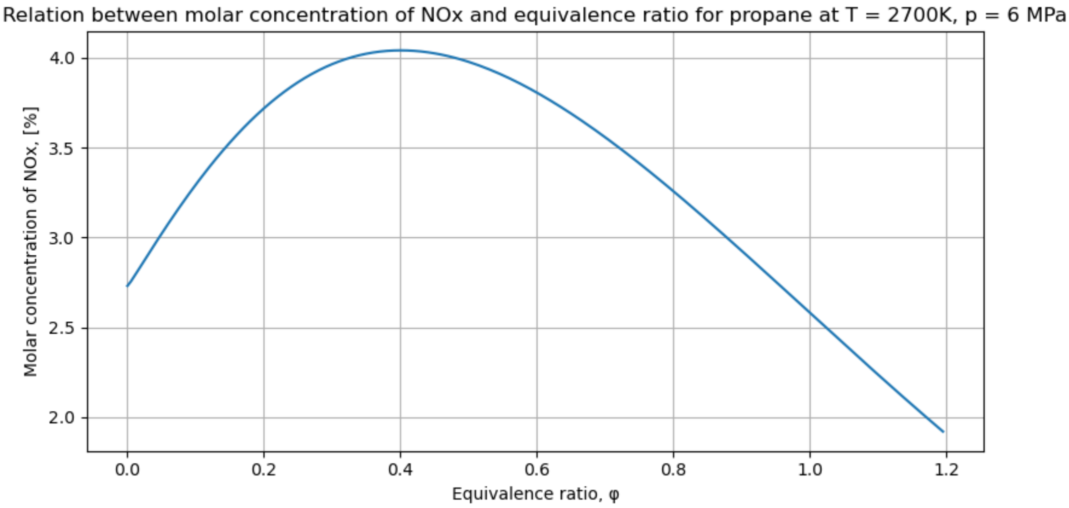

Figure 7: Concentration of NO_x in the engine from case 3 - PROPANE

4 Conclusions

The concentration of NOx rises with increasing temperature. These characteristics can be observed for both mixtures. As the carbon content in the mixture increases (and consequently the molar mass), a higher percentage of NOx in the exhaust gases is observed. Therefore, it can be inferred that to meet EU standards and adhere to current trends in reducing NOx emissions in exhaust gases, it is advisable to use mixtures with the simplest hydrocarbons possible at lower temperatures, which in this case is methane at 2100K.

5 References

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