NO_x AND EXTREMELY LOW TEMPERATURES OF CHARGING

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Abstract

The basis of basic research consists in the influence monitoring of unconventional (extremely low temperatures) charging intercooling on the selected ecological and economical parameters of a turbocharged internal combustion engine in the specific operational conditions (periodic starts and stops). The paper deals with the influence of the mentioned temperatures from the point of view of the harmful gaseous emissions production with focus on NOx.

The theoretical analysis, consequential mathematical modelling (in Fluent) of the utilizing of the extremely low temperatures of charging after the intercooler in the range from 30°C to near above zero temperatures of the turbocharged engine should define the changes trends in its power parameters and exhaust gas emissions production mostly NOx. At the same time it should consider the influence of the extremely low temperatures of charging on the engine inner corrosion at the periodic engine starts and stops. The mathematical model should allow alternatively solving possible risks resulting from the proposal newness and originality. From the proposal it is expected to obtain more effective energy utilization, the decrease of the environment ecological load compared with the standard solution and the possibility of creation of the permanent sustainable energetic system. The possibilities of the design solution for the system of extremely low temperatures of air fuel mixture are also presented in the paper.

Keywords: *nitrogen oxides, theoretical analysis, extremely low temperatures, free enthalpy, combustion temperature*

1. Introduction

The term nitrogen oxides NO_x means a group comprising mainly nitric oxide NO and nitrogen dioxide NO_2. NO_2 is the key component from the point of harmful influence and the environmental legislation is based on the assumption that the entire amount of NO_x oxidize into this component during its stay in the atmosphere. But the main component emitted by the combustion engine is NO. Equilibrium concentration of the nitrogen dioxide based on the conditions inside the engine cylinder is extremely low, so the term nitrogen oxides in the field of combustion engines mean particularly nitric oxide.

2. Nitrogen oxides NO_x

Nitric oxide NO arises by the chain reaction described by Zeldovich mechanism:

$$N_2 + O \leftrightarrow NO + N, \tag{1}$$

$$O_2 + N \leftrightarrow NO + O. \tag{2}$$

A key process in the presence of nitrogen oxides in the exhaust gases is relatively high occurence of the equilibrium concentration of NO in the work cycle phase with the high temperature, followed by a dramatic decrease of the reaction rate of decomposition of NO.

The deceleration of NO decomposition reaction is so sudden, that the term the freeze of NO concentration is used for its description. The value of NO equilibrium concentration maximum decreases with the reduction in combustion temperatures and thus the NO production rate decreases. Consequently the NO concentration in the exhaust gases decreases. The value of the maximum pressure does not have the direct influence on the chemical reactions, but it influences the reaction temperatures. The highest temperatures are reached in a slightly reach mixtures, but there is the lack of oxygen in these areas. This lack of oxygen inhibits the production of NO_x. Production maximum is shifted to the slightly lean mixtures area with the air excess cofficient of about 1.15. The position of the maximum of NO equilibrium concentration is consistent with the position of maximum temperature in the combustion chamber. In reality, however, the production maximum is moved on. The higher temperature, the more close the actual concentration of NO to the concentration determined according to equilibrium. The actual content of each component of mixture during the reaction lies between the starting content of this component in the input components of the reaction and its equilibrium content for an immediate state and concentration conditions.

As mentioned above, nitrogen dioxide NO_2 is produced secondarily from previously produced nitric oxide. At the normal temperature of the flame and process balance the NO_2/NO ratio must be relatively small. Experimental data show that this assumption is correct for spark ignition engines (at compression ignition engines the ratio can be of 10-20% of all emitted nitrogen oxides). According to Heywood the approximate mechanism of NO_2 formation is following. NO in the flame zone can be quickly converted by the following reaction:

$$NO + H_2O \rightarrow NO_2 + OH, \tag{3}$$

$$NO_2 + O \rightarrow NO + O_2. \tag{4}$$

This reaction runs until NO_2 created in the flame zone reduces its temperature by mixing with the cold gases.

3. Gaseous emissions production analysis

Calculation of the equilibrium composition of combustion products will be used to analyse the temperature influence of charging mixture on the combustion products composition. The calculation will be done through the special software (Fig. 1). The theoretical constant volume heat cycle (also Otto cycle) will be considered for the calculation. The calculation is based on the minimizing of the free enthalpy. The basis of the minimalization of free enthalpy for single case is to find such composition of the exhaust gases which has the minimum enthalpy at given temperature and pressure. Minimalization is done by the iterative calculation of gas composition and temperature. We will consider the combustion of octane with air at the stoichiometric ratio.

Fig. 1. Dialog box of the program

Combustion products consist of the following components: CO_2, CO, C_g, C_s, H_2O, H_2, OH, H, O_2, O, N_2, NO, N.

The set values can be seen in Fig. 2.

Fig. 2. Set input values for the calculation

The input parameters for the calculation are the following:

- compression ratio EPS = 12,
- inverse value of the excess-air coefficient FI = 1/1.69 = 0.592,
- mass fraction of combustion products in the mixture F = 0.0005,

- mixture pressure before compression P1 = 1.76 bar,
- mixture temperature before compression T1 (K),
- choice of the fuel type PALIVO = 3 (natural gas).

The engine is fitted with the charging air intercooler with the possibility of changing the charging air temperature within the range from 30°C to 0°C with the step of 5°C. We will input the single value of charging air temperature for the single calculation. Fig. 3 shows the calculation results for the charging air temperature of 5°C, where the calculated amount of single components can be seen.

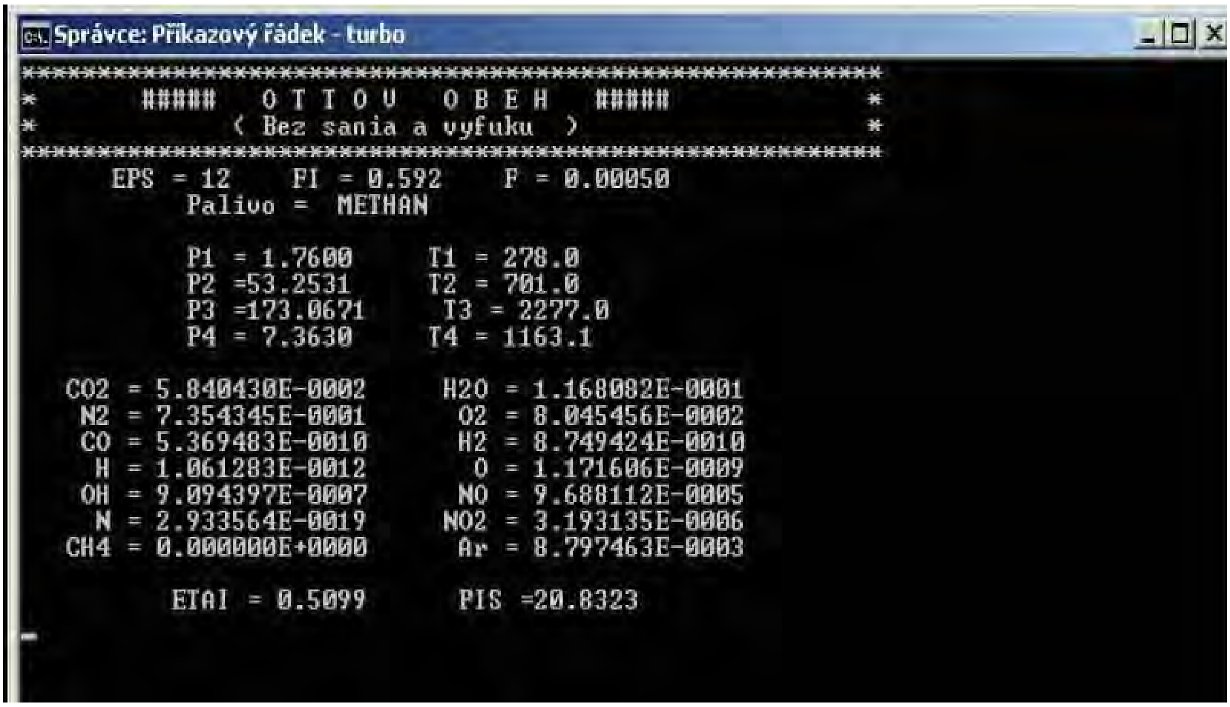

Fig. 3. Calculation results for the charging air temperature of 5°C

Table 1 and 2 show the calculated results of equilibrium concentration of single combustion products for the single values of charging mixture temperature. The results are represented through the mass fraction of single components.

Tab. 1. Equilibrium concentration of combustion products

Temperature of charging mixture (K)	N ( )	NO ( )	NO_2 ( )	CO ( )	CO_2 ( )	O ( )
273	2.36E-19	9.31E-5	3.17E-6	4.71E-10	5.84E-2	1.04E-9
278	2.93E-19	9.69E-5	3.19E-6	5.37E-10	5.84E-2	1.17E-9
283	3.63E-19	1.01E-4	3.22E-6	6.11E-10	5.84E-2	1.32E-9
288	4.49E-19	1.05E-4	3.24E-6	6.95E-10	5.84E-2	1.48E-9
293	5.54E-19	1.09E-4	3.26E-6	7.89E-10	5.84E-2	1.66E-9
298	6.82E-19	1.13E-4	3.29E-6	8.94E-10	5.84E-2	1.86E-9
303	8.39E-19	1.17E-4	3.31E-6	1.01E-9	5.84E-2	2.08E-9

Tab. 2. Equilibrium concentration of combustion products

Temperature of charging mixture (K)	O_2 ( )	OH ( )	H ( )	H_2 ( )	H_2O ( )
273	8.05E-2	8.44E-7	9.02E-7	7.79E-10	1.17E-1
278	8.05E-2	9.09E-7	1.06E-12	8.75E-10	1.17E-1
283	8.05E-2	9.79E-7	1.25E-12	9.82E-10	1.17E-1
288	8.05E-2	1.05E-6	1.46E-12	1.10E-9	1.17E-1
293	8.04E-2	1.13E-6	1.71E-12	1.23E-9	1.17E-1
298	8.04E-2	1.22E-6	2.00E-12	1.38E-9	1.17E-1
303	8.04E-2	1.31E-6	2.34E-12	1.54E-9	1.17E-1

As already mentioned, the cooling of the charging mixture reduces the combustion temperature, which is crucial for reducing NO_x emissions. This fact was the assumption for reducing NO_x emissions at extreme cooling of the charging mixture. The assumption was confirmed by the analysis.

Figure 4 shows the dependency of the mass fraction of NO in the exhaust gases on the value of the charging mixture temperature. As it can be seen the decrease in temperature results in the decrease in the NO emissions production. The simulation results shows that the decrease in mixture temperature from 30°C to 0°C results in the decrease of NO formation about 20.69%, what is interesting result.

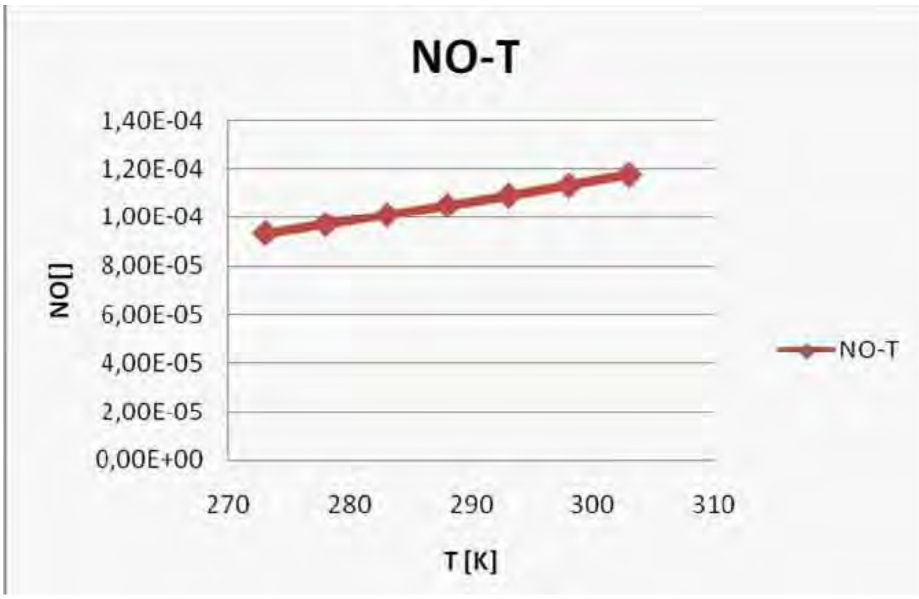

Fig. 4. Calculation results for the amount of NO

As already mentioned NO_2 emissions are not the priority in the evaluation of NO_x emissions at internal combustion engines.

Figure 5 shows the direction of change in the amount of NO_2 emissions is the similar as in the previous case. But the decrease in NO_2 emissions is not so significant. Decrease in mixture temperature from 30°C to 0°C means the decrease in NO_2 emissions about 3.92%.

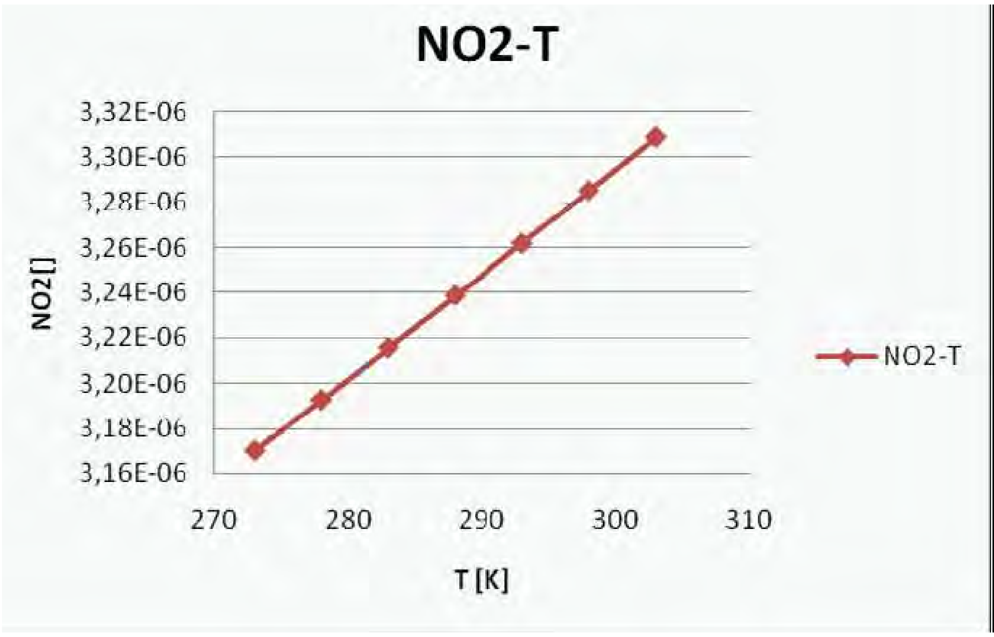

Fig. 5. Calculation results for the amount of NO2

The calculation results for the amount of CO are shown in Fig. 6.

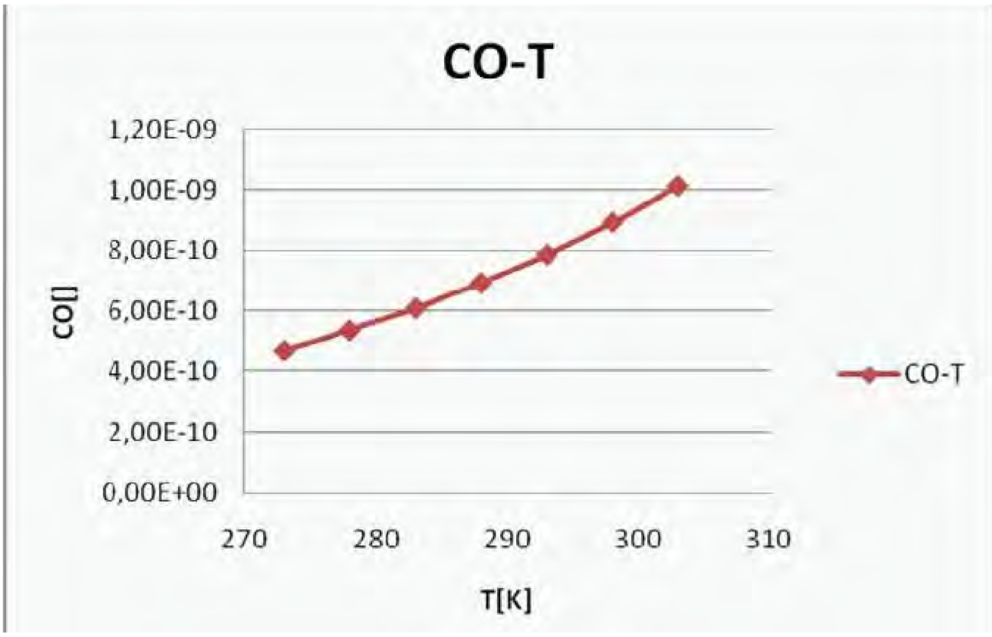

Fig. 6. Calculation results for the amount of CO

The result is that the CO production decreases about 53.47% with the decrease in mixture temperature from 30°C to 0°C.

Figure 7 shows the analysis results for the CO_2 emissions and Fig. 8 results for O emissions.

CO_2 emissions increase about 1.7% with the decrease of mixture temperature from 30°C to 0°C. This increase is not significant and is resulting from the decrease of CO.

Results show that the O emissions decrease about 49.88% with the decrease of mixture temperature from 30°C to 0°C.

From the point of view of design solution it is expected to use a liquid-air intercooler with the liquid cooled by a special system.

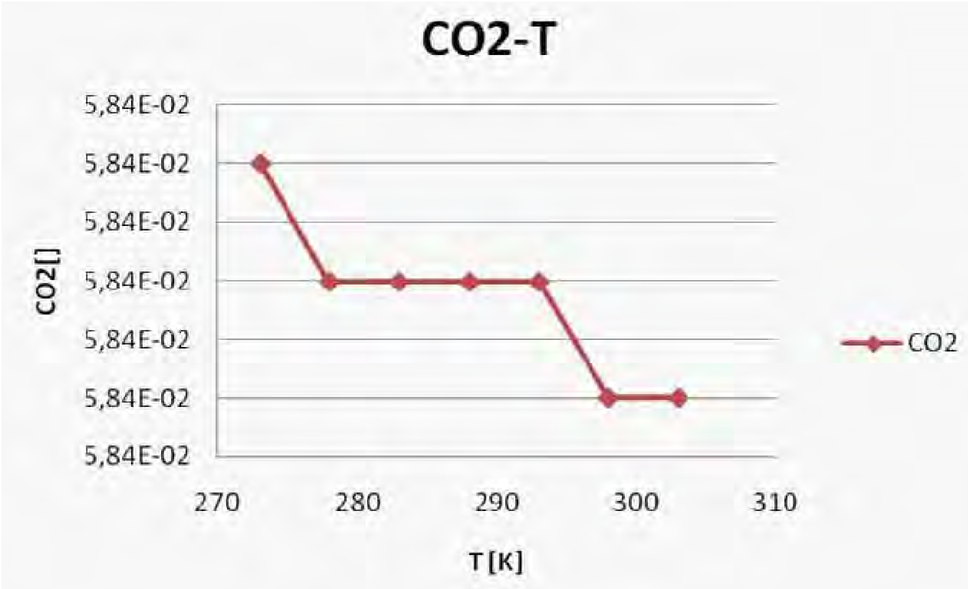

Fig. 7. Calculation results for the amount of CO2

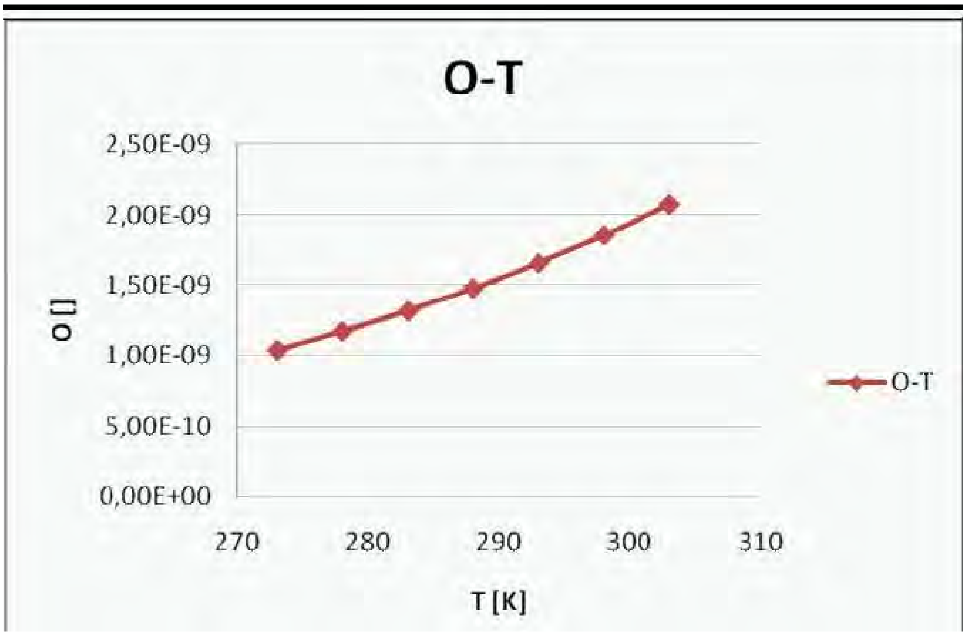

Fig. 8. Calculation results for the amount of O

4. Conclusion

The paper deals with the influence analysis of the extremely low temperatures of charging mixture in the range from 30°C to 0°C on the emissions production.

Results show that the mentioned decrease in mixture temperature mean the decrease in NO production about 20.69%, NO_2 about 3.92%, CO about 53.47%, O about 49.88% and the increase in CO_2 emission about 1.7%.

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