

Comparative analysis of exhaust emissions from a compression-ignition engine fueled with mixtures of rapeseed oil with n-hexane and diesel fuel during selected phases of the WLTP test

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The article presents the differences in emissions of a passenger car with a compression-ignition engine fueled by vegetable fuel – rapeseed oil with n-hexane and diesel fuel. Emission tests were carried out on a chassis dynamometer in selected phases of the World Harmonized Light Vehicle Test Procedure. Carbon monoxide, carbon dioxide, nitrogen oxides, total hydrocarbons and non-methane hydrocarbons were measured based on the WLTC Class 3b driving cycle. The effect of engine operating conditions on exhaust emissions when fueled with the fuels studied was described. A regression model was developed to estimate the level of pollutants in the exhaust gas.

Key words: *exhaust emission, WLTP, compression-ignition engine, vegetable fuel, regression model*

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1. Introduction

In order to protect life and health, reducing the harmful effects of internal combustion engines on the environment is a priority. Reducing emissions can therefore be considered a fundamental in the context of internal combustion engine development. By developing new vehicles, internal combustion engine manufacturers must meet constantly tightening emission standards. For many years, legislative procedures have been based on the use of driving cycles. This tests both speed changes and a wide range of loads under varying operating conditions. Currently, the World-wide Harmonized Test Procedure for Light Vehicles is used, which was developed based on actual driving data to simulate the most common daily driving conditions [3, 13].

The real operating conditions of internal combustion engines are largely undefined. The essence of emission measurements, in addition to replicating real conditions, is therefore to ensure their high accuracy and repeatability. In order to eliminate factors that affect the discrepancies in the values of the results, the tests should be performed under repeatable conditions, which include the same test environment, the use of the same test method, the use of the same test equipment and instruments, and, in the case of mapping, the test cycle should also be performed by the same operator. The repeatability of the measurement results is also due to the repeatability of the operating states of the internal combustion engine. The operating states of the engine that characterize emissions are determined by the engine speed, engine load or its thermal state, and in the case where the test engine is installed in a vehicle, by the vehicle speed and motion resistance. Measurements under laboratory conditions carried out on a chassis dynamometer, ensuring the repeatability of the motion resistance, make vehicle speed the main variable determining engine operating states [1, 6, 7, 12, 13].

However, so many factors affecting the level of pollutant emissions call into question their repeatability. The cost of conducting tests is often higher than the cost of the measuring equipment and the electricity used during the tests, or the working gases used. This affects the number of measurements performed. Issues of repeatability of emission tests are described in works [2, 6, 11, 13].

In the face of costly scientific research, it is reasonable to use learning algorithms that allow the construction of predictive models that, based on available empirical data, can predict the results of future experiments with high probability. As a result, it becomes possible to reduce the number of actual studies to the most promising ones. It allows the identification of hidden relationships in complex data sets that could go unnoticed using traditional methods of analysis [5].

Research on exhaust emissions is also an extremely important aspect of the energy transition. A growing number of studies have focused on comparing emissions from alternative energy sources versus traditional internal combustion engines. This is related to the positive impact of using bio-fuels on the environment. The use of replacement fuels that do not require structural or regulatory changes to the engine requires the development of a fuel with physical properties similar to those of conventional fuel. Solutions based on esterification processes or additives to vegetable oils are well known. The use of plant-based fuels significantly reduces carbon dioxide emissions, also taking into account their absorption during the growth phase of raw materials. In compression ignition engines, a decrease in particulate matter emissions is observed. However, the use of substitute fuels can also lead to increased nitrogen oxide emissions, especially during periods of high load. It is therefore important to test fuels under real driving conditions, based on current test procedures [4, 8–10, 14–16].

This paper combines the above challenges, focusing on the evaluation of emission relationships when running on mixtures of rapeseed oil with n-hexane based on selected WLTP test phases and the development of a regression model.

2. Materials and methods

The test vehicle was a Fiat Qubo passenger car with a 1.3 Multijet four-cylinder diesel engine. The engine complied with the Euro 5 standard. Basic information about the test object is shown in Table 1.

Table 1. Parameters and technical data of the Fiat Qubo passenger car with a 1.3 Multijet engine

| Parameter | Value |
|----------------------------|----------------------|
| Engine displacement | 1248 cm ³ |
| Fuel type | Diesel |
| Compression ratio | 16.8:1 |
| Emission standard | Euro 5 |
| Power | 55 kW |
| Max. power rpm | 4000 rpm |
| Max torque | 190 Nm |
| Max. torque rpm | 1750 rpm |
| Number of gears | 5 |
| 1 st gear ratio | 3.64:1 |
| 2 nd gear ratio | 1.95:1 |
| 3 rd gear ratio | 1.28:1 |
| 4 th gear ratio | 0.98:1 |
| 5 th gear ratio | 0.77:1 |
| Final drive ratio | 3.56:1 |
| Tire size | 185/65 R15 |

In the study, a mixture of rapeseed oil with a 20% addition of n-hexane (RONhex) was used. The added compound is a hydrocarbon produced during the distillation of crude oil. It is a component of the light gasoline fraction. Due to its physicochemical properties, it is used as a solvent in the chemical industry. Its addition affects the parameters of rapeseed oil, including surface tension, density, or viscosity, thus bringing its properties closer to those of conventional fuels. Its addition allows rapeseed oil to be used at ambient temperatures of sub-zero. The addition of n-hexane improves the atomization properties of the fuel in the combustion chamber, which promotes the combustion process and leads to higher engine efficiency. It also reduces the risk of damage to the injection system and other fuel system components, allowing rapeseed oil to be used without the need for engine modifications [4, 8–10]. Diesel fuel (DF) was used as the reference fuel. An auxiliary fuel tank was located in the vehicle, which allowed for a quick change of fuel mixtures and did not affect the amount of fuel in the main tank. The basic physicochemical properties of the fuels tested are presented in Table 2.

Table 2. Basic physicochemical properties of the tested fuels [9]

| | Diesel Fuel | RONhex |
|--|-------------|--------|
| Density at 20°C [kg/m ³] | 840 | 879 |
| Surface tension at 20°C [mN/m] | 29.15 | 27.70 |
| Kinematic viscosity index at 40°C [mm ² /s] | 2.7 | 11.70 |
| Flash point [°C] | 72 | < 40 |
| LC cetane number [-] | 51.2 | 75.6 |
| Calorific value [MJ/kg] | 43 | 9.4 |

The tests were conducted based on selected phases of the WLTP test. The condition of the vehicle and its preparation corresponded to the procedure recommendations. The tests were conducted on an unhomologized test stand, a diagram of which is shown in Fig. 1, which consisted of a Dynorace DF4FS-HLS two-axle chassis load dynamometer. To reproduce the driving cycle, a computer with implemented software was used, using the OBDII system to communicate with the vehicle's ECU. Using the system, the following were recorded:

- vehicle speed
- engine speed
- torque.

The test stand also included an AVL SESAM i60 FT measurement system, which recorded exhaust gas concentrations. The system's measuring probe was placed in front of the catalytic converter. During the tests, the concentration of the following substances was tested:

- concentration of carbon monoxide (CO) and carbon dioxide (CO₂)
- concentration of nitrogen oxides (NO_x divided into NO and NO₂)
- concentration of hydrocarbons (THC) and non-methane hydrocarbons (NMHC).

The stand was not built in a climate chamber, which made it impossible to control environmental conditions. Measurements were made under the following laboratory conditions:

- temperature (23.6–24.8°C)
- humidity (45–57.8%)
- atmospheric pressure (984.8–990.4 hPa).

Measurements were made based on the WLTC Class 3b driving cycle. Three runs were made for each of the fuels tested.

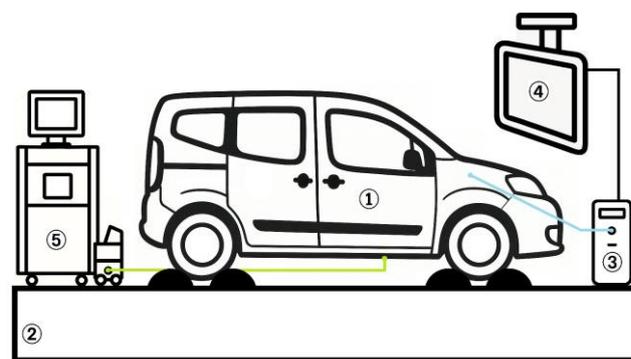


Fig. 1. Test stand (1 – Fiat Qubo passenger car, 2 – Dynorace DF4FS-HLS chassis dynamometer, 3 – PC with implemented WLTC test cycle, 4 – additional screen, 5 – AVL SEASAM i60 FT)

3. Results

The test travel speed results were linearly interpolated, and then a Savitzky-Golay filter was applied. The average travel speed (AV), standard deviation (SD) and coefficient of variation (CV) were calculated for each fuel. The results are shown in Table 3.

Table 3. Parameters of the driving cycles

| Parameter | DF | RONhex |
|-----------|-------|--------|
| AV [km/h] | 46.35 | 46.21 |
| SD [km/h] | 1.49 | 1.43 |
| CV [%] | 7.8 | 7.6 |

The results obtained (7.8% variability for DF and 7.6% variability for RONhex) indicate high repeatability of measurements. The average values of speed and torque for each fuel are shown in Fig. 2 and Fig. 3.

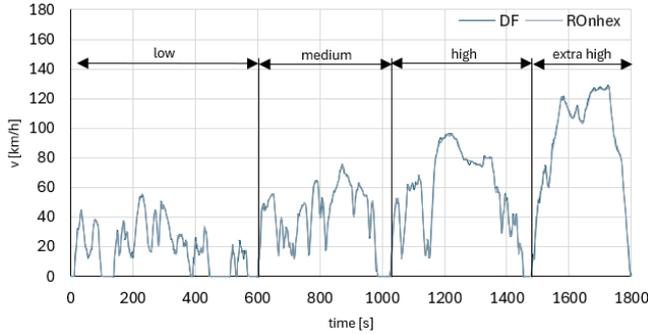


Fig. 2. Average speed during the WLTC driving cycle

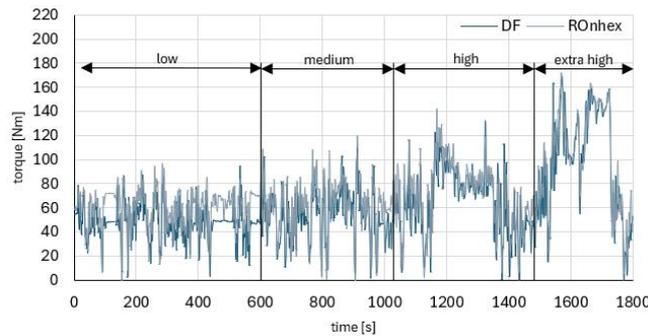


Fig. 3. Average torque during the WLTC driving cycle

In the analysis of the exhaust gas concentration results, a median filter was used to reduce impulse noise and a Savitzky-Golay filter to smooth the data. The results of the filtered and averaged measurements for each fuel type are shown in Fig. 4–17.

The highest CO concentrations were recorded for RONhex in the low phase (the average concentration reached 932.26 ppm and was 68.83% higher relative to DF in this phase) and for DF in the extra high phase (715.21 ppm and was 207.14% higher relative to RONhex). The high CO concentration in the early phases of the cycle for rapeseed oil with n-hexane addition is due to the lower temperature and incomplete combustion process, which, combined with the lower volatility of rapeseed oil, results in poorer fuel evaporation. On the other hand, the higher viscosity relative to diesel fuel negatively affects the fuel atomization process. This results in a less efficient combustion process. As the load and combustion temperature increase, this effect is offset, thanks in part to the oxygen content of the RONhex mixture, resulting in lower CO concentrations. In the case of DF, at higher loads, the fuel mixture becomes richer, and the lower oxygen content results in a higher CO concentration. The course of CO concentra-

tion over the WLTC cycle is shown in Fig. 4, while the average values over each cycle are shown in Fig. 5.

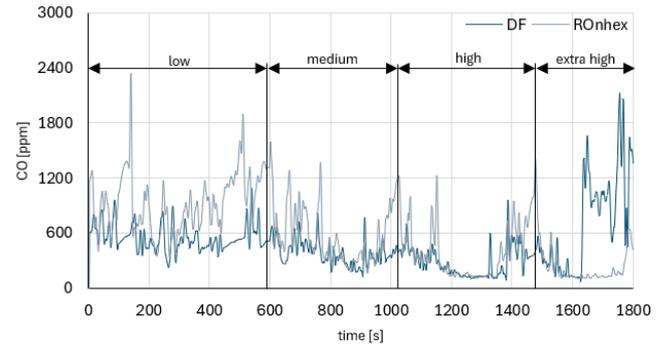


Fig. 4. CO concentration during the WLTC driving cycle

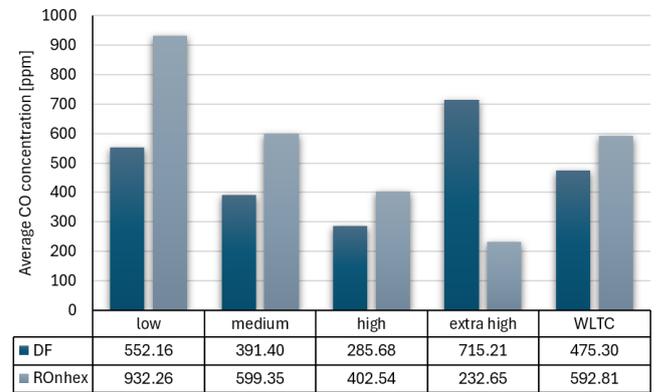


Fig. 5. Average CO concentration during each cycle

For both fuels tested, the highest CO₂ and NO_x concentrations were recorded in the phases characterized by the highest loads. The average CO₂ concentration in each phase was lower for RONhex (by 9.65% relative to DF throughout the cycle). The lower CO₂ concentration is mainly due to the difference in the chemical composition of the fuels tested. Diesel fuel contains more carbon per unit weight, which is associated with a higher heating value, as well as higher CO₂ emissions. In contrast, the increase in concentration with load is mainly due to the increased dose of fuel delivered. Figure 6 shows the course of CO₂ concentration over the WLTC cycle, and the average values for each cycle are shown in Fig. 7.

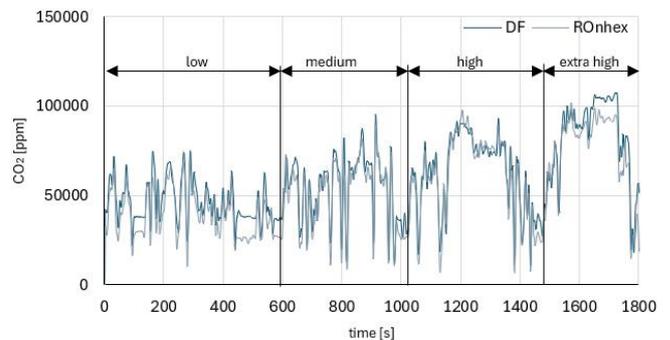


Fig. 6. CO₂ concentration during the WLTC driving cycle

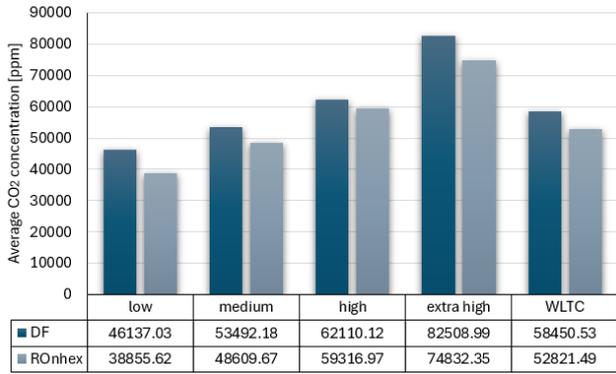


Fig. 7. Average CO₂ concentration during each cycle

The difference in average NO_x concentration throughout the cycle did not exceed 0.05%. At the same time, it was noted that in the low, medium and high phases it was lower for RONhex (by 15.9%, 8.13%, 0.77%, respectively) and in the extra high phase for DF (by 12.91%). This phenomenon is due to the difference in the chemical composition of the fuels - the presence of oxygen in rapeseed oil, and therefore the higher concentration of oxygen in the combustion process and the higher flame temperature. On the other hand, the increase in concentrations in subsequent phases is related to the increase in combustion temperature. Figures 8 and 9 show the course and average values of NO_x concentrations in each cycle.

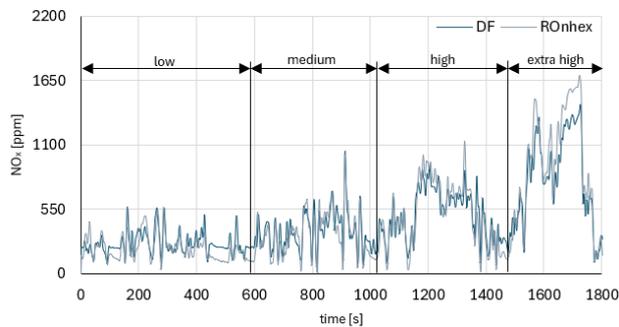


Fig. 8. NO_x concentration during the WLTC driving cycle

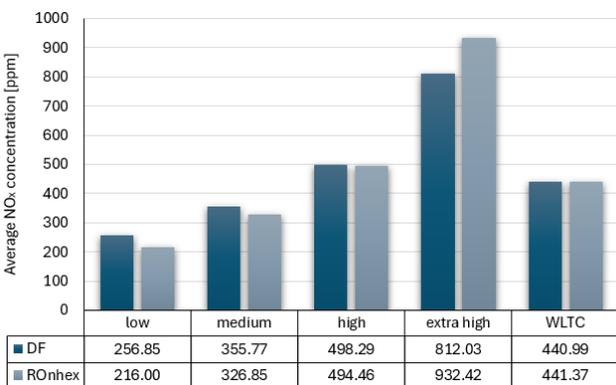


Fig. 9. Average NO_x concentration during each cycle

In the case of NO, the concentration throughout the cycle was 2.05% higher for DF than for RONhex. When considering the case of NO₂ concentration, the difference due to the presence of oxygen in the rapeseed oil, which pro-

motes the oxidation of NO to NO₂, again becomes apparent. Throughout the cycle, the NO₂ concentration was 16.26% higher for RONhex relative to DF. Figures 10 and 12 show the waveforms of NO and NO₂ concentrations during the WLTC cycle. The average values of NO and NO₂ concentrations in each cycle are shown in Fig. 11 and Fig. 13.

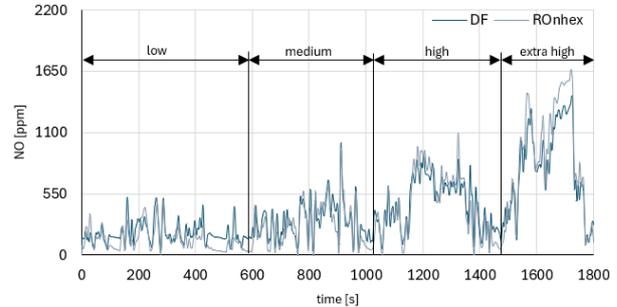


Fig. 10. NO concentration during the WLTC driving cycle

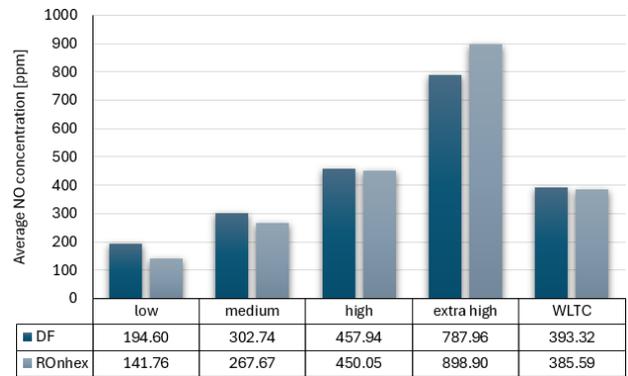


Fig. 11. Average NO concentration during each cycle

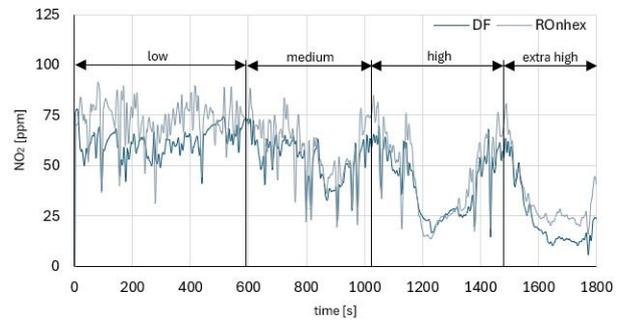


Fig. 12. NO₂ concentration during the WLTC driving cycle

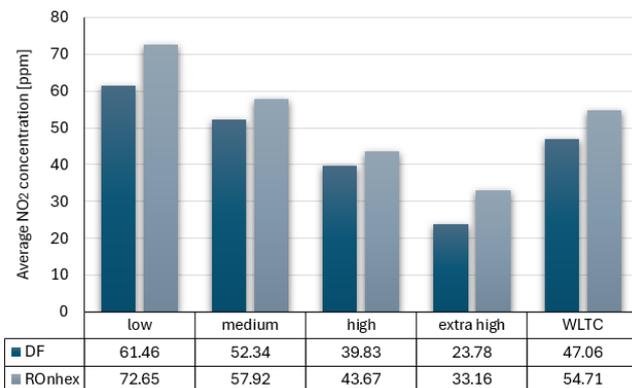


Fig. 13. Average NO₂ concentration during each cycle

For hydrocarbon exhaust concentrations, the highest concentrations were observed for RONhex in the low phase (the average concentration reached 109.76 ppm for THC and 242.77 ppm for NMHC), while for DF in the extra high phase (359.91 ppm for THC and 736.53 ppm for NMHC). For the tested concentrations in the extra high phase, a large deviation from the mean was observed in the case of DF (the extreme value of the upper distribution was 17 times higher than the average value in the case of THC, 16 times in the case of NMHC). This relationship was not observed for RONhex. The concentrations of THC and NMHC in the WLTC cycle are shown in Fig. 14 and 16, respectively. In contrast, the values of the average concentration are shown in Fig. 15 and Fig. 17.

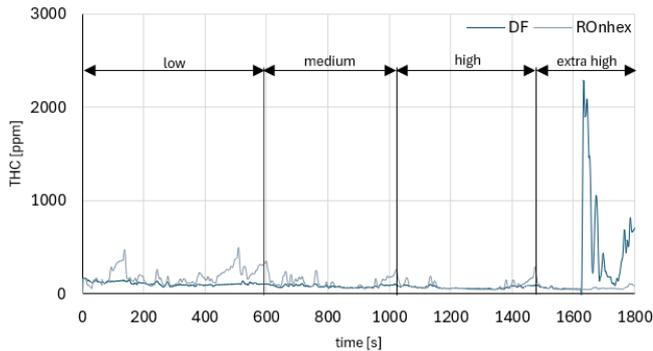


Fig. 14. THC concentration during the WLTC driving cycle

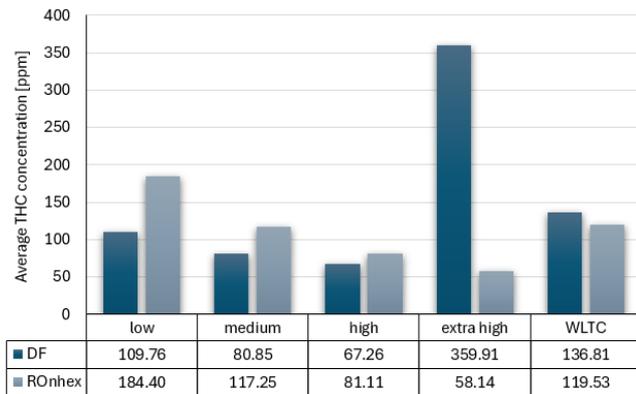


Fig. 15. Average THC concentration during each cycle

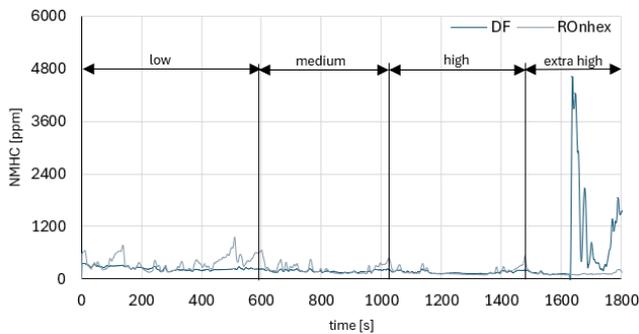


Fig. 16. NMHC concentration during the WLTC driving cycle

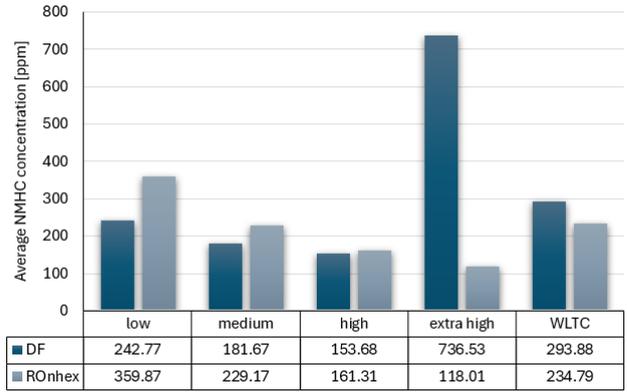


Fig. 17. Average NMHC concentration during each cycle

In further analysis, a predictive model was developed to forecast NO_x concentrations. Its purpose was to estimate the level of pollutants based on input (independent) variables - vehicle speed, engine speed and engine load. The highest R^2 coefficient of determination was obtained for both fuels tested, using the Random Forrest model. This is a versatile algorithm, used in datasets, for classification and regression purposes, due to its ability to model complex, non-linear relationships between variables. Table 3 shows the results of fitting the obtained predictive models using metrics for assessing the quality of regression models - mean absolute error (MAE), root mean squared error (RMSE). Figure 18 shows the actual and predicted values plot for both cases considered. Meanwhile, Fig. 19 and Fig. 20 correlate the above results with vehicle speed for DF and ORhex, respectively.

Table 3. Metrics for evaluating the quality of regression models

| Parameter | DF | RONhex |
|------------|--------|--------|
| R^2 | 0.9537 | 0.9466 |
| MAE (ppm) | 56.16 | 57.38 |
| RMSE (ppm) | 78.91 | 80.52 |

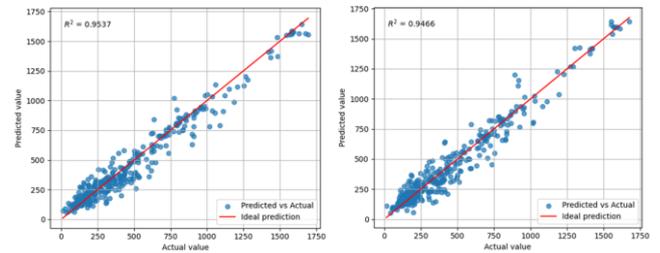


Fig. 18. Actual and predicted values plot (DF – left, RONhex – right)

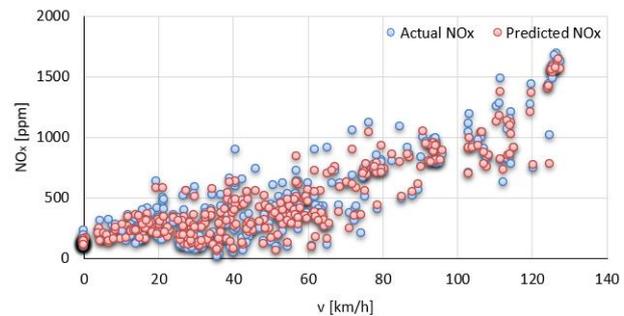


Fig. 19. Comparison of predicted values and actual NO_x concentrations for DF

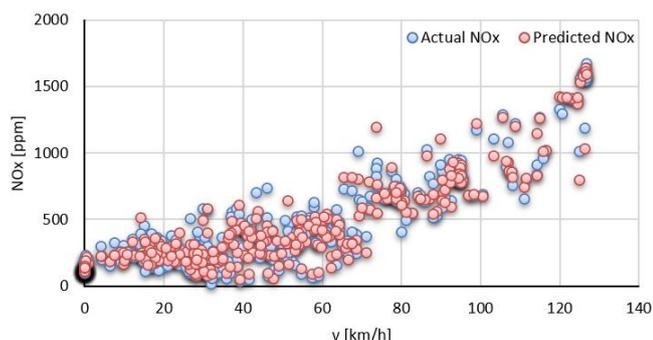


Fig. 20. Comparison of predicted and actual values of NO_x concentration for RONhex

A comparison of the model used for both fuels showed a lower coefficient of determination R^2 , and higher prediction errors for RONhex. This indicates that the model generates more stable predictions with smaller deviations from actual values for DF.

4. Conclusions

The study was able to measure the concentrations of exhaust emissions for diesel fuel and a mixture of rapeseed oil with 20% n-hexane additive, based on the WLTC driving cycle.

When measuring CO and NO_2 , the concentration of these components is higher for RONhex. Lower loads result in lower temperatures and incomplete combustion, which, combined with the lower volatility of rapeseed oil, results

in poorer fuel evaporation, and the higher viscosity compared to diesel fuel has a negative effect on the atomization process. This results in a less efficient combustion process and higher CO concentrations. As the load and combustion temperature increase, this effect is compensated by the oxygen content in RONhex, unlike DF, where at higher loads the fuel mixture becomes richer. The lower oxygen content causes an increase in CO concentration. In the case of NO_2 concentration, the oxygen content in rapeseed oil promotes the oxidation of NO to NO_2 , resulting in a higher concentration than in DF.

Similarly, in the case of hydrocarbon exhaust concentrations, RONhex had the highest concentrations in phase I of the cycle, in contrast to DF, whose maximum concentration in the last phase of the cycle was significantly higher than the average value (almost 17 times for THC and 16 for NMHC) and the values obtained for RONhex. CO_2 and NO concentrations increased with vehicle load and were higher for DF.

The study developed a predictive model to predict NO_x concentration values based on vehicle speed, engine speed and engine load. The model used had a high predictive capability.

A further stage of research envisages the analysis of individual cycle phases, especially in the context of studying the stability of the combustion process in phases characterized by low loads for RONhex. The research is also planned to continue by applying more complex predictive models.

Nomenclature

| | | | |
|---------------|--------------------------|--------|--|
| AV | average | OBDII | on-board diagnostic II |
| CI | compression ignition | RMSE | root mean squared error |
| CO | carbon oxides | RONhex | rapeseed oil with 20% n-hexane |
| CO_2 | carbon dioxides | SD | standard deviation |
| CV | coefficient of variation | THC | total hydrocarbons |
| DF | diesel fuel | v | vehicle speed |
| ECU | engine control unit | WLTC | Worldwide Harmonized Light Vehicles Test Cycle |
| MAE | mean absolute error | WLTP | Worldwide Harmonized Light Vehicles Test Procedure |
| NMHC | non-methane hydrocarbons | | |
| NO_x | nitrogen oxides | | |

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