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Toxicity of Exhaust Fumes (CO, NO_x) of the Compression-Ignition (Diesel) Engine with the Use of Simulation

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Abstract: Nowadays more and more emphasis is placed on the protection of the natural environment. Scientists notice that global warming is associated with an increase of carbon dioxide emissions, which results inter alia from the combustion of gasoline, oil, and coal. To reduce the problem of pollution from transport, the EU is introducing increasingly stringent emission standards which should correspond to sustainable conditions of the environment during the operation of motor vehicles. The emissivity value of substances, such as nitrogen oxides (NO_x), hydrocarbons (HC), carbon monoxide (CO), as well as solid particles, was determined. The aim of this paper was to examine, by means of simulation in the Scilab program, the exhaust emissions generated by the 1.3 MultiJet Fiat Panda diesel engine, and in particular, carbon monoxide and nitrogen oxides (verified on the basis of laboratory tests). The Fiat Panda passenger car was selected for the test. The fuels supplied to the tested engine were diesel and FAME (fatty acid methyl esters). The Scilab program, which simulated the diesel engine operation, was the tool for analyzing the exhaust toxicity test. The combustion of biodiesel does not necessarily mean a smaller amount of exhaust emissions, as could be concluded on the basis of information contained in the subject literature. The obtained results were compared with the currently valid EURO-6 standard, for which the limit value for CO is 0.5 g/km, and for NO_x − 0.08 g/km, and it can be seen that the emission of carbon monoxide did not exceed the standards in any case examined. Unfortunately, when analyzing the total emissions of nitrogen oxides, the situation was completely the opposite and the emissions were exceeded by 20–30%.

Keywords: exhaust emission; emission standards; simulations; WLTP; NEDC; sustainability

1. Introduction

Currently, the impact of human activity on the natural environment is increasingly subjected to analysis [1,2]. The preservation of clean air is essential for the comfort of life and human health [3,4]. The contaminants around us have a major impact on the environment, causing, among other things, the greenhouse effect, the ozone hole, but also many of civilization's diseases, such as cancer, asthma, and allergies [5,6]. In the face of the huge popularity of passenger cars and the wide use of trucks and other means of transport, attempts to minimize this phenomenon are becoming a huge problem [7,8].

The goals of transportation policy are more and more important for the policy of sustainable development [9,10]. The combination of a dynamic economy and social integrity should focus on the consistency of human actions with the requirements of the ecosystem [11,12]. This type of strategy defines sustainability as meeting the needs of not only current, but also future generations [13]. Sustainable economic growth forces the need to analyze the relationship between transport, investments, and the determination of the degree of air pollution [14,15]. Transport is an important factor facilitating social, economic, and environmental development, but emissions of the resulting pollutants appears to be a side effect [16,17].

Protection of air purity and activities related to the reduction of greenhouse gas emissions from transport are a priority of the climate and energy policy of the European Union bodies [18,19]. Regardless of improvements in vehicles and in the automotive industry, transport still has a negative impact on air quality [20,21]. Emissions of substances, such as carbon dioxide, carbon monoxide, nitrogen oxides, aromatic hydrocarbons, as well as harmful substances in the form of solid particles originated from the transport sector, are now significantly higher than in 1990 [22–24]. Therefore, from time to time, stricter limits for exhaust emissions from motor vehicles are introduced as a result of concern and care for the natural environment [25,26].

To reduce the intensity of the problem, the European Parliament has been updating EURO standards [27,28] for many years to reduce the toxicity emitted by vehicles, such as cars, trucks, and buses, excluding aircraft and ships. These standards are subject to change and the limit values being introduced are reduced, as shown in Table 1, in order to mobilize car concerns to look for new, better technological solutions that will constitute a lower burden for the natural environment [29,30].

Table 1. Acceptable values of individual exhaust components in Euro standards (compression ignition, car category: M).

Standard	CO [g/km]	PM [g/km]	NO_x + THC [g/km]
EURO-1	3.16	0.14	0.70
EURO-2	1.00	0.08	0.56
EURO-3	0.64	0.05	0.30
EURO-4	0.50	0.009	0.23
EURO-5	0.50	0.005	0.70
EURO-6	0.50	0.0045	0.56

Different standards have been applied for each vehicle. These standards determine the value of emissivity of substances such as nitrogen oxides (NO_x), total hydrocarbon (THC), hydrocarbons (HC), carbon monoxide (CO), as well as matter particles (PM) [25,31]. Currently, the tightening of regulations concerning the reduction of emission of toxic compounds in engine exhaust, and a decrease of fuel consumption and greenhouse gas emissions are the main factors controlling the direction of automotive construction development [25,32,33].

In recent years, standards for the diesel engine have been severely tightened [34,35]. The basic method for reducing toxins is the use of the common rail fuel injection [36,37]. Six EURO standards have been created so far, as shown in Table 1, at intervals of several years, in order that car manufacturers can keep pace with the development of new technologies and adapt their models to legal requirements regarding toxin emissivity [38].

In order to analyze, monitor, and reduce pollutant emissions from transport, the New European Driving Cycle (NEDC) test was introduced [39,40], followed by the WLTP (Worldwide Harmonized Light Vehicle Test Procedure) [41,42].

In 2017, the regulation of Global Technical Regulation No. 15 came into force, which is a more appropriate way for development and planned implementations in the field of emission testing, concerning, among others, gaseous and particulate pollutants. The main legislative objective of this act is related to the reduction of the permissible values of CO_2 emissions and reduction of fuel consumption of vehicles [43,44].

Determination the actual emission of pollutants from vehicles was introduced as a result of efforts to reduce the discrepancy between the results of laboratory tests and the results of road tests [45,46]. Emission measurement devices in real conditions are already widely available. This is a legal requirement that is valid throughout the EU. This is related to the need for further research on the precise determination of the relationship between real emissions from vehicles in road conditions and emissions determined in laboratory conditions [44,47,48].

The actual fuel consumption, and thus its emission of pollutants into the atmosphere while driven on the road, depends to a large extent on individual driving behavior [49,50], route characteristics [51], traffic flow [52], vehicle load, and external circumstances [53,54], such as temperature, air resistance, and acceleration [55,56]. Analyses of the results of measurements and tests presented in the literature allow the assessment of the impact of the transported cargo on the road emission parameters [57,58]. The increase in the load applied to the power unit during operation results in an increase of CO_2, NO_x, and PM emissions [59], while the reduction of the vehicle speed causes reduction of emissions [60].

In connection with the above, the construction and use of computer simulation models for determining and comparing the values of emitted exhaust components in the context of two NEDC and WLTP driving tests is significant [61].

Computer simulations find more and more supporters among representatives of science. This is confirmed by the growing number of publications, in which simulations serve as a method for verifying research hypotheses. "Computer simulation" is a method based on performing experiments on models that describe existing or designed systems in order to get knowledge about the time dependence behavior of the investigated system. A computer program, that is a formal representation of the model of the tested system, is a tool that uses computer simulation to achieve a research goal [62,63].

As the European Union's inspection bodies have shown, road transport still remains unrivaled in the transport of goods [22]. Nevertheless, more and more European countries such as the Netherlands, Norway, and Germany intend to withdraw vehicles with combustion engines from sale and prohibit their use in cities in the coming years. Despite the implementation of new laws and publicizing the situation, the problem remains unsolved, and people choose their own convenience, ignoring the social and environmental consequences.

The aim of the paper is to examine, by means of simulation in the Scilab program, the exhaust emissions generated by the 1.3 MultiJet Fiat Panda diesel engine, in particular carbon monoxide and nitrogen oxides. The simulation took place in the vehicle's working conditions as well as during the driving test generated by NEDC and WLTP, using fuels and biofuels. The engine was chosen for the analysis due to the fact that it is one of the most popular engines with low capacity. Depending on the car brand, these engines have different markings, although in a large part their construction is unified (Fiat, Opel, Lancia).

The conducted research was part of the preparations for the participation of the facility in the research project "Preventive measures to reduce the adverse health impact of traffic-related air pollution (PrevenTAP)" [64]. The knowledge thus gained was a key element in the said project due to conducting experiments with research animals, such as rats, carried out under very stringent conditions in terms of animal welfare and under the control of veterinary services. Before conducting the actual experiment, it was necessary to demonstrate that the methodology being prepared is safe towards animals, also with the use of further simulations involving the diesel engine module and other elements of the test station. The data obtained from the simulation were used to develop a real control system for the control of the research station which would enable the introduction of regulated exhaust stream drawn from the exhaust system during the operation of the engine in front of and past the solid particle filter, into the air streams supplied to the test chambers. In this case, the size of the exhaust stream ducts—electronically controlled valves for the regulation of the exhaust streams—and the capacity of the fans for the chambers, etc. were selected. The results of these experiments are being analyzed for the preparation of subsequent publications. The detailed instructions for the applied engine were also used in the works under the project "Green fuels and human health toxicity of engine emission from 1st and 2nd generation biodiesel fuels" and were allowed to maintain very stable atmospheric parameters in test chambers [65–70].

2. Materials and Methods

The Fiat Panda passenger car was selected for the test (Table 2). In the 2012 version, it has a 4-cylinder in-line engine with a displacement of 1251 cm^3. The maximum power is 66 hp and the maximum torque of the drive system is 200 Nm. The fuel tank holds 35 L. According to the manufacturer, the fuel consumption in the urban cycle is 5.2 L/100 km and in the extra-urban cycle 3.6 L/100 km. The vehicle's drive is transmitted to the front. The engine is connected to the manual gearbox, which allows acceleration from 0 to 100 km/h in about 13 s. The maximum speed of the Fiat Panda is 165 km/h.

Table 2. Basic technical data of the Fiat 1.3 MultiJet engine used in the simulation [71].

Parameter	Unit	Value
Cylinder layout	-	in-line
Number of cylinders, c	-	4
Type of injection	-	direct, multistage
Cylinder work order	-	1—3—4—2
Compression ratio, e	-	17.6
Diameter of the cylinder, D	mm	69.6
Piston stroke, S	mm	82
Engine displacement, Vss	cm^3	1251
Maximum engine power, Ne	kW	66
Engine rotational speed for its maximum power, nN	rpm	4000
Maximum engine torque, Me	Nm	200
Engine rotational speed for its maximum torque, nM	rpm	1750
Rotational speed of idle gear, nbj	rpm	850 ± 20

The fuels applied in the examined engine include [72] diesel and fatty acid methyl esters (FAME), as shown in Table 3.

Table 3. Basic properties of the fuels applied. FAME: fatty acid methyl esters.

Parameter	Diesel	FAME
Carbon content [%]	86.5	78.0
Hydrogen content [%]	13.4	12.0
Oxygen content [%]	0.0	10.0
Calorific value [MJ/kg]	44.0	37.0
Air demand [g/g]	14.5	12.5

The Scilab program, which simulated the diesel engine operation, was the tool for analyzing the exhaust toxicity test. It is a free scientific package, which was created mainly for conducting mathematical research. The program allows work in many areas, such as signal processing, statistics, linear algebra, and matrices, and can create diagrams, graphs, and 2D and 3D animations, and, most importantly, has the Xcos editor, which is used to build models and mechanical systems [73]. The general simulation scheme (developed in a few modules) of vehicle operation for the WLTP test, NEDC, and simulation of the consumption of two fuels—diesel fuel and FAME—is shown in Figure 1.

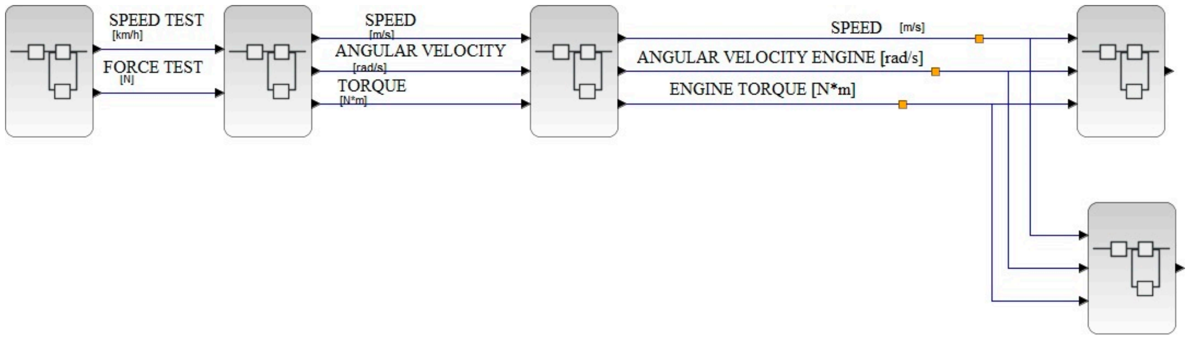

Figure 1. General scheme of the developed simulation of the vehicle operation under the Worldwide Harmonized Light Vehicle Test Procedure (WLTP) or New European Driving Cycle (NEDC) tests.

Due to the functionality of the software enabling creation of hierarchical structures of created projects, the developed simulation was built of the following modules performing specific tasks:

- "WLTP NEDC"—The module generates simulation control signals in accordance with the momentary values described in the documents of WLTP driving tests (RCG – Random Cycle Generator) and NEDC [74].
- "Gearbox"—The module simulates the behavior of the actual transmission system, including vehicle wheels (wheel dynamic diameter during movement), main transmission (gear ratio), and gearbox (gear shifting).
- "Limits for engine"—The module is responsible for monitoring the instantaneous values of rotational speeds and torque calculated during the simulation. In the event of the exceeding of admissible ranges, the module for further simulation steps transfers of the extreme values adopted for the correctness of calculations.
- "Calculations for diesel"—The module is based on the characteristics of hourly fuel consumption and the hourly air demand as a function of rotational speed and torque introduced for simulation of the selected engine.
- "Calculations for FAME"—This module performs calculations in the same way as for diesel but takes into account the characteristics of emissions of carbon monoxide and nitrogen oxides for the operation of a FAME driven engine [71,75].

The scheme of the emissivity calculation block of the selected engine, determined in accordance with the WLTP and NEDC driving tests for selected pollutants, is shown in Figure 2.

The New European Driving Cycle (NEDC) test was introduced in the 1990s. It involves the study of exhaust emissions and fuel consumption while driving a car in laboratory conditions, as close as possible to natural conditions. The vehicle is placed on special chassis dynamometers that imitate the real road. It is subjected to conditions such as acceleration and deceleration, as well as driving at a certain speed. The driving simulation during the NEDC test is divided into two parts. The first one includes urban driving [76,77], lasts 13 min, and the distance travelled is 4 km. The car slowly accelerates to 50 km/h and then the vehicle stops at the given time. These activities are repeated 4 times. The second part reflects off-road driving, takes 6 min and 40 s, and the car travels a distance of 7 km. It is based on accelerating the car to 70, 100, and 120 km/h. In this cycle, the vehicle does not stop, but only decreases the speed. The results show the average fuel consumption as well as the average emission of harmful substances and CO_2.

In order to perform even more effective emission measurements and to actualize the emissivity results, the WLTP (Worldwide Harmonized Light Vehicle Test Procedure) was developed. During the tests, more factors were taken into account, such as the average temperature at which the car works (13 °C), and the impact of equipment and configuration of engine versions and transmissions [78]. The research of a given model in the WLTP cycle will be based on tests in many variants, and the result will be the interval between the lowest and the highest emission versions [79,80].

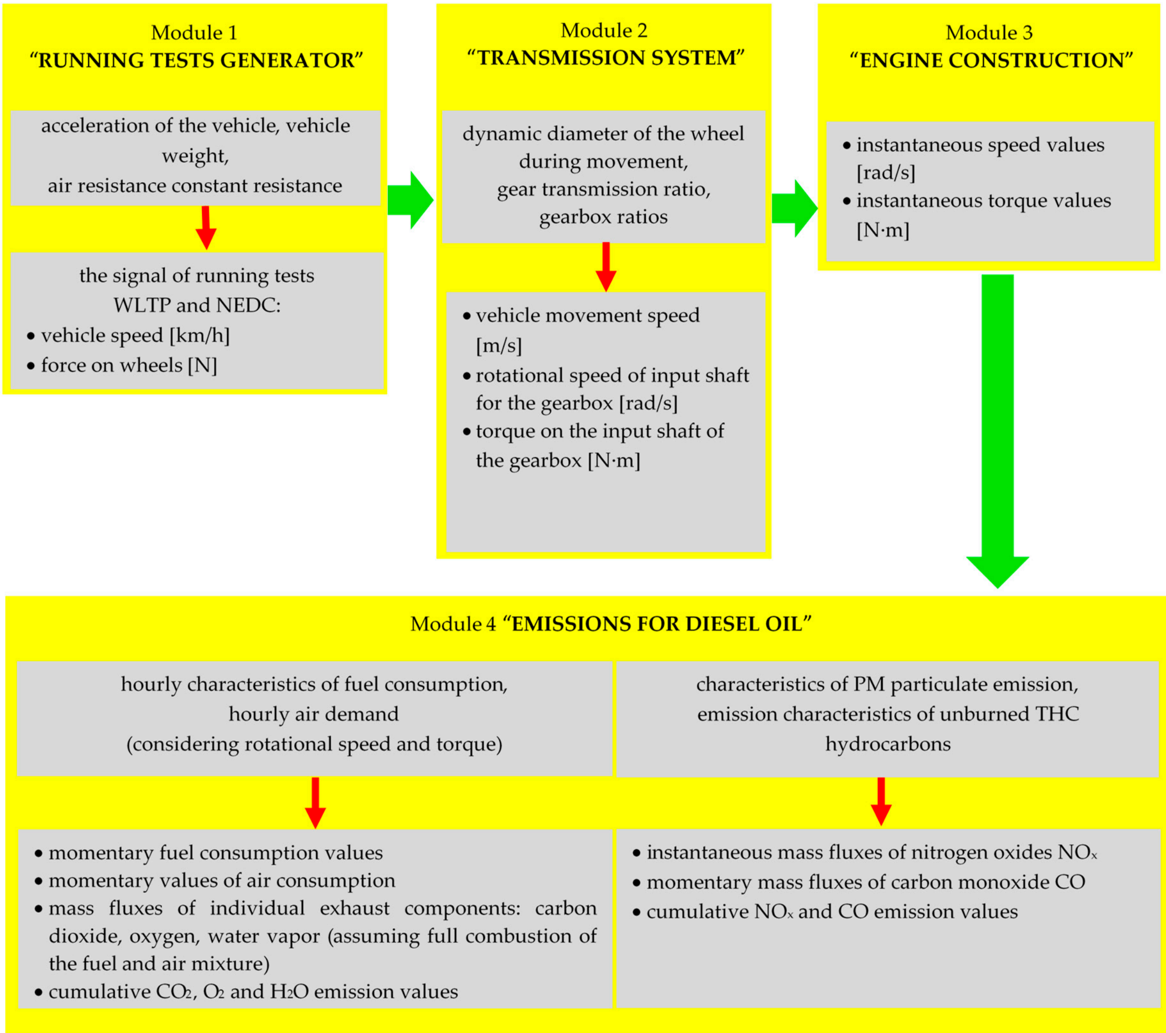

Figure 2. Diagram of simulation model on the basis of which the mass exhaust values were calculated.

The WLTP cycle differs from the NEDC test in both the duration and the driving scenario. The duration of the test is 30 min. In addition, the vehicle travels about 23 km, and for 13% of the duration of the WLTP test the vehicle remains stationary. The test consists of four parts: (1) This part lasts 589 s, and the vehicle covers a 3 km distance, accelerating to 56.5 km/h and reaching an average speed of 18.9 km/h. The vehicle is stationary for 26.5% of the test time. (2) This stage lasts 433 s and its purpose is to determine the average speed. The vehicle covers 4.7 km, accelerating to 76.6 km/h, and reaching the average speed of 39.4 km/h. In this part, the vehicle is stationary for 11.1% of the time. (3) This part lasts 455 s, the vehicle covers 7.2 km, accelerating to 97.4 km/h, and maintains the average speed of 56.5 km/h. The vehicle is stationary for 6.8% of the time. (4) The last part is a test at very high speeds. The test lasts 323 s, the vehicle covers 8.3 km, reaching a top speed of 131.3 km/h and maintaining the average speed of 94 km/h. The vehicle is stationary for 2.2% of the duration of the test [81–83].

3. Results and Discussion

The emissivity simulation of the selected diesel engine for the vehicle movement in the WLTP and NEDC driving tests allowed for the simulation experiment to be carried out using various conditions of the start/stop system as well as supplying the motor with diesel and FAME. Presented below are the results of the simulation work in the form of time-weighted traces and the comparison of fuel consumption parameters, air consumption, and carbon dioxide and nitrogen oxide emissions, taking into account the variability of the input parameters of the simulation.

Figure 3 presents the results of emissivity simulation of the selected diesel engine for the WLTP test with the start/stop system disabled and powered with (A) diesel and (B) FAME in the form of momentary courses: mass emission stream of carbon monoxide (CO [g/s]), mass emission stream of nitrogen oxides (NO_x [g/s]), total emission of carbon monoxide (CO [g]), total emission of nitrogen oxides (NO_x [g]).

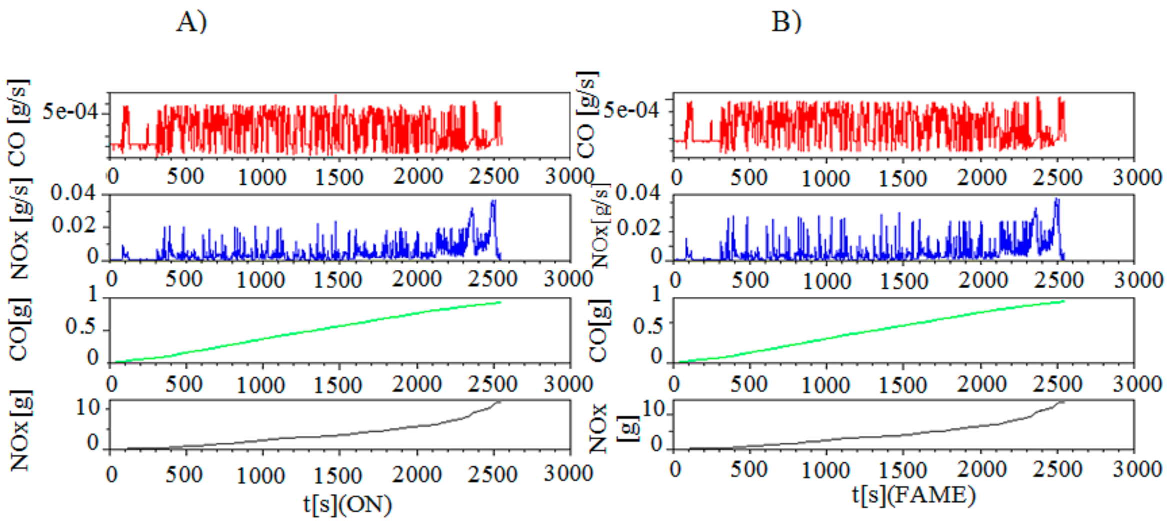

Figure 3. Results of the work of the simulation block "Calculations for diesel" responsible for the motor simulation—WLTP test; start/stop system disabled (see references in the text): (**A**) diesel fuel (ON); (**B**) fatty acid methyl esters (FAME).

The momentary courses of the mass emission stream of CO and nitrogen oxides are very similar in the case of the examined fuels, however, when analyzing total emissions, differences can be seen. In the case of carbon monoxide during the combustion of diesel, the final emission reaches the value of 1 g/s, while in the case of esters it is about 0.7 g/s. As for the total emission of nitrogen oxides, the situation is reversed—higher values (12 g/s) appear when combusting FAME.

3.1. Simulation Results for the WLTP (RCG) Test—Start/Stop System Enabled

Figure 4 shows the simulation results for the WLTP (RCG) test with the start/stop system enabled and powered by (A) diesel fuel and (B) FAME, in the form of momentary waveforms. In this case, the values for total emissions are close to the value of the test with the start/stop system disabled, and the difference is apparent when testing the mass emission stream of carbon. At the beginning of the measurement, the course of the emission curves differs—the curves are doubled to the maximum value and then suddenly drop to the zero value. After 300 s, the measurement is carried out continuously, without any disturbances. This change is caused by the structure of the test—during the first stage the vehicle is stationary for more than one-quarter of the time.

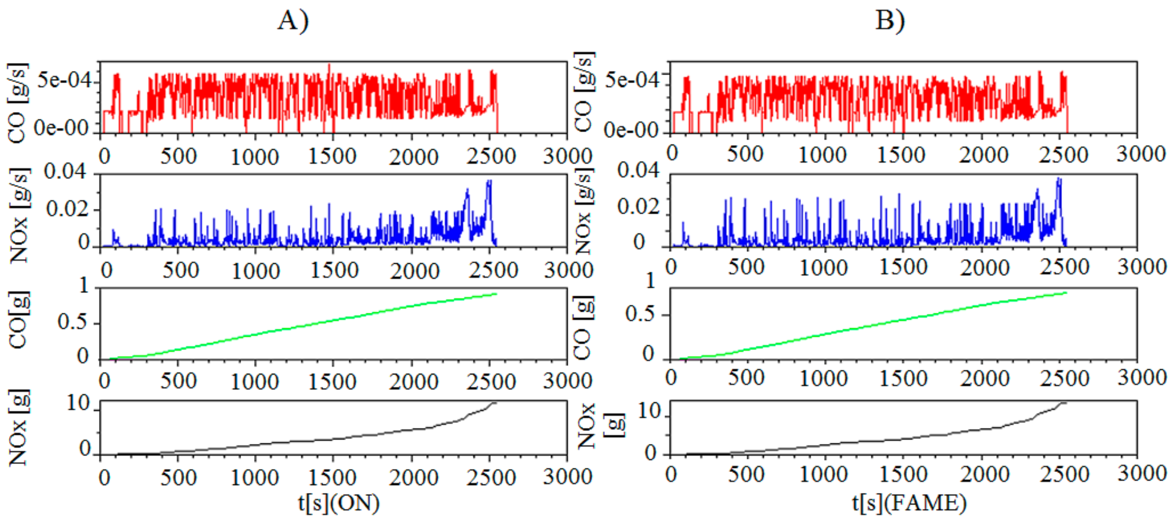

Figure 4. Results of the work of the simulation block "Calculations for diesel" responsible for the motor simulation—WLTP test; start/stop system enabled (see references in the text): (**A**) diesel fuel (ON); (**B**) fatty acid methyl esters (FAME).

3.2. Simulation Results for the NEDC Test—Start/Stop System Disabled

Below, Figure 5 shows the results for the simulation performed with the NEDC test, with the start/stop system disabled. The dependences examined by this test show the same relationships as in the WLTP test, i.e., the total carbon monoxide emission is significantly higher in the case of diesel fuel combustion, and the carbon monoxide emissions are greater from the combustion of fatty acid esters.

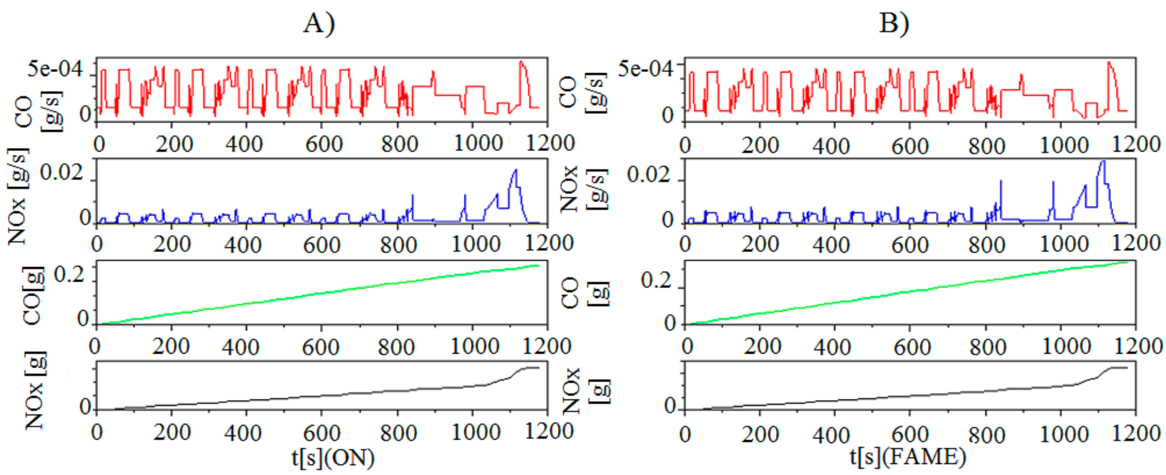

Figure 5. Results of the work of the simulation block "Calculations for diesel" responsible for the motor simulation—NEDC test; start/stop system disabled (see references in the text): (**A**) diesel fuel (ON); (**B**) fatty acid methyl esters (FAME).

3.3. Simulation Results for the NEDC Test—Start/Stop System Enabled

In the last case, as shown in Figure 6, of the NEDC simulation, with the start/stop system enabled, it can be seen that when analyzing the mass stream of carbon monoxide, it is shown exactly at which moment the vehicle stops and starts, so that the unit emissions during the start-up rapidly increase and then they decrease. The total CO emission in this case is twice as high in the case of diesel fuel combustion, and the total emission of nitrogen oxides reaches higher values in the case of FAME combustion.

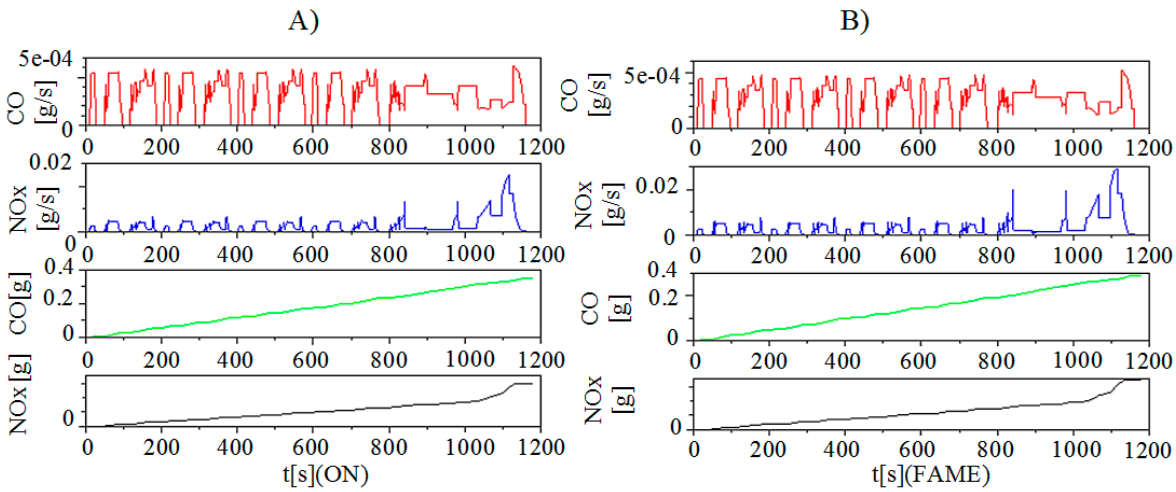

Figure 6. Results of the work of the simulation block "Calculations for diesel" responsible for the motor simulation—NEDC test; start/stop system enabled (see references in the text): (**A**) diesel fuel (ON); (**B**) fatty acid methyl esters (FAME).

3.4. Comparison of Results

The simulation of driving tests compliant with the WLTP and NEDC parameters for the selected vehicle enabled the introduction of modifications of the working conditions, including switching off and on the start/stop system, applying various fuels—diesel fuel and FAME—and selecting the driving test. Table 4 presents a collection of results of fuel demand and air demand as well as emission of carbon monoxide and nitrogen oxides for conducted simulations, including WLTP or NEDC driving tests, with the start/stop system enabled or disabled and diesel fuel or FAME supply.

Table 4. Summary of results of simulations.

Distance in the Test [km]	**11.03**				**34.68**			
Driving test applied	NEDC	NEDC	NEDC	NEDC	WLTP	WLTP	WLTP	WLTP
Start/stop system	OFF	OFF	ON	ON	OFF	OFF	ON	ON
Fuel applied	ON	FAME	ON	FAME	ON	FAME	ON	FAME
Fuel consumed [kg]	0.406	0.482	0.359	0.427	1.24	1.47	1.22	1.45
Air consumed [kg]	13.0	13.0	12.1	12.1	36.8	36.8	36.5	36.5
Carbon monoxide emission CO [g]	0.413	0.340	0.351	0.290	0.941	0.764	0.921	0.748
Nitrogen oxide emission NO_x [g]	0.92	1.07	0.91	1.05	3.52	3.82	3.52	4.12

The chart of the results of the study shows a slight difference between the combustion of diesel and FAME. The results of test emissions in a unit of mass per kilometer are very similar, however it should be remembered that during the WLTP test, the vehicle travels a much longer distance, in a longer run, almost without stops, which contributes to its greater accuracy and higher total values [84–86].

The results of the research are surprising as it turns out that burning biodiesel does not necessarily mean a smaller amount of exhaust emissions, as could be concluded, as shown in Table 3, on the basis of information contained in the subject literature. During the combustion of FAME, the amount of carbon monoxide emissions was lower than during the combustion of diesel and was within the limits of the EURO standards. Unfortunately, this situation does not apply to nitrogen oxides, the emission of which during the combustion of biodiesel was higher. Significant differences between emissivity tests can be seen in the fuel and air consumption, where it is about three times higher for the WLTP test for a longer distance traveled in the examination [87].

The results show that the impact of using the start/stop system on CO and NO_x emissions is higher in the NEDC test, mainly due to a longer idling period compared to the WLTP test [88].

What is important, when comparing the obtained results with the currently applicable EURO-6 standard, for which the limit value for CO is 0.5 g/km, and for NO_x—0.08 g/km [76] (n26), it can be noticed that the emission of carbon monoxide does not exceed the standards in any case, as shown in Table 5. Unfortunately, when analyzing the total emissions of nitrogen oxides, the situation is completely the opposite and the emissions are exceeded by 26–49%.

Table 5. Emissions of carbon monoxide and nitrogen oxides in comparison to EURO-5 and EURO-6.

Distance in the Test [km]	11.03				34.68			
Driving test applied	NEDC	NEDC	NEDC	NEDC	WLTP	WLTP	WLTP	WLTP
Carbon monoxide emission CO [g/km]	0.04	0.03	0.03	0.03	0.03	0.02	0.03	0.02
EURO-6 CO [g/km]	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5
Nitrogen oxide emission NO_x [g/km]	0.0810	0.097	0.083	0.095	0.101	0.110	0.101	0.119
EURO-5 NOx [g/km]	0.180	0.180	0.180	0.180	0.180	0.180	0.180	0.180
EURO-5 NOx Standard exceeded by [%]	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
EURO-6 NOx [g/km]	0.080	0.080	0.080	0.080	0.080	0.080	0.080	0.080
EURO-6 NOx Standard exceeded by [%]	1.25	21.25	3.75	18.75	26.25	37.50	26.25	48.74

4. Conclusions

Due to increasingly restrictive emission standards for toxic exhaust components, there is a growing need for research into the construction and regulation of engines, as well as for measuring equipment. These tests are important from the point of view of science and industry. These analyses affect the development of legal regulations and the development of motorization.

On the basis of the conducted research it can be concluded that:

1. The WLTP test is more accurate than the NEDC test because it refers to 'normal' driving conditions. The results of pollution measurements carried out with this test are more actual, refer to EURO-6 standards, and may affect the improvement of air quality.
2. Differences in the measurements between tests are:
    - In the case of total CO emissions tests, according to the WLTP test, for the cases of EURO-5 and EURO-6, the emission limits had not been exceeded in any of the tests.
    - In the case of total NO_x emission tests, according to the WLTP test, the emissions are increased by 26–49% (for NEDC from 1.25–18.75%, the tested 1.3 MultiJet Fiat Panda diesel engine was subject to approval according to the NEDC test—accordingly to the production year).
    - Simulations were carried out on the basis of literature information that contained the results of experimental measurements for a vehicle of unknown technical condition and mileage. The accuracy of the obtained simulation results is influenced by the accuracy of the data reported in the literature source.
3. Results of the conducted research provide useful indicators for more economically efficient technologies for the use of fuels and biofuels.
4. Despite the introduction of increasingly restrictive legal norms, outdated tests and procedures are still used for measurements, mainly for economic reasons.
5. The developed computer simulation is the universal tool that can be used to estimate the emissions of toxic compounds for each type of engine (the operational characteristics of the engine is required).
6. Computer simulations extended to many representative vehicles could be the basis for reliable estimation of the actual fluxes of harmful substances during traffic, while most often simulations of traffic emissions are based upon accepted average values.

This type of research provides knowledge about the scale of greenhouse gas and other air pollutant emissions generated by transport and can be an indication for actions aimed to reduce emissions to assure sustainable development. Sustainable transport development should take into account ecological, social, and economic objectives; therefore, such analyses will allow the understanding of the essence of the problem in the light of environmentally friendly transport policy.

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