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The Development of CO_2 Instantaneous Emission Model of Full Hybrid Vehicle with the Use of Machine Learning Techniques

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Abstract: Road transport contributes to almost a quarter of carbon dioxide emissions in the EU. To analyze the exhaust emissions generated by vehicle flows, it is necessary to use specialized emission models, because it is infeasible to equip all vehicles on the road in the tested road sections with the Portable Emission Measurement System (PEMS). However, the currently used emission models may be inadequate to the investigated vehicle structure or may not be accurate due to the used macroscale. This state of affairs is especially related to full hybrid vehicles, since there are none of the microscale emission models that give estimated emissions values exclusively for this kind of drive system. Several automakers over the past decade have invested in hybrid vehicles with great opportunities to reduce costs through better design, learning, and economies of scale. In this work, the authors propose a methodology for creating a CO_2 emission model, which takes relatively little computational time, and the models created give viable results for full hybrid vehicles. The creation of an emission model is based on the review of the accuracy results of methods, such as linear, robust regression, fine, medium, coarse tree, linear, cubic support vector machine (SVM), bagged trees, Gaussian process regression (GPR), and neural network (NNET). Particularly in the work, the best fit for the road input data for the CO_2 emission model creation was the GPR method. PEMS data was used, as well as model training data and model validation. The model resulting from this methodology can be used for the analysis of emissions from simulation tests, or they can be used for input parameters for speed, acceleration, and road gradient.

Keywords: CO_2 emission; emission modelling; vehicle emission; full hybrid; electric vehicles; passenger cars; machine learning

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1. Introduction

Proper mobility planning in accordance with decarbonization policies must consider a general increase in mobility demand projected toward the use of hybrid and electric vehicles and the increased use of public transport and shared mobility instead of conventional private conventional vehicles [1,2]. Several studies in the literature focus on the analysis of best practices starting from the modification of infrastructures and traffic volumes, while others focus on the assessment of transport demand with particular reference to travel habits that have recently been modified by the advent of the COVID19 pandemic [3,4].

As climate change is showing its impact across Europe, the European automotive market is turning to all-electric vehicles. The growing footprint of electric cars is helping to reduce the level of carbon dioxide emissions into the atmosphere [5]; however, there has also been a strong growth in the registration of full hybrid vehicles.

From January to July 2021, the European light vehicle market grew 19.0% from its low point in 2020. At the same time, full hybrid registrations (excluding PHEVs and mild

hybrids) increased by 65.6%. At the national level, Italy, France, and Poland all doubled their hybrid registrations [6].

Due to the fact that the permissible emission limits of pollutants with regard to air quality standards are increasingly exceeded, there is a need to develop new models to assess emissions from road transport to adequately estimate the impact of vehicle traffic on the overall emission of harmful exhaust components. To adequately reflect real conditions, the effects of emissions on a local scale should be taken into account, using modern technologies to measure exhaust emissions. To estimate the impact of, for example, intelligent traffic control systems, dynamic speed limits or various types of intersections on the emission of pollutants, specific driving systems, the calculations should be sufficiently sensitive to the characteristics of vehicle traffic under real operating conditions [7,8].

Vehicle exhaust emission models should reflect the local vehicle structure, driving characteristics, and atmospheric conditions to provide reliable results [9]. Measurement methodology is also a key issue in the conduct of emission tests. So far, tests have been performed using methods such as laboratory tests, tunnel tests, remote sensing, or mobile measurement on board a vehicle [10–14]. However, for the development of microscopic models, many road tests are needed, e.g., with the use of PEMS systems. The use of this system has increased significantly in recent years [15,16]. Studies also show that the PEMS system is a reliable source for obtaining data on actual vehicle emissions compared to laboratory tests [17]. The results of road tests on exhaust emissions differ significantly from those obtained during transient dynamometer tests in controlled conditions [18]. Furthermore, vehicle exhaust emission tests showed that current emission values have changed significantly in the last few years with the introduction of new engine solutions and exhaust gas treatment systems, influencing the variability and increased sensitivity of the results [19]. In order to assess the impact of changes in road traffic, e.g., driver behavior on speed limits, traffic lights, the occurrence of intersections, it is necessary to develop special models that will give a reliable prediction of emissions.

Due to the fact that full hybrid vehicles and their emission specifications are different compared to conventional combustion engine vehicles [20] in this work, the authors propose a methodology for the creation of a new emission model for this type of vehicle. Full hybrid vehicle within a specific range of engine operation when, in fact, the combustion engine is not working, but the electric engine powers the vehicle and emits zero emissions. For vehicle operation, especially when the vehicle speed is high, there can be a state in which electric and combustion engines work at the same time, or the combustion engines work separately. In general, the level of emission of harmful exhaust components for NOx, PM, THC, and CO is relatively low compared to the previous generation internal combustion engines due to the configuration and catalytic system of the latest engine system. However, due to the consumption of hydrocarbon fuel, there are still CO_2 emissions that affect global warming. Based on the literature review, there is no work that focuses on modeling CO_2 emissions for full hybrid vehicles on a microscale. Furthermore, actual existing emission models for micro-scale, especially when emission map is taken under consideration, wrongly indicate emission hotspots, since for some range of vehicle speed, which occurs especially in the urban cycle of vehicle operation, there is actually no emission when the electric engine is working. Given the above, this work concerns the presentation of the methodology for the CO_2 development emission model for a full hybrid vehicle. The creation of an emission model is based on the review of the accuracy results of methods, such as linear, robust regression, fine, medium, coarse tree, linear, cubic support vector machine (SVM), bagged trees, Gaussian process regression (GPR), and neural network (NNET). Particularly in the work, the best fit for the road input data for the CO_2 emission model creation was the GPR method. The obtained emission model is a microscale model, so that means that it can be useful, e.g., in the case of a detailed analysis of emissions on a particular part of the road. The overall flow chart of the research is presented in Figure 1.

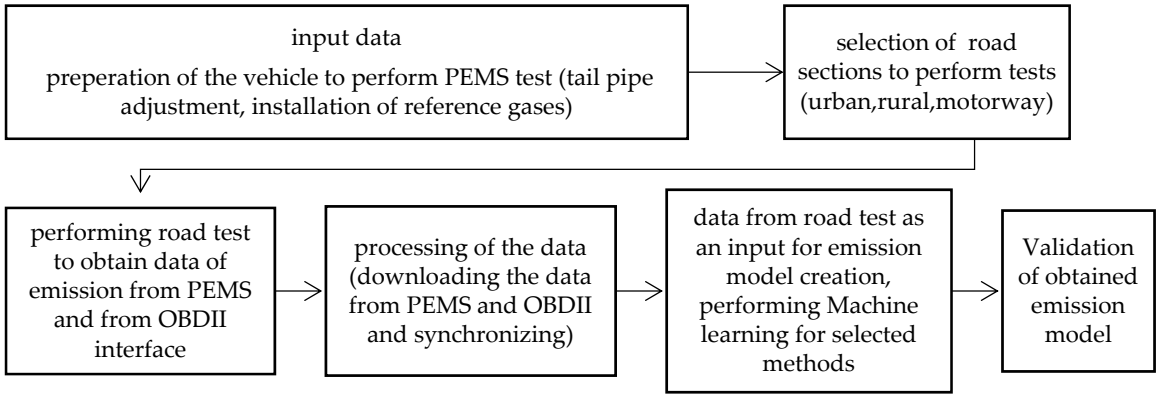

Figure 1. Flow chart of research.

2. Emission Models-Description

In general, it is possible to classify models for estimating road traffic and related emissions considering different scales of accuracy, namely: macroscopic (regional), mesoscopic (local), and microscopic (intersections, road sections).

Macroscopic models are based mainly on the average driving speed parameter on the analyzed road section [21]. They are based on the dependence presented in Equation (1):

$$F = A + \left(\frac{B}{V}\right) + C \cdot V + D \cdot V^2 \quad (1)$$

where:

A,B,C,D—coefficients selected depending on the type of vehicle and road,
V—average travel speed (km/h),
F—fuel consumption (l/100 km).

Macroscopic models are used to estimate fuel consumption and the environmental impact of road transport. They allow the determination of the impact of total energy consumption by projects and road infrastructure development strategies and the assessment of the impact of greenhouse gas emissions on the studied area. Some environmental impacts are local, regional, or global, and they can be either short-term or long-term [22]. Macroscale emission models allow for the determination of the large-scale transport impact of a region (regional, in the transport corridor).

The current macroscale emission model approach used to quantify harmful exhaust emissions is based on two calculation steps. The first stage consists of selecting a set of emission factors that determine the amount of emissions for given traffic conditions, while the second stage is the assessment of vehicle activity in the analyzed area. The emissions are calculated by multiplying these two steps.

Microscopic models for calculating emissions require a large amount of data based on the continuous measurement of basic vehicle parameters, such as speed, acceleration, terrain gradient, and position coordinates [23]. They calculate the instantaneous emission in a specific time unit, usually 1 (s). Many microscale models have been developed that calculate emissions based on the results of microsimulation models based on: measuring power, speed and a combination of these parameters.

An exemplary model for the micro scale proposed in [24] is based on the relationship between emission and driving speed. The results show that exhaust emissions and fuel consumption increase with increasing speed, even when vehicle traffic is delayed. Such a phenomenon cannot be described by models based on vehicle power [25]. Exampled micro scale emission model [26] is based on linear regression for velocity and acceleration and provides a relatively good fit to the raw data ($R^2 > 0.92$) for all measures of effectiveness (MOE). The regression results are sensitive to the test method used, i.e., the driving cycle

and the sample of vehicles selected to represent the composition of the vehicle fleet. This model is based on the Equation (2):

$$MOE = \sum_{i=0}^{3} \sum_{j=0}^{3} k_{i,j}^{e} \cdot V^{i} \cdot A^{j} \quad (2)$$

where:

MOE—instantaneous fuel consumption and emission of harmful exhaust compo nents,
$k_{i,j}^{e}$—regression model coefficients for *MOE*; for speed and for acceleration *j*,
V^{i}—speed (m/s),
A^{j}—acceleration (m/s^2).

Example emission models with division to micro- and macroscale for vehicles are presented in Table 1.

Table 1. Exampled emission models with division to macro and micro scale.

Scale	Emission Model	Description
macro	Computer Program to Calculate Emissions from Road Transport (COPERT)	EU standard vehicle emission calculator. It uses vehicle mileage, speed etc. [27]
	Handbook Emission Factors for Road Transport (HBEFA)	Application providing emission factor for different vehicle class [28]
	Motor Vehicle Emissions Simulator (MOVES)	Estimates emission for mobile sources at national, project and country scale [29]
	Emission Factors Model (EMFAC)	Computer model to estimate emission rate from motor vehicles for years 2000 to 2050 [30]
micro	Comprehensive Modal Emission Model (CMEM)	Power-demand model based on a parameterized analytical representation of emissions production [31]
	Passenger Car and Heavy-Duty Emission Model (PHEM)	Instantaneous vehicle emission model developed by the TU Graz covering different type of vehicles [32]
	Emissions from Traffic (EMIT)	Emissions calculations across large urban areas for dispersion modelling, allows to predict the impact of e.g., low emission zones [33]
	RoundaboutEM	Emission calculation from passenger cars for roundabout journeys [34]

Currently, there are only a few works that concentrate on machine learning methods for the creation of vehicle emission models. In the work [35], the authors analyze and group the data sets of emissions from diesel vehicles in a cluster and then develop neural network models. In the work [34] authors developed an emission model from a few vehicles powered by petrol, diesel, and LPG for the purpose of roundabout emission. When we consider hybrid vehicles, this work will be one of the very first to show methods to create an emission model of CO_2 using machine learning. Furthermore, the methodology and emission maps presented will be the first that are sensitive to the hybrid drive system.

3. Methodology

In the first stage of creating an exhaust emission model, it is necessary to collect an appropriate amount of data from the PEMS system. Before starting the vehicle road test, the tested vehicle was checked with the use of stationary exhaust gas analyzers, according to the periodic diagnostic test procedure. The results of the concentrations and amounts of harmful exhaust components of the vehicles tested were within acceptable limits. For the purpose of the work, a full hybrid vehicle has been chosen to see what the effect will be of creating machine learning emission models, especially on emission maps, since there are

some periods when the vehicle does not emit any emission since the combustion engine is not working. The vehicle used for road tests is presented in Figure 2. The vehicle was manufactured in 2020 and has Euro 6d emission standard, the engine capacity is 1497 cm^3 and is fueled with petrol. For the tested vehicle, aftertreatment system is TWC and electric motor in synchrony with permanent magnet, and traction battery is nickel-metal hydride. Maximum power of the electric motor is 45 Kw and maximum torque is 169 Nm.



Figure 2. View of a PEMS-equipped vehicle used for road testing.

For contemporary models of exhaust emissions, it is also necessary to distinguish between them due to the specificity of traffic during road tests. Microscale models are most often divided according to the type of road into urban, rural, and motorway. This division is important because if we also list the data obtained while driving through the indicated parts of the road, the created exhaust emission models will be more accurate. The test route for tests using the PEMS system is shown in Figure 3.

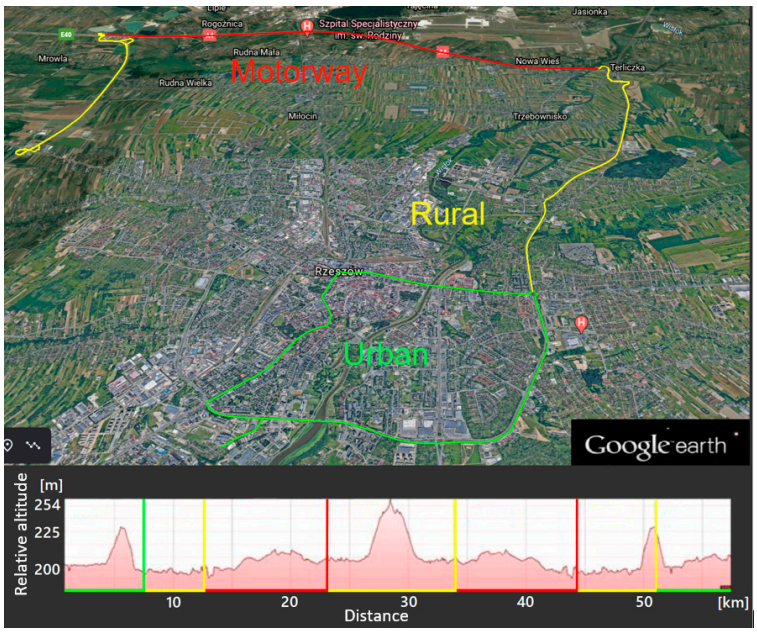

Figure 3. View of the test road with relative altitude graph.

For the collection of road emissions data, a route section was selected that included, as mentioned, urban, rural, and motorway parts. Details related to the road test are presented in Table 2.

Table 2. Specification of the on-road emission test.

Parameter	Data
Total distance (km)	55.79
Distance of the urban part (km)	16.10
Distance of the rural part (km)	19.88
Distance of the motorway part (km)	19.81
Average speed (km/h)	55.29
Urban average speed (km/h)	32.56
Rural average speed (km/h)	62.24
Motorway average speed (km/h)	102.76

The primary goal was to obtain a complete overview of vehicle emissions data under various road conditions. Driving tests were carried out in March 2021, the average ambient temperature was 6.42 °C and the average humidity was 70.83%RH. The PEMS system (OBS-2200) automatically recorded exhaust emission data and vehicle operating data. Additionally, in the vehicle, the OBD II system was connected to later verify the speed data with the GPS data of the PEMS system. The data were recorded at a frequency of 1 Hz, so that each sample generated about 4000 records. Each data record contained information on: speed, vehicle acceleration, fuel consumption, emission level of CO_2 exhaust components, humidity, air temperature, latitude, longitude, and altitude above sea level.

Exemplary distributions of speed/acceleration from a trip in off-peak traffic conditions are shown in Figure 4.

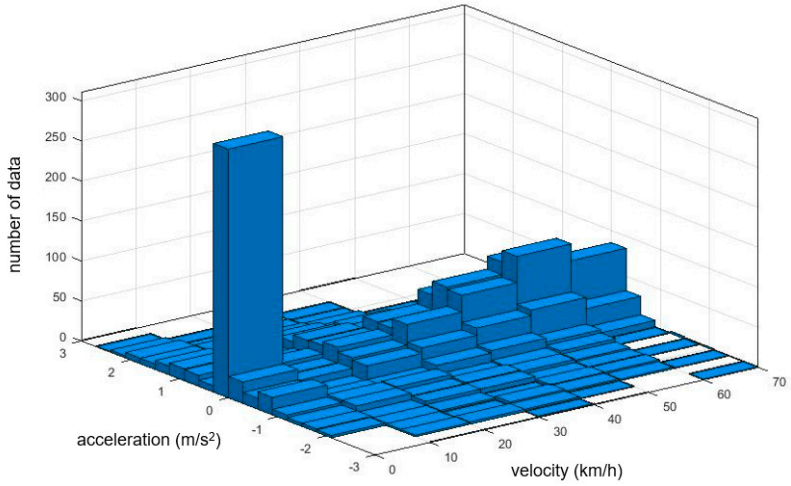

Figure 4. Exampled speed and acceleration distribution for urban part of road.

Emission models for the carbon dioxide data collected from the PEMS system were created in the Regression Learner application. Matlab's Regression Learner application allows to select the statistical method to find the most suitable regression model for researched case. Among the methods used, it can be distinguished between standard linear regression and more advanced methods using machine learning techniques. In the development of the models, the cross-validation method was also used. Five or ten times cross-validation is now recommended. With five-fold cross-validation, the data is randomly divided into 5 equal portions, of which the test set is one portion (example), while the remaining portions are used to construct the classifier. A ten-fold cross-validation was used to obtain the most accurate models for the tested data sample.

From the different methods of regression for the purpose of emission model creation, the following were assessed: linear, robust regression, fine, medium, coarse tree, linear, cubic SVM, bagged trees, Gaussian process regression (GPR) and neural network. For the analyzed exhaust emission data, the method of GPR was used due to the best results obtained. Unfortunately, in this method it is impossible to write the model equation, because the Gaussian process regression is nonparametric and is not limited by a functional form [36]. GPR calculates the probability distribution for all admissible functions that fit the emission data. The simplified emission model creation scheme is presented in Figure 5.

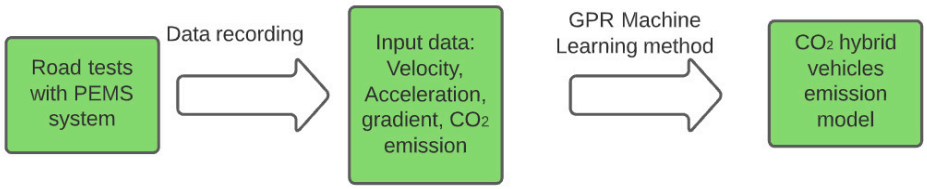

Figure 5. General overview of the emission model creation procedure sequence.

4. Results of Emission Model Validation

The evaluation and validation of the model is the most important part in the process of its creation because on this basis it can be stated to what extent the prepared model fulfills the assumed task. Validation of the obtained exhaust emission models was carried out on the basis of the results of instantaneous emissions, using data that were not used for the previous calibration of the model. Four widely used coefficients of forecast error assessment were used to validate the models obtained. *RMSE* (root mean square error), R^2 (Coefficient of determination), *MSE* (mean squared error), and *MAE* (mean absolute error).

The root mean square error is calculated on the basis of formula (3):

$$RMSE = \sqrt{\frac{1}{n}\sum_{t=1}^{n}\left(y_t - y_t^P\right)^2} \quad (3)$$

where:

n—number of samples,
y_t—forecast,
y_t^P—observed values.

The mean squared error (*MSE*) and *MAE* (mean absolute error) is calculated based on the formulas (4) and (5):

$$MSE = \frac{1}{n}\sum_{t=1}^{n}\left(y_t - y_t^P\right)^2 \quad (4)$$

$$MAE = \frac{1}{n}\sum_{t=1}^{n}\left|y_t - y_t^P\right| \quad (5)$$

where:

n—number of samples,
y_t—forecast,
y_t^P—observed values.

The coefficient of determination is calculated based on the formula (6):

$$R^2 = \frac{\sum_{t=1}^{n}\left(\hat{y}_t - \overline{y}\right)^2}{\sum_{t=1}^{n}\left(y_t - \overline{y}\right)^2} \quad (6)$$

where:

R^2—coefficient of determination,
y_t—forecast,

$\hat{y}_t$—predicted values of the dependent variable,
$\overline{y}$—average value of the actual dependent variable.

The first part of choosing the best machine learning method for CO_2 emission prediction was to compare different methods of machine learning regression. Table 3 presents the methods of researched regression analysis. The lowest value of RMSE, MSE and MAE and at the same time the highest value of R^2 was for the Gaussian process regression (Exponential GPR) so that this method was chosen for later creation of emission model.

Table 3. Result of emission modeling with different machine learning techniques.

Type of Model	RMSE (Validation)	R^2 (Validation)	MSE (Validation)	MAE (Validation)
Tree, Fine tree	1.1813	0.59	1.3955	0.71621
Tree, Medium Tree	1.2422	0.55	1543	0.8211
Tree, Coarse Tree	1.3053	0.51	1.7039	0.89876
Linear Regression (linear)	1.3948	0.43	1.9454	1.0258
Linear Regression (Robust Linear)	1.4189	0.42	2.0133	1.0026
Stepwise Linear Regression	1.3632	0.46	1.8584	0.99398
Linear SVM	1.4232	0.41	2.0256	1002
Cubic SVM	1.3524	0.47	1.8289	0.87705
Esemble, Bagged Trees	1.1929	0.59	1.423	0.8447
Gaussian Process Regression (Exponential GPR)	1039	0.69	1.0795	0.7066
Neural Network (Three-layered Neural Network)	1.2559	0.54	1.5773	0.87841

In the first stage, validation was carried out based on analysis of the scatter plots of the data between the predicted and observed data. In Figure 6 we can see the Gaussian process regression efficiency of prediction for CO_2 emission data.

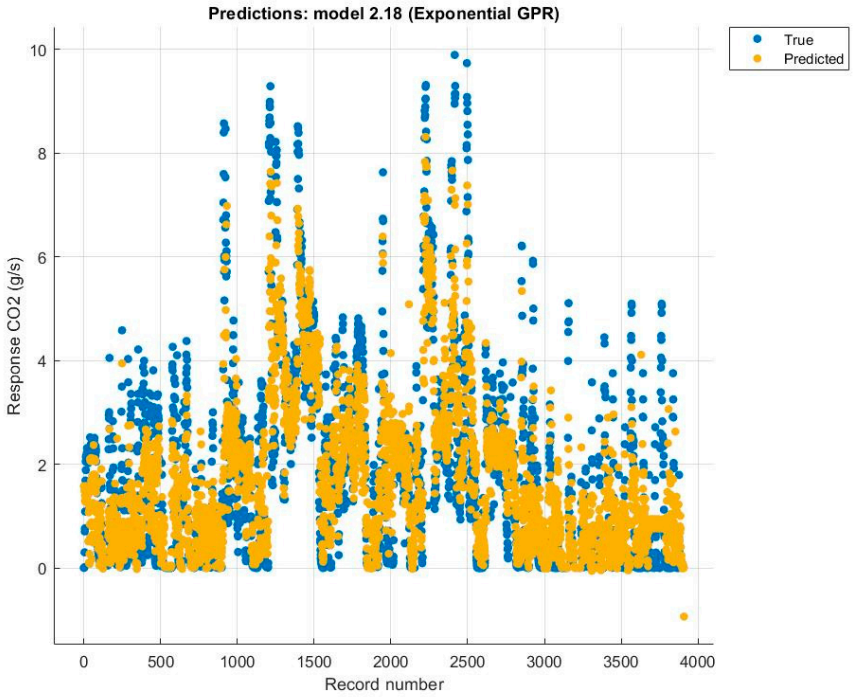

Figure 6. Prediction performance of CO_2 emission for a selected Exponential GPR computational model.

An exemplary graph of scatter points of predicted and observed data is shown in Figure 7. For the analysis of the data scatter plot, it is important to check which point clouds are arranged in the obtained data points and whether there are large numbers of outliers for them.

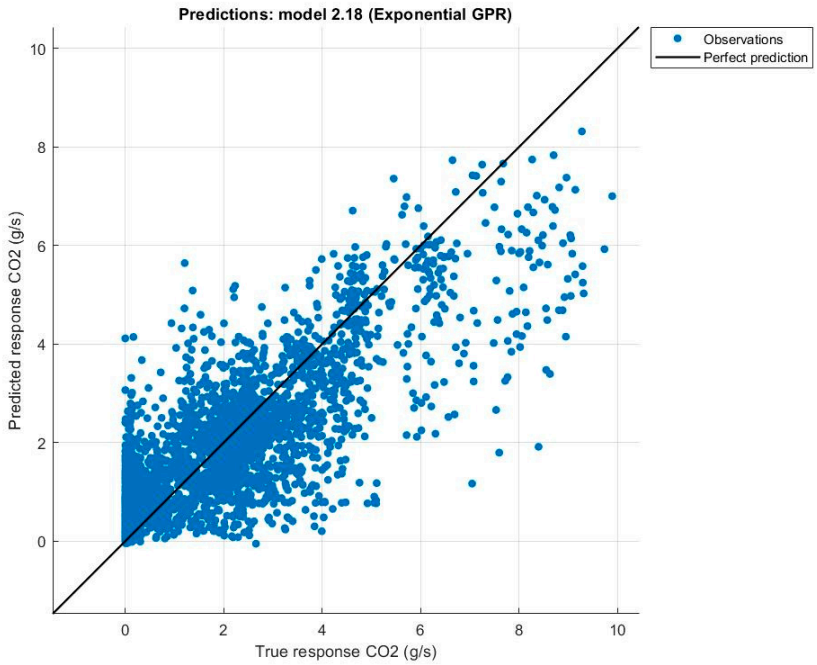

Figure 7. Predicted vs. true response scatter plot for the CO_2 emissions.

For the analysis of the data scatter plot, it is important to check which point clouds are arranged in the obtained data points and whether there are large numbers of outliers for them.

The Figure 8 of residuals also confirms that the models can be considered adequate because the data on them do not fit into any patterns and are distributed in such a way that their clusters go to the middle of the diagram.

The last part of the model validation was the verification of the real CO_2 emission data from the road to the predicted data for the entire research road path. The main challenge in modeling CO_2 emissions for a full hybrid vehicle was to obtain the right evaluation of the emission map, as this is one of the most important factors for the microscale emission model. The most important thing was to caption sectors where there was actually zero emission, since the engine was not running and the vehicle was only powered by an electric motor. Based on Figure 9, it can be seen that the emission map as well as the PEMS data as well as the prediction data of the model are very similar and also the ranges of the emission values are very similar. The greatest number of zero emission zones activities of the tested hybrid vehicle is in the urban part (dark blue parts). Actually, the CO_2 emission from models is showing a lower frequency of zero emission ranges of vehicle operation, but also reflects it in some part in a good level. Also, the sum of emissions for the whole road is very similar: for the PEMS real road data, the sum of CO_2 is 6421.46 g and for predicted data, it is 6423.42 g. As we can see from Figure 9 for the speed occurring in the city centers, there is very low emission of CO_2 or there is none. The highest emission occurs for part of the motorway due to the high load of the combustion engine.

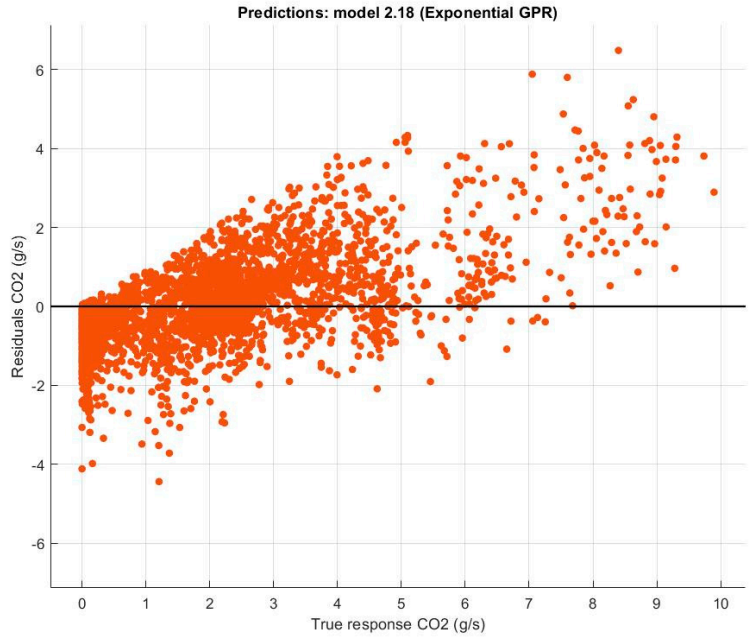

Figure 8. Residuals vs. predicted response scatter plot for the CO_2 emissions.

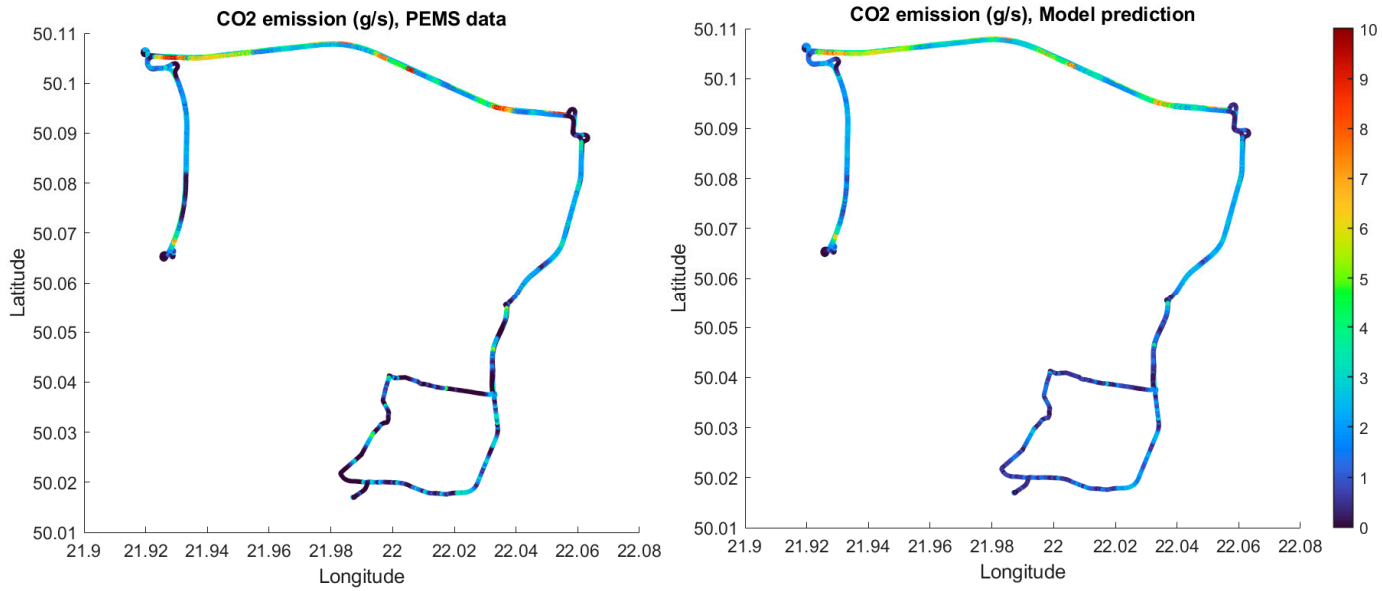

Figure 9. Comparison of emission map for the real data (PEMS) and the model prediction data for CO_2 emission.

In Figure 10, an instantaneous emission of CO_2 obtained from PEMS during or-road test is presented and also predicted data from emission model. Based on Figure 10 it can be seen that as well as for low and for high speeds, there is relatively good mapping of the real word CO_2 emission to the predicted one. For the period of 3700–3800 s there is a visible gap between these two datasets, but there can obviously be more of that error and it is justified. This state of affairs is because hybrid vehicles and their use of combustion engines cannot be fully reflected by emission models, especially when we put just velocity, acceleration, and road gradient as an input of predictors. The fuel consumption and in consequence CO_2 emission are related to more factors, such as: level of battery, speed, acceleration, use of accessories such as air conditioning, etc.

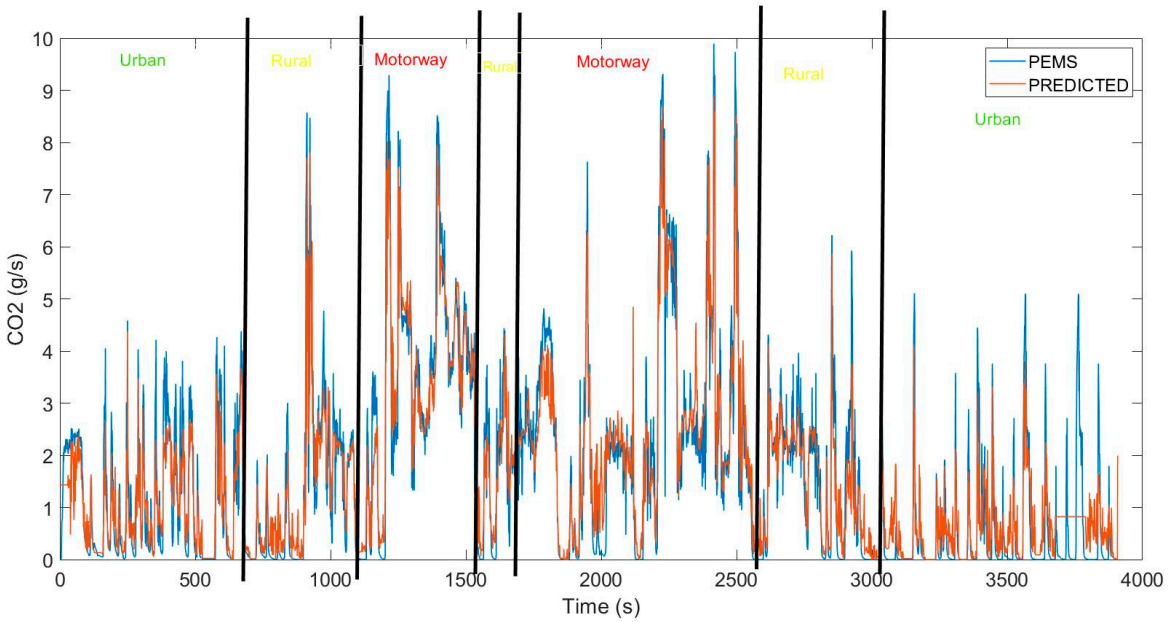

Figure 10. Instantaneous emission of CO_2 for real road data from PEMS and predicted model data.

The differences in emissions obtained from road tests (PEMS) and model calculations are shown in Figure 11. Based on Figures 10 and 11 we can see that relatively some differences in the emission obtained have been observed, both from the PEMS and the computational model. The largest single gap can be visible for the rural road section—around -6 g/s. Some gaps have also been observed in the rest of the road sections, urban and motorways, up to 3–-3 g/s. The highest density of differences can be noted for the urban section, as mentioned before—period 3700–3800s.

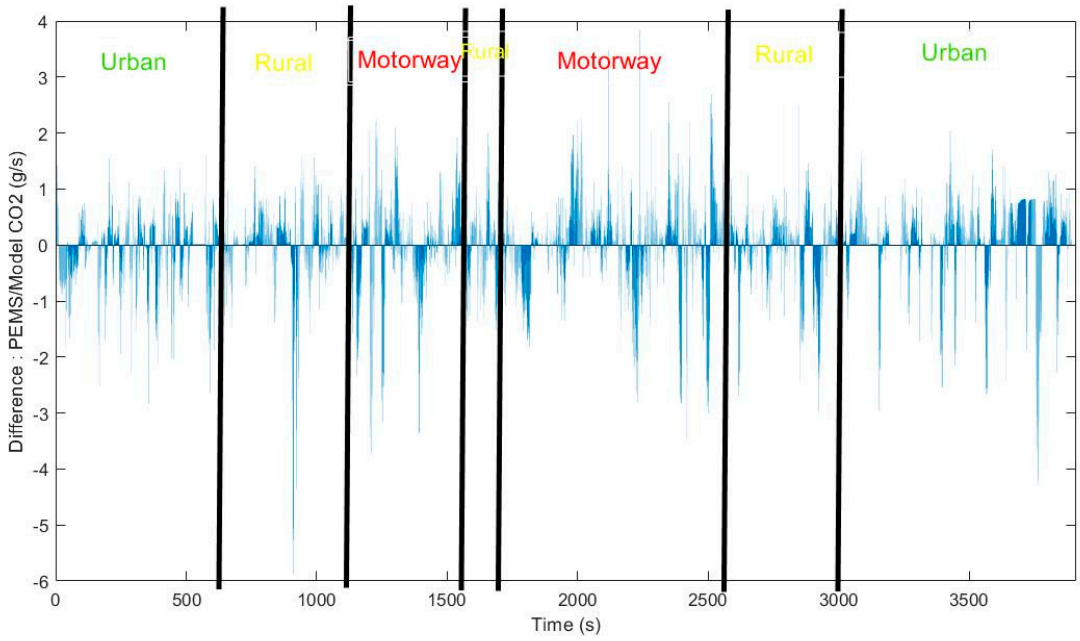

Figure 11. Differences of CO_2 emissions obtained results from PEMS and emission model calculation.

The obtained emission model of CO_2 can be directly used as an application which requires only speed, acceleration, and gradient obtained from the road test. The use of this emission model is especially recommended for micro-scale road modelling, e.g., in the Vissim software. From every simulation performed, it is possible to have an output

related to the movement of the simulation vehicles and it is easily accessible. Because of that, it would be possible to create viable emission maps to detect the hotspots of emission from hybrid vehicles on the investigated part of the road which can be modeled as a simulation model.

5. Conclusions

In the coming years, a further significant increase in the number of vehicles is expected, which will worsen the condition of the natural environment and adversely affect the health of the population, especially in urban areas [37–39]. Such a situation will lead to increased congestion. In the case of simulation analyzes of emissions, it is necessary to create national and regional emission models on a micro scale, because they give detailed results of emissions generated by vehicles passing, for example, through selected arteries of city streets. In this case, the COPERT macroscale models available to the public and currently used in Poland seem to be insufficient, especially when it is necessary to analyze the emission from the hybrid vehicle.

Computational emission models show great potential for their further use for output data, e.g., from vehicle traffic simulation models. Thanks to this, road designers, already at the design stage of a given road section, can obtain in detail the future forecasted results of the emission of harmful exhaust components, which may have an impact on road passersby or as a result of the dispersion of these gases on local residents, by simulating the forecast road traffic.

On the basis of the outputs of the work, it can be concluded:

- CO_2 emissions from hybrid vehicles are not strictly correlated with speed and acceleration because in some range of vehicle operation there is no emission, because combustion engine is not working.
- Machine learning methods are sufficiently sensitive to learn and create emission CO_2 models for this kind of vehicle emission activities,
- Due to the variability of CO_2 emission from the hybrid vehicle, there is a gap in the existing emission models, as they do not provide reliable results, especially when it comes to emission maps.
- Machine learning regression techniques can give an adequate emission model for full hybrid vehicles, especially for the Gaussian process regression technique.
- The main issue of modelling CO_2 emissions among hybrid vehicles touches urban roads, since there is the highest value and share of electric motor usage.
- The developed emission modelling methodology can be used in terms of microscale vehicle movement modeling to later create, for example, map on emission of researched part of the road to find zones with the lowest and highest CO_2 emissions, and thus to develop more beneficial solutions to reduce these emissions.

Future research plan regarding developing of the emission model includes performing road test in e.g., different ambient temperature, because it has direct influence on duration of cold start emission and on battery capacity.

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Abbreviations

CO	Carbon monoxide
CO_2	Carbon dioxide
GPR	Gaussian process regression
LPG	Liquified petroleum gas
MAE	Mean Absolute Error
MOE	Measures of effectiveness
MSE	Mean squared error
NNET	Neural network
NOx	Nitrogen oxides
PEMS	Portable Emission Measurement System
PHEV	Plug-in hybrid electric vehicle
PM	Particulate matter
R^2	Coefficient of determination
RMSE	Root mean square error
SVM	Support vector machine
THC	Total hydrocarbons

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