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Vehicle Hydrocarbons' Emission Characteristics Determined Using the Monte Carlo Method

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Abstract

Hydrocarbons (HCs) are products of incomplete combustion process which can occur during operation of the internal combustion engines (Flagan and Seinfeld 1988; Wallington et al. *Meteorologische Zeitschrift*, *17*(2), 109–116, 2008). Incomplete combustion process affects the fuel consumption and engine performance (Baskar and Senthilkumar *Engineering Science and Technology, an International Journal*, *19*, 438–443, 2016; Rakopoulos and Giakoumis 2009) also the emission of unburned HCs affects the emissions of the other air pollutants (Jung et al. *Journal of Environmental Sciences*, *54*, 21–32, 2017; Wang et al. *Journal of Environmental Sciences*, *46*, 28–37, 2016; Kerbachi et al. *Energy Procedia*, *136*, 388–393, 2017). This paper presents the methodology for the investigation of HC amount emitted from internal combustion engines. It can be used for estimation of the emission factors, emissions from various vehicles and engine types, also carrying out the environmental impact assessment of various vehicles. The HC emission characteristics is defined as the dependency between the measured HC emissions (specific distance emission) and the vehicle's velocity. The Monte Carlo simulation allows determining the HC emission's characteristics from internal combustion engines. In the paper, five emission characteristics determined using the consecutive Monte Carlo simulations are given. In each case, the characteristic is fit using the 7th degree (order) polynomial regression. The goodness of fit is assessed using Ramsey's RESET test, and the $RMSE$. The authors find application of the proposed methodology in various types of the internal combustion engines to assess their environmental properties.

Keywords Air pollution · Emission · Light-duty vehicle · Semi-ignition engine · Monte Carlo simulation

1 Introduction

Road transport is the one of the most important sources of pollutants released into the air [10, 17]. Results given by Lelieveld et al. [36] indicate that the air pollution emitted from the land traffic has important contribution to the premature mortality, in both groups of countries: developed and developing. An analysis given by Dedoussi and Barrett [13] highlights that the road transportation sector has significant contribution to the exposure to $PM_{2.5}$ particulates, and they are in 29% the result of the nitric oxides' emission and in 33%—usage of the ammonia in after-treatment technologies.

The number of intensive studies on the road transportation sector's environmental effects is also a result of the recent industrial affair commonly called *Dieselgate* [3, 6, 8]. Scientific investigations started to focus not only on the context of the air quality and health (e.g., [22, 23, 33, 57]), but also at the road transportation's emission limitation problems [16], and at the issues associated with environmental properties of the internal combustion engines [51].

Environmental properties of the internal combustion engines are not necessarily associated with the road transportation. In a broader context, studies on the marine internal combustion engines are devoted to the nitric and sulphuric oxides primarily [9, 29, 35]; however, the methodology

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based on the emission characteristics, presented in this paper, does not depend on the selected air pollutant.

The emission of unburned HCs can be taken into consideration as the engine's combustion performance indicator. During the incomplete combustion process, the HC emission affects the emissions of other pollutants, especially ultrafine particles and nitric oxides [28, 30, 56]. On the contrary to the nitric oxides, carbon monoxide or soot, the increase of the HC emission is observed also during the deceleration [28, 45]. Moreover, results given in [1, 58] and [55] show that the driving in congestion (urban peak) results with significant increase of HC emission. The HCs released into the air can cause negative health effects and also contributes to the ground-level ozone concentration or smog [37, 41].

Presented results find the transportation sector significant in the context of air quality and human health impact. More accurate determination of the HC emissions from this sector can help to carry out the detailed quantitative assessment of the air emission impact taking into account the negative health effects of smog episodes.

2 Materials and Methods

The emission is usually estimated using two variables: 'emission factor' and 'activity of the emission source' [19, 47, 48, 52]. In case of the road transportation sector, the emission factor is the average emission of pollutant released into the air as a result of driving the particular distance or combustion of the particular amount of fuel. The HC emission inventory from the vehicles is determined as follows:

$$E_{\mathrm{HC}} = \sum_{i,j,k} \left(EF_{\mathrm{HC},j,k} \times A_{j,k} \right), \tag{1}$$

where: E_{HC}—emission of hydrocarbons [g]; EF—emission factor [g $\cdot$ km^{-1}]; i—engine performance, e.g. accordingly to the European emission standards; j—emission source (vehicle type: passenger car, light-duty vehicle, hard-duty vehicle, machinery, and other); k—fuel type (e.g. gasoline, diesel oil, CNG); $A_{j,k}$—activity for the emission source, distance-driven j [km].

Emission factors are various and depend on the technology, year of production, style of driving and many other variables. It causes that the emission factors are widely applied to assess the engines' environmental properties.

2.1 Specific Distance Pollutant Emission

Apart from emission factors (1), the air pollutants' emissions can be also used for determining the environmental impact of vehicles. The measured value $\hat{E}$ (see Eq. 2) is known as the specific distance pollutant emission (SPDE). SPDE, defined as the averaged emission per the vehicle's mileage, is obtained in the laboratory by measuring the real time emission using the exhaust gases' analyzer. The 'emission' is defined as the total mass of particular pollutant released into the air [12].

Mathematically, SPDE (further notation: $\hat{b}$) is a derivative of emission with respect to the distance travelled by the vehicle. The distance travelled is measured using the chassis dynamometer. SPDE is associated with the particular distance associated with the driving cycle (see Section 2.3).

$$\hat{b} = \frac{\hat{E}}{\hat{s}} = \frac{V_{\mathrm{mix}} \cdot Q_{\mathrm{HC}} \cdot k_{\mathrm{H}} \cdot C_{\mathrm{HC}} \cdot 10^{-9}}{s}, \tag{2}$$

where: $\{\hat{\cdot}\}$—average value; $\hat{E}$—emission, measured by exhaust gas analyzer [g]; s—vehicle's distance measured by the chassis dynamometer [km]; V_{mix}—volume of the diluted exhaust gas [m^3/test], corrected to the standard conditions ($T = 293$ K, $p = 101.33$ kPa); Q_{HC}—density of the analysed HCs at standard conditions [kg/m^3]; k_{H}—humidity correction factor [dimensionless], for HCs $k_{\mathrm{H}} = 1$; C_{HC}—concentration of the HCs in the diluted exhaust gas measured by the exhaust gas analyzer and corrected by the amount of HCs contained in the dilution air [ppm].

Parameter $\hat{b}$ can be also expressed as a dynamic value (variable over time) depending on the engine operating state processes which is usually characterized by (operator notation used):

- engine load—$M_e(t)$,
- engine speed—$n(t)$,
- engine thermal state—$T_s(t)$, expressed as the set of engine parts' temperatures and factors operating on its systems such as coolant and lubricating oil, and
- environmental conditions—$G(t)$:

$$\begin{aligned} b(t) &= \Xi_M[M_e(t), n(t), T_s(t), G(t)] \qquad (3)\\ &= \Xi_v[v(t), A(t), T_s(t), G(t)], \qquad (4) \end{aligned}$$

where: Ξ_M—operator using the engine load; Ξ_v—operator using the vehicle's velocity $v(t)$; $A(t)$—matrix which contains information about vehicle motion resistance connected with the shape and other properties of the surface [7].

The SPDE ($\hat{b}$) can be then expressed together with the time series of the vehicle's velocity ($\hat{b}$ vs. $\hat{v}$). This kind of dependency is defined as *emission characteristics*.

2.2 Laboratory Equipment

Empirical tests are conducted on a Citroën Berlingo light-duty vehicle, equipped with a semi-ignition engine. The vehicle's velocity is investigated using a chassis dynamometer EMDY 48 (Schenck-Komeg, one roller of 48″ diameter) [50], and HC emission—using exhaust gases analyzer FIA-725A, MEXA 7200 (Horiba) [25]. The measurements took place at the Automotive Industry Institute in Warsaw. Equipment used in the tests was in accordance with the requirements of the Directive of the European Parliament and Council on vehicles homologation testing [15] also the metrological and technical requirements for instruments measuring vehicle exhaust emissions [27]. Among various types of tests, e.g. FTP 75, HWFET, Stop and Go and Autobahn [14, 18], the chosen procedure is in line with the Rule No. 83 ECE [54].

2.3 The NEDC Driving Cycle

The pseudo-random road traffic conditions are modelled in the form of a stochastic process $v(t)$ which is established as the NEDC driving cycle (Fig. 1) [2, 40, 42, 54].

The NEDC driving cycle is a version of the former driving test named EC+EUDC [38, 45, 53]. The last update of the cycle took place in 1997. The NEDC driving cycle is elaborated to simulate the statistically average use of vehicle in Europe. It consists of the two parts from which EC simulates urban driving, and EUDC—extra urban. Before the test, the vehicle is allowed to soak for at least 6 h at a test temperature of 20–30 °C. It is then started and allowed to idle for 40 s. The beginning of the sampling starts after 40 s from the start of the cycle. The length of the cycle is 1, 220 s on the distance of 11, 007 m, including the idle period. Average vehicle's velocity is 9 m/s (32.5 [km/h]), and maximal—33 m/s (120 km/h). In 2000, the idling period has been eliminated, i.e. engine starts at 0 s and the emission sampling begins at the same time. This modified cold-start procedure is referred to as the New European Driving Cycle (NEDC).

2.4 Stochastic Model

The multidimensional stochastic process of phenomena accompanying the operation of a vehicle $Y(t)$ applies to the HC emission and fuel consumption primarily:

$$Y(t) = [E_{\mathrm{HC}}, G_{\mathrm{f}}]^{\top}, \tag{5}$$

where: E_{HC}—intensity of HC emissions; G_{f}—intensity of fuel consumption.

Considering processes $v(t)$ and $Y(t)$ as functions of the time, it can be considered that the notations $v(t)$ and $Y(t)$ are equivalent. Assuming the ergodicity of $v(t)$ and $Y(t)$, means:

$$\lim_{\tau\to\infty} E\left\{\left[\frac{1}{\tau}\int_{t_0}^{t_0+\tau}\{\cdot\}dt - \mu_{\{\cdot\}}\right]^2\right\} = 0, \tag{6}$$

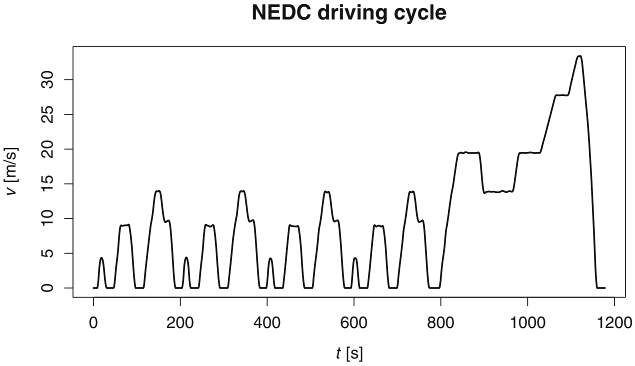

Fig. 1 The NEDC driving cycle

where: $\{\cdot\}$—$v(t)$ or $Y(t)$; $\mu_{\{\cdot\}}$—expected value of $v(t)$ or $Y(t)$ (*constant*); t_0—start of averaging process; τ—length of the averaging process.

There is possible to determine their average values ($\hat{v}$ and $\hat{Y}$) in the expected time frame (t_α, t_ω), as below:

$$\hat{v}(t_\alpha, t_\omega) = \frac{1}{t_\omega - t_\alpha}\int_{t_\alpha}^{t_\omega} v(t)dt, \tag{7}$$

$$\hat{Y}(t_\alpha, t_\omega) = \frac{1}{t_\omega - t_\alpha}\int_{t_\alpha}^{t_\omega} Y(t)dt. \tag{8}$$

SPDE ($\hat{b}$) is defined as the ratio of particular pollutant's emission concentration and the vehicle's velocity. Thus, the average specific distance pollutant emissions are expressed as follows:

$$\hat{b} = \frac{\hat{E}(t_\alpha, t_\omega)}{\hat{v}(t_\alpha, t_\omega)}. \tag{9}$$

Considering the average specific distance pollutant emissions as a function of average velocity as well as the time of the start and finish of the averaging process:

$$\hat{b} = f(\hat{v}(t_\alpha, t_\omega), t_\alpha, t_\omega). \tag{10}$$

Assuming that the t is the random variable, in particular, t_α and t_ω, then the SPDE ($\hat{b}$) should be treated as a random function. The dependency $\hat{b}$ vs. $\hat{v}$ is simultaneously characteristic of the HC emission process.

Monte Carlo simulation (e.g. [24, 39, 43]) gives the possibility of determining the stochastic characteristics of vehicle pollutant emissions expressed as the form of dependence between $\hat{b}$ and the average vehicle velocity $\hat{v}$. Similarly, it is possible to consider one–dimensional characteristic dependencies between the SPDE and other values, e.g. the average value of the module of acceleration or the average value of the module of the product of velocity and acceleration. There is also a possibility of determining multidimensional characteristics of air pollutants' emissions.

A fundamental quality of the proposed method for determining characteristics is the ability to obtain information about the examined object on the basis of a single implementation of the stochastic process. Thus, the Monte Carlo method has been applied in line with the initial, historical intention of its creators [39].

Registration of the processes of pollutant emission concentrations was processed digitally, eliminating significant errors and conducting low-pass filtration. The Golay–Savitzky filter [49] was used in filtration, with the following averaging parameters: two-sided use of two points and a second degree approximating polynomial (smoothing).

2.5 Quantitative Assessment

Characteristics are fitted to the $\hat{b}$ vs. $\hat{v}$ dependency using the polynomial regression for each from five independent Monte Carlo simulations. Influential observations are rejected from the models if their Cook's distances exceeded 2. Cook's distances [5, 11, 21] are calculated using procedure implemented in statistical language `R` [44]. The correctness of the analytical model forms is checked using Ramsey's RESET test [32, 46] implemented in the `lmtest` library [26].

To carry out a quantitative assessment of all SPDE simulations, the root mean square error ($RMSE$) is calculated:

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(b_i(\hat{v}_i) - \hat{b}(\hat{v}_i))^2}, \tag{11}$$

where: $RMSE$—root mean square error of the $\hat{b}$; i—the number of speed's averagings; $\hat{v}_i$—the i-th averaged speed; $\hat{b}$, the average SPDE value obtained from the one series series.

3 Results and Discussion

Figure 2 shows the processed HC emission concentration processes using Golay–Savitzky low-pass filtration [49]. The emission is automatically calculated by registering the volume of air flow used by the engine (2). The processes of the air flow through the engine is subject to the same digital processing procedures as the pollutant emission concentration processes.

The registered vehicle's velocity processes as well as the HC emission concentrations are used to determine pollutant emission characteristics.

The determined characteristics using five consecutive Monte Carlo simulations (MC_1, MC_2, MC_3, MC_4, and MC_5) presented in the figures below (Figs. 3, 4, 5, 6 and 7). The figures show the original series of the lab measurements (grey points) with the determined HC

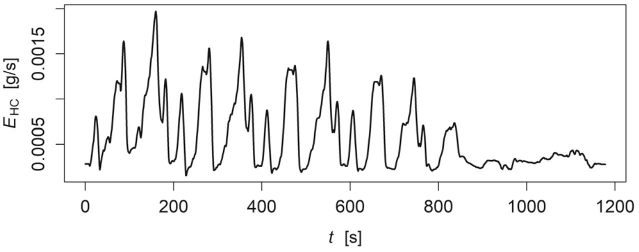

Fig. 2 The time series of the hydrocarbons' emission intensity E_{HC} [g/s]

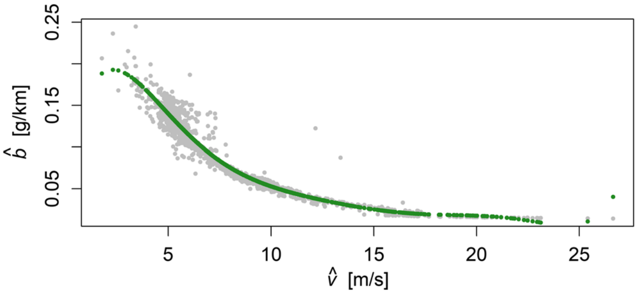

Fig. 3 Simulation 1 (MC_1). $\hat{b}$ [g/km]) vs. $\hat{v}$ [m/s]. Characteristics added

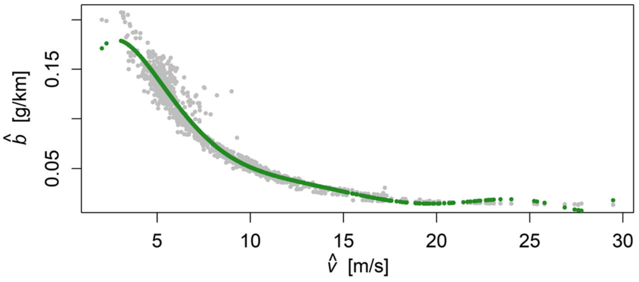

Fig. 4 Simulation 2 (MC_2). $\hat{b}$ [g/km]) vs. $\hat{v}$ [m/s]. Characteristics added

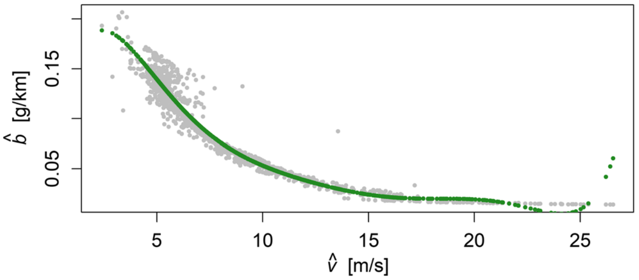

Fig. 5 Simulation 3 (MC_3). $\hat{b}$ [g/km]) vs. $\hat{v}$ [m/s]. Characteristics added

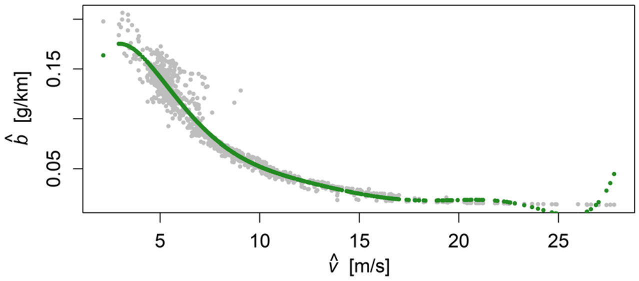

Fig. 6 Simulation 4 (MC_4). $\hat{b}$ [g/km]) vs. $\hat{v}$ [m/s]. Characteristics added

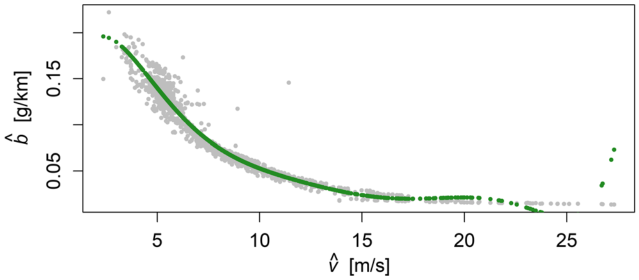

Fig. 7 Simulation 5 (MC_5). $\hat{b}$ [g/km]) vs. $\hat{v}$ [m/s]. Characteristics added

Table 1 The qualitative assessment of the Monte Carlo simulations of the $\hat{b}$ vs. $\hat{v}$ dependency

Simulation	R^2	$RMSE$	RESET (p-value)
MC_1	0.9092	0.0114	0.5557
MC_2	0.9303	0.0102	0.0329
MC_3	0.8932	0.0111	$8.022 \cdot 10^{-9}$
MC_4	0.9260	0.0107	0.2040
MC_5	0.9058	0.0106	$9.06 \cdot 10^{-13}$

For each simulation is applied the polynomial fit of 7th degree (order). Ramsey RESET test's p value indicates the correctness of fit

emission characteristics (green line). The goodness of fit is performed using the coefficient of determination (R^2), $RMSE$, and the p value of the Ramsey's RESET Test. They are presented in Table 1. The parameters of the determined characteristics are given in Table 2.

Repeatability and reproducibility is characteristic for the Monte Carlo simulation. Basing on previously gained knowledge [7, 31, 34] is possible to conclude about the process. In the case of HCs released from the light-duty vehicles' semi-ignition engines, the characteristic is the significant characteristic's decrease along with the increase of the average vehicle velocities (Figs. 3–7). Obtained results confirm the finding given in [1] and [45] on non-typical behavior of the HCs in comparison to the another pollutants (e.g. nitric or sulphuric oxides).

4 Conclusions and Outlook

Characteristics of pollutant emissions in the form of a dependences between specific distance emissions and average velocity are a valuable source of information about the environmental properties of vehicles in their operating conditions. The characteristics significantly facilitate the combustion process performance and help to determine emission factors in various operational states of the internal combustion engines.

Without an awareness of these characteristics it is not possible to balance pollutant emissions for road traffic, and thus also assess the negative impact of the road transportation on the environment and human health.

The methodology presented in this paper uses the fixed function of speed over time together with the measured time series of the pollutant released into the air. That means the methodology is not dependent on the measured pollutant nor the combusted fuel. It can be considered for application to various types of internal combustion engines, including marine or aeronautical.

The potential application for the proposed method is broad. It can be used to study many objects, not only technical ones, for which the co-dependence of processes

Table 2 The parameters of obtained emission characteristics ($\hat{b}$ vs. $\hat{v}$ regressions)

Sim.	β_0	β_1	β_2	β_3	β_4	β_5	β_6	β_7
MC_1	0.0959	−1.3791	0.7036	−0.0731	0.0923	0.1650	−0.0358	0.0923
MC_2	0.0957	−1.3203	0.7309	−0.1817	0.0554	0.1486	−0.0852	0.1144
MC_3	0.0923	−1.3611	0.7225	−0.0997	0.1272	0.1795	0.0345	0.1044
MC_4	0.0932	−1.2747	0.7004	−0.1505	0.0364	0.1737	−0.0388	0.1131
MC_5	0.0946	−1.3514	0.7404	−0.1268	0.0859	0.1805	−0.0191	0.1277

Polynomial fit in form: $\hat{b}_i = \beta_0 + \sum_{n=1}^{k=7} \beta_n \cdot (\hat{v}_i)^n$

describing the object is characteristic and expressed as the postulated determination or confirmed correlation.

The emission characteristics elaborated with using the collected data are determined by application of the Monte Carlo method and the polynomial regression. The repeatability and reproducibility of the presented methodology can be easily found by analyzing their shapes—decreasing along with the increasing velocity. The significant increases of the characteristics at the right tails can be explained with the expected HC emission increase during the engine clutch [1].

The proposed methodology is characterized by the low sensitivity to various pseudo-random conditions occurring during carrying out the experiments. That means the determined characteristics do not depend on the applied methodology. This result of the simulation research confirms the effectiveness of this method in determining characteristics of the emission produced by car engines.

It is possible to significantly expand the test programme to encompass other properties of the considered stochastic process.

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