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The emission of BTEX compounds during movement of passenger
car in accordance with the NEDC

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Abstract

The results of the research in the field of benzene, toluene, ethylbenzene and xylene isomers (BTEX) concentrations in exhaust gases of spark ignition engines under different operating conditions are presented in this paper. The aim of this paper is to gain a clearer insight into the impact of different engine working parameters on the concentrations of BTEX. The experimental investigation has been performed on the SCHENCK 230W test stand with the controlled IC engine. The engine operating points have been chosen based on the results of a simulation and they are considered as the typical driving conditions according to the New European Driving Cycle. Concentration levels of BTEX compounds in exhaust gas mixtures have been determined by gas chromatography technique by using the combination of Supelcowax 10-Polyethylene glycol column and the PID detector. Based on the experimental research results, the emission model of BTEX compounds has been defined by the simulation of movement of a Fiat Punto Classic passenger car in accordance with the NEDC cycle. Using the results obtained within the simulation, the official statistics on the number of gasoline-powered cars on the territory of the Republic of Serbia and the European Commission data on the annual distance traveled by car, the amounts of BTEX compounds emitted annually per car have been estimated, as well as the emissions of the entire Serbian car fleet.

Keywords: aromatic compounds; driving cycle; exhaust gases; engine testing; emission model
1. Introduction

The permanent increase in the need for various forms of energy leads to constant environmental degradation. The energy sector is the largest source of air pollution resulting from human activity, mainly from the combustion of fossil fuels (International Energy Agency, 2016). Constant emissions of pollutants into ambient air affect the global processes by increasing concentration levels of pollutants, distribution and allocation between basic environmental compartments, biotic and abiotic matrix. The consequences of uncontrolled emissions of pollutants are related to the presence of large amounts of various gases in the atmosphere, like CO₂, SO₂, CH₄, NₓOᵧ, and VOC (Alyuz and Alp, 2014). In addition to these compounds, there is a large number of specific hazardous and carcinogenic substances in the atmosphere. Air pollution has many unwanted effects, the extent of which is determined by the concentration levels of different pollutants. There is a wide range of negative health impacts, adverse impacts on vegetation, climate change, acidification of atmospheric precipitations, and eutrophication of water bodies (Bernstein et al., 2004; Bobbink et al., 2010; Künzli et al., 2000; Tong et al., 2016).

A significant part of environmental air pollution and a wide range of health hazards originate from motor vehicle emissions (Caprino and Togna, 1998; Poorfakhraei et al., 2017). This has induced strong legislative efforts to reduce the harmful vehicle emissions. The notably reduced traffic emissions have been achieved by new engine technologies, exhaust aftertreatment, and newly developed, reformulated fuels. However, only a part of the exhaust compounds are legally regulated, such as nitrogen oxides (NOₓ), carbon monoxide (CO), total hydrocarbons (HC), and particulate matter (PM). On the other hand, more specific, carcinogenic compounds, such as BTEX, remain largely unregulated (Westphal et al. 2010).
The most recent European Union ecological standards related to the exhaust gases of motor vehicles from Euro 1 to Euro 6, which is being applied since September 2014, are focused on the lowering of the greenhouse gas emissions: CO₂, CO, N₂O₅, suspended particles and total HCs (Diesel Net, 2018). The results of many experimental researches, including the results of this study, point to high concentration levels of BTEX aromatic compounds in motor vehicle exhaust gases (Lan and Minh, 2013; Macedo et al., 2017; Truc and Kim Oanh, 2007). These high concentrations appear as a result of the substitution of lead, an anti-detonator, by aromatic compounds in unleaded fuels with the purpose of increasing the octane number (Truc and Kim Oanh, 2007). Octane number is one of the main parameters used in quality control of gasoline and provides information about the resistance to auto-ignition (Rankovic et al., 2015). The chemical structure of hydrocarbons in gasoline has great influence on detonation. BTEX are very resistant to self-detonation, which is why they are used as octane number increasers in unleaded fuels (Mendes et al., 2012). Consequently, the problem of the presence of lead in the environment has been replaced by a new, and possibly greater, problem of BTEX compounds. It has only recently been recognized that benzene added to unleaded petrol in order to maintain vehicle performance may be a worse threat to human health than the lead it had displaced (Colls, 2002).

BTEX have become the common components in the atmosphere of most urban areas (Murena, 2007; Zalel et al., 2008), and their negative impacts on environmental and public health have already caused general concern (Moolla et al., 2015; Rezazadeh et al., 2012; Tohon et al., 2014). They are highly reactive in the troposphere, and therefore play an important role in the atmospheric chemistry (Atkinson, 2007). These compounds have been recognized as the important photochemical precursors for tropospheric ozone and organic aerosols (Barletta et al., 2008; Liu et al., 2009; Zhang et al., 2012). Aromatic BTEX can be seriously toxic at both short- and long-term exposures.
Benzene is the most harmful compound from the BTEX group, which has been categorized by the International Agency for Research on Cancer (IARC) as a known human carcinogen (Group 1) (Bayliss et al., 1997; Demirel et al., 2014; Maltoni et al., 1989; Mehlman, 2008).

The other BTEX compounds have also been identified as neurotoxic (Chen et al., 2011; Fustinoni et al., 2010), carcinogenic and mutagenic at concentration levels found in urban environment (Bono et al., 2003). Exposure to BTEX compounds causes symptoms such as tiredness, confusion, weakness, drunken-type actions, memory loss, nausea and loss of appetite (Edokpolo et al., 2014; Romieu et al., 1990; Tunsaringkarn et al., 2012).

1.1. The New European Driving Cycle- NEDC

A driving cycle is a fixed schedule of vehicle operation which allows emission tests to be conducted under reproducible conditions (Barlow et al., 2009). Driving cycles are usually defined in relations of vehicle speed as a function of time. The emission levels are dependent upon many parameters, including the vehicle-related factors such as model, size, fuel type, technology level and mileage, as well as the operational parameters such as speed, acceleration, gear selection and road gradient. (Franco et al., 2013; Tzirakis et al., 2006.) For that reason, different driving cycles have been developed for different types of vehicles such as cars, vans, trucks, buses, and motorcycles. It is also useful to note that driving cycles may be used for a variety of purposes other than emission measurements, such as engine testing or drivetrain durability.

The New European Driving Cycle (NEDC) is a driving cycle designed to estimate the emission levels of car engines and fuel economy of passenger cars. The NEDC is a stylized cycle, with periods of acceleration, deceleration and constant speed, and it is supposed to represent the typical usage of a passenger car in Europe. The cycle is divided into two main
parts. The first part simulates driving of a motor vehicle in urban areas, while the second part is reserved for simulation of driving on the open road. The first part of NEDC consists of four repeated ECE-15 Urban Driving Cycles (UDC) with a total length of 4,052 km and driving time period of 13 minutes, as shown in Figure 1. The average speed in the urban part of the cycle is 19 km/h, while the maximum speed is 50 km/h. The second part, an Extra-Urban driving cycle (EUDC), consists of 13 stages and lasts 400 seconds, with a top speed of 120 km/h (Fig. 1) (Agudelo et al., 2016; Barlow et al., 2009). The NEDC is used for type approval of light-duty vehicle models in the European Union.

![Fig. 1. The New European Driving Cycle (NEDC)](image)

The purpose of this cycle is to simulate vehicle and engine operation that usually occurs during the regular exploitation of passenger cars. In this way, the values measured during this cycle to a large extent reflect the real impact of vehicles on the environment and natural resources.

1.2. Engine testing

Engine testing is an expensive and complex process that requires a lot of research time and engagement, complicated measuring equipment and skilled manpower. For the purposes of this study, it was necessary to examine the toxicity of combustion products generated during
engine operation. The internal combustion engine basically works in a wide range of engine speeds (Antoni et al., 2013, Fu et al., 2014). If we add to this the fact that the engine can operate at varying loads (Karthikeya Sharma et al., 2015, Rahman et al., 2015), which also have a relatively wide operating range, it may lead us to a simple conclusion on a practically infinite number of possible combinations and setpoints. However, in the practical use of engines, particularly in the use of motor vehicles, not all combinations of engine speeds and loads are possible (Chen et al., 2016; Yunus Khan et al., 2015). The selection of characteristic setpoints is a very complex process, because it is necessary to know the features of the motor-vehicle-environment system. It means that for the motion of a motor vehicle, two different engines will run at different operating points. In order to obtain the desired setpoints for this experimental research, it was necessary to establish the operating regimes which are of fundamental significance.

Obtaining these interesting points can be done in two different ways. The first is an empirical determination through experiments with real motor vehicles, while the other way would be reserved for retrieving the setpoints via numerical simulations. Specifically, in this paper a numerical simulation was selected for the finding of characteristic operating points of the engine. The carried-out simulations of the internal combustion engine as the drive unit were presented in detail in Dorić Phd thesis. The results of the simulations presented in (Dorić, 2012) were the input parameters for further investigation.

As can be seen from Fig. 2, the operating points are connected to form an operating line. This operating line represents engine regimes during passenger car driving in accordance with the NEDC requirements. It is evident that the largest part of the engine operating regime is reserved for medium speeds and very low loads. The presented figure of engine operation was used in the selection of setpoints for analyzing the toxicity of the engine in experimental testing. It is easy to observe the commonly used operating points during the IC engine
exploitation in urban areas, as can be seen in Fig. 2. These regimes are mostly set at the low levels of load, around 10 to 30% of full load, to be more specific.

Fig. 2. The operating points of IC engine selected in order to meet the power requirements of urban driving (source: Dorić, 2012)

Considering that full engine load is not expected during exploitation of vehicles in urban areas, it can be concluded that full load is not relevant from the viewpoint of this research. Also, it would be unrealistic to expect the toxicity of all operating points through which the engine is running during simulation to be examined. There are many operating points where engine works for very short periods of time. On the other hand, there are many points at which the engine is kept running longer and more frequently passes through them. These points represent the focus of our experimental research.

The main intention of this paper was to quantify the pollution formation of BTEX compounds from a vehicle engine, and the focus of our research was placed on engine regimes that are expected most in the urban exploitation of vehicles. To ensure the reproducibility of the experimental tests, the NEDC was selected as the pattern of driving of passenger cars in urban driving conditions. Based on the results of emission measurements at characteristic operating points of the cycle, the quantities of BTEX compounds emitted have been assessed during the movement of a Fiat Punto Classic (FPC) passenger car in accordance with the NEDC pattern.
2. Materials and methods

During the experimental research, the emission characteristics of a naturally aspirated Oto engine with the specifications given in Table 1 have been investigated, with the purpose of predicting the quantities of BTEX compounds emitted during the movement of FPC passenger car in accordance with the NEDC.

Table 1
Main engine data

<table>
<thead>
<tr>
<th>Engine model</th>
<th>1.1 EFI (Electronic Fuel Injection)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Engine type</td>
<td>In-line, 4-stroke</td>
</tr>
<tr>
<td>Bore and stroke</td>
<td></td>
</tr>
<tr>
<td>Total engine displacement</td>
<td>1.1 L</td>
</tr>
<tr>
<td>Firing order</td>
<td>1-3-4-2</td>
</tr>
<tr>
<td>Compression ratio</td>
<td>10:1</td>
</tr>
<tr>
<td>Valves per cylinder intake/exhaust</td>
<td>1/1</td>
</tr>
<tr>
<td>Aspiration</td>
<td>atmospheric</td>
</tr>
<tr>
<td>Injection system</td>
<td>multipoint</td>
</tr>
<tr>
<td>Peak power @ 6000 RPM</td>
<td>40 kW</td>
</tr>
<tr>
<td>Peak torque @ 3500 RPM</td>
<td>60 Nm</td>
</tr>
<tr>
<td>Engine speed</td>
<td>1000-6000 rpm</td>
</tr>
<tr>
<td>Testing load range</td>
<td>10-50%</td>
</tr>
<tr>
<td>Fuel</td>
<td>Europremium unleaded gasoline</td>
</tr>
<tr>
<td>Emission standard</td>
<td>Euro 4</td>
</tr>
<tr>
<td>Exhaust gas control</td>
<td>TWC (Three-way catalyst)</td>
</tr>
</tbody>
</table>

2.1. Test stand

For this experimental investigation, a special category of ECU (Engine Control Unit), which is programmable in order to achieve different working parameters, has been used. These ECUs do not have a fixed behavior, but can be reprogrammed by the user. The examples include adding or changing the turbocharger, adding or changing the intercooler, changing the exhaust system, and converting to run on alternative fuel. As a consequence of these changes, the ordinary ECU may not provide the appropriate control for the new configuration. In these situations, a programmable ECU can be wired in. These can be programmed or mapped with a laptop connected by a serial or USB cable while the engine is running. The programmable ECU may control the amount of fuel to be injected into each cylinder. This
varies depending on the engine's RPM (Revolutions per Minute) and the position of the accelerator pedal (or the manifold air pressure). The engine tuner can adjust this by bringing up a spreadsheet-like page on the laptop where each cell represents an intersection between a specific RPM value and an accelerator pedal position (or the throttle position, as it is called). In this cell, the number corresponding to the amount of fuel to be injected is entered. This spreadsheet is often referred to as the fuel table or the fuel map. By modifying these values while monitoring the exhausts while using a wide band lambda probe to see if the engine runs rich or lean, the tuner can find the optimal amount of fuel to be injected into the engine at every different combination of RPM and throttle position. This process is carried out at a SCHENCK 230W dynamometer, giving the tuner a controlled environment to work in. An engine dynamometer gives a more precise calibration for racing applications. Tuners often utilize a chassis dynamometer for street and other high performance applications. Another parameter that is mappable and has been used for this article is the closed loop lambda. With the closed loop lambda, the ECU monitors a permanently installed lambda probe and modifies the fueling to achieve stoichiometric (ideal) combustion. On the traditional petrol-powered vehicles this air-fuel ratio is 14.7:1 (Colls, 2002; Liu et al., 2015; Wang et al., 2015).

The schematic layout of the experimental equipment used to define BTEX compounds emission model is shown in Fig. 3.

**Fig. 3.** The schematic layout of the experimental setup: 1, engine; 2, dynamometer; 3, dynamometer controller; 4, high-speed data acquisition board; 5, pressure transducer; 6, Voyager Mobile GC; 7, ECU; 8, computer 1; 9, computer 2.
2.2. Measurements of BTEX concentrations

The target compounds have been analyzed in exhaust gas samples by the Perkin Elmer Photovac Voyager-mobile GC. The Voyager uses the principles of gas chromatography (GC) to separate and identify volatile organic compounds. The Voyager mobile GC employs a unique set of analytical columns and preprogrammed temperatures and flow rates to optimize the separation of complex VOC mixtures found in exhaust gases. The sample components become separated from one another as they are carried through the column due to the differences in their rates of interaction with the sorptive material. For the separation of sample components the Supelcowax10-Polyethylene glycol (PEG) column has been used.

In order to accurately quantify the target compounds, before each sampling set calibration of the Voyager has been carried out using the authentic Messer Techogas standard of BTEX gases prepared in Ultra Zero nitrogen as a balance gas. The concentrations of all BTEX compounds in the prepared gas standard were approximately 1 vol. ppm (benzene 1.02 ± 0.100, toluene 0.945 ± 0.095, ethylbenzene 0.988 ± 0.099, m-xylene 0.958 ± 0.096, p-xylene 0.979 ± 0.098 and o-xylene 0.964 ± 0.096). During the calibration process, the Tedlar bag, filled with the prepared gas standard, is connected to the Voyager using the gas bag adapter. The built-in pump of the Voyager during 20 s takes sufficient quantity of the sample at the pressure of 1 atm (101325 Pa). As the compounds elute from the column, they are detected by the photoionization detector (PID). A triangle-shaped peak results for each compound whose integrated area under the peak is proportional to the concentration of the compound. The onboard microprocessor of the Voyager converts the area into parts-per-million or parts-per-billion. A plot of the detector response versus time results in a chromatogram, where the retention time of each peak indicates an individual compound’s identity and the area under the peak indicates its concentration. The chromatogram of the calibration standard is stored in the Voyager’s library, which contains the retention time, peak area and concentration of each compound.
target analyte. The ratio of peak area to concentration represents the compound’s sensitivity.

When an unknown sample is run, peak retention times are compared to the retention times of the library compounds. If they match within the specified window, the peak is identified as the corresponding compound of interest. The peak area is then divided by the sensitivity of that compound to determine its concentration.

Ideally, each compound will be retained in the column for a different period of time, having a unique retention time (benzene 284.3 s, toluene 482.0 s, ethylbenzene 825.1 s, p.m-xylene 854.4 s and o-xylene 1105.0 s). Due to the difficulties in resolving the chromatography peaks, the results for m-xylene and p-xylene are represented as a sum. The limit of detection (LOD) of the applied method is 0.01 ppm.

Before conducting the experimental procedures of measuring the BTEX concentrations in exhaust gases of IC engine, proper values of the operating points during driving in urban areas were defined. A simulation has been performed in order to achieve the values of vehicle speed from the NEDC, which are described in Figure 1. After choosing the powertrain, defining the motor vehicle type and the velocity profile it became possible to calculate the engine speed. These values are clearly defined areas in which the engine operates during exploitation in the city and outside the city run. The velocity profile which is used when driving a motor vehicle under the conditions of NEDC has been taken as an input parameter of the simulation. The conventional aspirated gasoline engine was adopted as the drive unit. This engine was also used in the experimental research. In addition to the chosen engine, an adequate transmission system and the necessary tires were selected, as well as the coefficient of drag, the vehicle’s weight and other essential parameters. The engine speed-time dependence during movement of the FPC passenger car in accordance with the NEDC is shown in Fig. 4.
The characteristic operating points have been defined in accordance with the fact that a passenger car in urban driving moves in conditions of low and medium levels of engine load. This parameter had a constant value of 10% during our experimental measurements. The value of the lambda factor was maintained at the value of 1 by using the lambda probe in order to achieve optimal conditions for the combustion of fuel-air mixture. The stoichiometric ratio ($\lambda=1$) corresponds to the mass of air needed to completely oxidize a mass of fuel, namely 14.7 g of air for 1g of fuel (Colls, 2002; Liu et al., 2015; Wang et al., 2015). The speed of the experimental engine was varied in the range from 950 to 4000 rpm. Based on the engine speed-time dependence, the operating points that correspond to the conditions of stoichiometric mixture ($\lambda = 1$) and low load (10%) have been defined. Commercial Euro premium unleaded gasoline, has been used as motor fuel. After defining the characteristic operating points, measurements of concentration levels of BTEX compounds were carried out in controlled conditions. The sampling of exhaust gases has been conducted on an experimental engine exhaust pipe in order to determine the concentration levels of BTEX compounds in the mixture of exhaust gases. The sampling process lasted for 20 seconds, and the analysis of each portion of the exhaust gas lasted 20 minutes.
2.3. Predicting the amount of BTEX compounds emitted during the NEDC

In order to predict the amount of BTEX compounds emitted during the corresponding driving cycle, the dominant factor to be considered is the fuel combustion as the primary source of BTEX emissions into the atmosphere. To overcome the resistance to movement at any speed, the drive wheels require adequate power ($P = F \cdot v$). Bringing power over a period of time means spending a certain amount of energy for the realization of that power ($P = \frac{dE}{dt} \Rightarrow E = \int P \cdot dt$). The primary source of the energy of motion of a passenger car is fuel, the internal energy of which is transformed into the mechanical one inside the engine. The given engine energy enables the vehicle to overcome the resistance to movement. Fuel consumption on a road section depends primarily on the total energy required to overcome the resistance to movement in that section. Considering the type of resistance, the total energy depends on the parameters of the vehicle and the ground, their interactions and the conditions in which the vehicle is moving. Based on the relationship between energy and power, the expression for the total energy required for the movement of vehicles on a given road section at the given conditions can be reached by:

$$P_T = \frac{dE}{dt} \Rightarrow E = \int_0^T P_T(t) \cdot dt$$  \hspace{1cm} (1)

where:

- $E$ – the energy required for the movement of the vehicle in the time interval $T$
- $P_T$ – the power required for the drive wheels (generally changes over time with the changing modes of movement and external conditions)

Considering the fact that the power required on the wheels must be equal to the total sum of the partial power required to overcome the individual components of the resistance to movement, the same relation can be applied to energy:
\[ E = E_f + E_{ar} + E_{py} + E_a = \int_0^T P_f(t) \cdot dt + \int_0^T P_{ar}(t) \cdot dt + \int_0^T P_{IN}(t) \cdot dt + \int_0^T P_a(t) \cdot dt \tag{2} \]

where:

326 \( E_f \) – the energy required to overcome the rolling resistance

327 \( E_{ar} \) – the energy required to overcome air resistance

328 \( E_{IN} \) – the energy required to overcome the resistance of inertia (kinetic energy)

329 \( E_a \) – the energy required to overcome the resistance of the rise/climb

330 Considering that \( P = F \cdot v \), and taking into the account the expressions for calculating specific movement resistances \( (F_f, F_w, F_{IN}, F_a) \), the expressions for the partial energy spent for their overcoming can be reached.

331 The energy required to overcome the rolling resistance:

\[ E_f = f \cdot G \cdot \int_0^T v \cdot dt = f \cdot G \cdot S \tag{3} \]

332 where:

333 \( S \) – the total distance traveled \( S = \int_0^T v \cdot dt \)

334 \( G \) - gravitational force \((9.81 N \cdot kg^{-1})\)

335 \( f \) - the coefficient of rolling resistance

336 \( v \) - vehicle speed

337 The energy spent for overcoming the rolling resistance is linearly proportional to the force of the rolling resistance \( (F_t = F \cdot G) \) and the length of distance. Different types of pneumatics have different values of coefficient \( f \). The approximate values of the coefficient \( f \) on a hard surface are:
\( f_0 = 0,01 \) – for passenger cars

\( f_0 < 0,01 \) – for commercial vehicles (Clark and Dodge, 1979; Holmberg et al., 2012)

The energy required to overcome the air resistance:

\[
E_w = \frac{1}{2} \cdot \rho \cdot C_w \cdot A \cdot \int_0^T v^3 \cdot dt = \frac{1}{2} \cdot \rho \cdot C_w \cdot A \cdot v^2 \cdot S
\]  

(4)

where:

\( \rho \) - the density of air

\( C_w \) - the empirical air resistance-drag coefficient

\( A \) - the frontal area of the vehicle

The energy required to overcome the resistance of inertia:

\( v(0) \Rightarrow E_{IN} = \Delta E_K = \frac{m \cdot v^2}{2} \)  

(5)

Where \( m \) represents the total mass of the vehicle, including the driver.

The energy required to overcome the resistance of inertia of the vehicle during acceleration is equal to the kinetic energy to be submitted to the vehicle. Parts of the cycle, in which the speed is increased, therefore, contribute to an increase in fuel consumption, in proportion to the weight of the vehicle.

The energy required to overcome the resistance of the climb:

\[
E_\alpha = G \cdot \sin \alpha \int_0^T v \cdot dt = G \cdot \sin \alpha \cdot S = G \cdot H
\]

(6)

where:

\( H = S \cdot \sin \alpha \) – the height of climbing

The energy consumed in overcoming the resistance of the climb is linearly proportional to the vehicle weight \( G \) and the height of climbing \( H \).
3. Results and discussion

Based on the results of BTEX emission measurements in controlled experimental conditions, the concentration profiles of BTEX compounds that are emitted during movement of the FPC passenger car in accordance with the NEDC driving pattern have been defined.

Table 2 shows the results of BTEX compound concentration measurements at different RPMs of the experimental engine under the conditions of low engine load and adjusted stoichiometric ratio in air-fuel mixture. The measurements were carried out five times under the same conditions, and all results were averaged over the five measurements.

### Table 2
The results of BTEX compound concentration level measurements at different RPMs

<table>
<thead>
<tr>
<th>RPM</th>
<th>10% engine load</th>
<th>Mean</th>
<th>SD</th>
<th>min</th>
<th>max</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>950 rpm</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Benzene (ppm)</td>
<td>16.5</td>
<td>0.645755</td>
<td>15.8</td>
<td>17.3</td>
<td></td>
</tr>
<tr>
<td>Toluene (ppm)</td>
<td>55.2</td>
<td>4.852007</td>
<td>49.95</td>
<td>62.3</td>
<td></td>
</tr>
<tr>
<td>Ethylbenzene (ppm)</td>
<td>11.6</td>
<td>2.279693</td>
<td>8.2</td>
<td>14.3</td>
<td></td>
</tr>
<tr>
<td>m,p-xylene (ppm)</td>
<td>44.3</td>
<td>5.008792</td>
<td>38.3</td>
<td>51.6</td>
<td></td>
</tr>
<tr>
<td>o-xylene (ppm)</td>
<td>12.6</td>
<td>3.621567</td>
<td>9.7</td>
<td>17.9</td>
<td></td>
</tr>
<tr>
<td>1500 rpm</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Benzene (ppm)</td>
<td>19.8</td>
<td>3.734157</td>
<td>16.3</td>
<td>25.5</td>
<td></td>
</tr>
<tr>
<td>Toluene (ppm)</td>
<td>50.7</td>
<td>14.76257</td>
<td>34.74</td>
<td>73.0</td>
<td></td>
</tr>
<tr>
<td>Ethylbenzene (ppm)</td>
<td>10.2</td>
<td>3.672073</td>
<td>6.62</td>
<td>15.2</td>
<td></td>
</tr>
<tr>
<td>m,p-xylene (ppm)</td>
<td>37.3</td>
<td>3.731019</td>
<td>33.85</td>
<td>43.2</td>
<td></td>
</tr>
<tr>
<td>o-xylene (ppm)</td>
<td>11.3</td>
<td>5.697105</td>
<td>4.2</td>
<td>17.2</td>
<td></td>
</tr>
<tr>
<td>2000 rpm</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Benzene (ppm)</td>
<td>22.4</td>
<td>0.215058</td>
<td>22.1</td>
<td>22.7</td>
<td></td>
</tr>
<tr>
<td>Toluene (ppm)</td>
<td>37.9</td>
<td>1.783255</td>
<td>35.4</td>
<td>40.2</td>
<td></td>
</tr>
<tr>
<td>Ethylbenzene (ppm)</td>
<td>9.0</td>
<td>1.091155</td>
<td>7.80</td>
<td>10.5</td>
<td></td>
</tr>
<tr>
<td>m,p-xylene (ppm)</td>
<td>31.2</td>
<td>2.68235</td>
<td>28.0</td>
<td>34.3</td>
<td></td>
</tr>
<tr>
<td>o-xylene (ppm)</td>
<td>10.1</td>
<td>0.815853</td>
<td>8.80</td>
<td>10.8</td>
<td></td>
</tr>
<tr>
<td>2500 rpm</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Benzene (ppm)</td>
<td>25</td>
<td>0.960234</td>
<td>23.93</td>
<td>26.48</td>
<td></td>
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<tr>
<td>Toluene (ppm)</td>
<td>42.8</td>
<td>4.836838</td>
<td>39</td>
<td>51</td>
<td></td>
</tr>
<tr>
<td>Ethylbenzene (ppm)</td>
<td>7.951</td>
<td>0.204775</td>
<td>7.659</td>
<td>8.2</td>
<td></td>
</tr>
<tr>
<td>m,p-xylene (ppm)</td>
<td>26.000</td>
<td>2.768429</td>
<td>22.2</td>
<td>30</td>
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<tr>
<td>o-xylene (ppm)</td>
<td>9.001</td>
<td>0.34886</td>
<td>8.41</td>
<td>9.301</td>
<td></td>
</tr>
<tr>
<td>3000 rpm</td>
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<td></td>
</tr>
<tr>
<td>Benzene (ppm)</td>
<td>25.5</td>
<td>4.919477</td>
<td>20.5</td>
<td>31.2</td>
<td></td>
</tr>
<tr>
<td>Toluene (ppm)</td>
<td>37.9</td>
<td>1.783255</td>
<td>35.4</td>
<td>40.2</td>
<td></td>
</tr>
<tr>
<td>Ethylbenzene (ppm)</td>
<td>9.0</td>
<td>1.091155</td>
<td>7.8</td>
<td>10.51</td>
<td></td>
</tr>
<tr>
<td>m,p-xylene (ppm)</td>
<td>31.2</td>
<td>2.68235</td>
<td>28</td>
<td>34.3</td>
<td></td>
</tr>
<tr>
<td>o-xylene (ppm)</td>
<td>10.1</td>
<td>0.815853</td>
<td>8.8</td>
<td>10.8</td>
<td></td>
</tr>
<tr>
<td>3500 rpm</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Benzene (ppm)</td>
<td>31.2</td>
<td>3.706885</td>
<td>24.64</td>
<td>33.52</td>
<td></td>
</tr>
<tr>
<td>Toluene (ppm)</td>
<td>34.3</td>
<td>3.497244</td>
<td>28.351</td>
<td>37.093</td>
<td></td>
</tr>
<tr>
<td>Ethylbenzene (ppm)</td>
<td>5.875</td>
<td>0.322885</td>
<td>5.345</td>
<td>6.143</td>
<td></td>
</tr>
<tr>
<td>m,p-xylene (ppm)</td>
<td>19.5</td>
<td>6.255953</td>
<td>13.1</td>
<td>29.3</td>
<td></td>
</tr>
<tr>
<td>o-xylene (ppm)</td>
<td>6.655</td>
<td>1.959352</td>
<td>4.51</td>
<td>9.82</td>
<td></td>
</tr>
</tbody>
</table>
### 4000 rpm

<table>
<thead>
<tr>
<th>Compound</th>
<th>Concentration (ppm)</th>
<th>Number of Data Points</th>
<th>Minimum</th>
<th>Maximum</th>
</tr>
</thead>
<tbody>
<tr>
<td>Benzene</td>
<td>35.5</td>
<td>5.61917</td>
<td>26.08</td>
<td>40.03</td>
</tr>
<tr>
<td>Toluene</td>
<td>31</td>
<td>5.82648</td>
<td>22.45</td>
<td>36.74</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>3.84</td>
<td>3.006884</td>
<td>1.04</td>
<td>8.75</td>
</tr>
<tr>
<td>m,p-xylene</td>
<td>12.2</td>
<td>5.842181</td>
<td>6.98</td>
<td>19.2</td>
</tr>
<tr>
<td>o-xylene</td>
<td>4.8</td>
<td>2.129641</td>
<td>2.52</td>
<td>7.98</td>
</tr>
</tbody>
</table>

The literature data point to the fact that BTEX accounts for roughly 95% of total VOCs emitted by the engine. In addition, toluene dominates (40–50%) all VOC emissions (Agarwal et al., 2015). The results of the quantification of BTEX compounds in the exhaust gas stream point to the domination of toluene emissions at almost all operating points (Fig. 5).

The results obtained from the experimental measurements point to a trend of decrease in concentration levels of almost all compounds of the BTEX group, except benzene. Namely, increasing the engine speed and therefore the piston speed increases the turbulence intensity of the flame during combustion (Brequigny et al., 2016). With higher RPM values, higher temperatures in the combustion chamber of IC engines are reached (Heywood, 1988; Kilicarslan and Qatu, 2017), which enables a more complete combustion of fuel under the conditions of sufficient amounts of oxygen, which is supplied by the wide lambda probe. The increase in concentration levels of benzene in the exhaust gas stream, together with higher
RPM, can be explained by simultaneous reaching of optimal conditions for the hydro-dealkylation of toluene and xylene to benzene at higher temperatures (Rabinovich and Maslyanskii, 1973; Alibeyli et al., 2003; ATSDR, 2007). In this way, at the expense of disappearance of a part of higher aromatics, there comes to a benzene formation in the exhaust gas stream. In their research for Ford Motor Company, Kaiser and associates demonstrated that pure toluene fuel generates a substantial amount of benzene emissions. This conversion contributes to the benzene enrichment in the exhaust gas stream since gasoline normally contains appreciable toluene and other higher aromatics (Kaiser, 1992). This confirms that dealkylation of substituted benzenes is a significant source of benzene emission.

By using the results of emission and concentration levels of BTEX compound measurements in characteristic operating points of the NEDC cycle, the concentration profiles of BTEX compounds have been defined in accordance with the energy requirements and fuel consumption during movement of the FPC passenger car in accordance with the given movement pattern.

In defining the concentration profiles we took on the zero emission in the parts of the cycle in which there are minimal energy requirements for the movement of the automobile, hence also minimal fuel consumption. Those are the stop periods, as well as the periods of deceleration during the NEDC.

The concentration profiles, defined based on the measurements of BTEX compound concentrations at different RPMs of the experimental engine, are shown in Fig. 6 a-e:
The concentration profiles, defined based on the data of BTEX compound emissions during different experimental engine operating regimes, have been used as the basis for the defining of the emission model. The emission model has been defined based on the energy requirements of the FPC passenger car during movement in accordance with the NEDC driving pattern. As a result of the emission model, the quantities of the BTEX compounds emitted have been determined. The FPC passenger car uses a 1.1 EFI engine, the emission characteristics of which have been bench-tested.

3.1. BTEX emission model

Fuel consumption has a dominant influence on the quantities of BTEX compounds emitted during the driving cycle. It is mainly dependent on engine speed, engine power, and air-to-fuel ratio. The engine power needed for the movement of a passenger car in accordance with the NEDC pattern is calculated as the sum of total tractive power requirement at the wheels and engine power requirement for accessories, such as air conditioning. The tractive power is gained by the sum of inertial driving resistance, rolling resistance, and air drag resistance. These terms depend on vehicle characteristics and on vehicle speed and acceleration.
The tailpipe emission rates for BTEX compounds in this paper are modeled as the fraction of the engine-out emission rates that leave the catalytic converter. The parameters used in calculations are shown in the Table 3.

### Table 3
The technical characteristics of the FPC passenger car and parameters required for the calculation

<table>
<thead>
<tr>
<th>Technical characteristic</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total vehicle weight [kg]</td>
<td>950</td>
</tr>
<tr>
<td>$c_w$ – the empirical air resistance coefficient</td>
<td>0.30</td>
</tr>
<tr>
<td>$A$ – the frontal area of the vehicle [m$^2$]</td>
<td>1.85</td>
</tr>
<tr>
<td>$f$ – the coefficient of rolling resistance</td>
<td>0.01</td>
</tr>
<tr>
<td>$\rho$ – the density of air [kg/m$^3$]</td>
<td>1.2</td>
</tr>
</tbody>
</table>

Taking into the account the technical characteristics of the FPC passenger car, given in the Table 3, the amount of energy required for the moving of the vehicle according to the NEDC pattern has been calculated. The energy requirements are shown in Fig. 7. Within the calculations, the component of overcoming the resistance of the climb has been neglected, since the focus of the assessment of the emitted concentrations of BTEX compounds is on largest European cities, the topography of which enables neglecting the aforementioned resistance component.

![Fig. 7](image) The energy requirement of the FPC passenger car during movement in accordance with the NEDC pattern

According to the simulation results, the specific fuel consumption in (g/kWh) during the NEDC for the FPC has been calculated. The results of the simulation are shown in Fig. 8.

![Fig. 8](image)
474 Fig. 8. The specific fuel consumption during the NEDC for the FPC

475 Based on the energy requirements for the movement of the FPC passenger car in accordance
476 with the NEDC pattern, and specific fuel consumption, the required fuel mass for moving in
477 accordance with the aforementioned pattern has been calculated. The results of the calculation
478 are shown in the Fig. 9.

482 Fig. 9. The required fuel mass for moving in accordance with NEDC for the FPC

485 Air consumption during the NEDC is obtained from the condition that for the combustion of
486 1g of fuel it is necessary to spend 14.7 g of air in stoichiometric conditions. The necessary
487 amount of air for the movement of FPC during NEDC cycle is shown in Fig. 10.
Fig. 10. The necessary mass of air for the movement of FPC during NEDC

The total amount of gas in the exhaust (n) formed during the combustion of fuel represents the sum of the quantities of burned fuel ($n_{fuel}$) and air spent ($n_{air}$) for the burning of stoichiometric air-fuel mixture:

$$n = n_{fuel} + n_{air}$$  \hspace{1cm} (7)

Considering the air-fuel mixture as an ideal gas, the volume of the exhaust gas can be calculated by using the Clapeyron equation:

$$V = \frac{nRT}{p}$$  \hspace{1cm} (8)

where:

- $n$- total amount of gas in the exhaust (mol)
- $V$- volume of exhaust gases ($m^3$)
- $R$- universal gas constant (8,314 J/molK)
- $T$- the average temperature of exhaust gases (600°C, 873°K)
- $p$- the pressure of sampled exhaust gases (101325 Pa)

The exhaust gas volume emitted during the NEDC, calculated by using the equation 8, is shown in Figure 11.
Based on the concentration dependences (Fig. 6. a-e) and fuel consumption during the NEDC of the FPC passenger car and exhaust gas volume - time dependence (Fig. 11.), the volumes of target BTEX compounds can be calculated by using equation 9.

\[
V_{B,T,E,X} = \frac{C_{B,T,E,X} \cdot V}{10^6}
\]  \hspace{1cm} (9)

where:

- \( V_{B,T,E,X} \) - volume of the target BTEX compound: benzene, toluene, ethylbenzene or xylene (m\(^3\))
- \( C_{B,T,E,X} \) - concentration of the target BTEX compound: benzene, toluene, ethylbenzene or xylene (ppm)
- \( V \) - volume of exhaust gases (m\(^3\))

The masses of the BTEX compounds emitted during the NEDC have been calculated by using the equation 10:

\[
m_{B,T,E,X} = \frac{p \cdot V_{B,T,E,X} \cdot M_{B,T,E,X}}{RT}
\]  \hspace{1cm} (10)

where:

- \( m_{B,T,E,X} \) - mass of the target BTEX compound: benzene, toluene, ethylbenzene or xylene (g)
$M_{B,T,E,X}$ - molar mass of the target BTEX compound: benzene, toluene, ethylbenzene or xylene (g/mol)

$V_{B,T,E,X}$ - volume of the target BTEX compound: benzene, toluene, ethylbenzene or xylene (m$^3$)

$R$ - universal gas constant (8,314 J/molK)

$T$ - the average temperature of exhaust gases (600°C, 873°K)

The masses of the BTEX compounds emitted during the NEDC are shown in Fig. 12. (a-e).
Fig. 12. The masses of BTEX compounds emitted during the NEDC

After completing the experimental testing and implementation of results in the appropriate movement model based on the NEDC pattern, the results of the total masses of BTEX compounds emitted are presented in the Table 4. Taking into the account the fact that the theoretical distance traveled during one cycle based on the NEDC pattern is 11023m, the mass of BTEX components emitted on 100 km can easily be calculated, as well as specific emissions in g/km in accordance with the adopted pattern of movement.
According to the official statistics data dated from 14th March 2014 in Serbia there have been registered 1770206 passenger cars, and approximately 40% of the total number use gasoline as motor fuel, i.e. 708082 (SORS, 2014). Considering the fact that in Serbia there are no exact data on the number of annual kilometers per car traveled, European commission data for the assessment of the BTEX compounds emitted on a yearly level have been used in this paper (Nemry et al., 2008). Namely, motor fuel passenger cars in Europe travel 16500 km a year, which means that a passenger car emits 676.5 g of benzene annually. In regard to the data in Serbia, that would amount to 479 t of benzene on a yearly level. We are talking about an extremely high quantity of group I carcinogenic substance, and considering the fact that for the carcinogen effects there are no small or safe doses, there is no threshold. It is supposed that the carcinogen effect occurs at any dose applied. This assumption is based on the knowledge of the biological evolution of cancer. All that is needed is a single molecule of a toxic substance to change a cell, giving it the possibility to develop itself into cancer. The development of cancer is a multi-step process which occurs over many years (Tanaka et al., 2013; Ibuki and Goto, 2004). As the dose (the concentration) grows, so does the risk, i.e. the possibility, of cancer development.

The estimated quantities of emissions for other components of the BTEX group are shown in Table 5.
Table 5

The estimated quantities of BTEX compounds emitted in Serbia per car annually

<table>
<thead>
<tr>
<th>Compound</th>
<th>The specific emission [g/km]</th>
<th>per car annually [g]</th>
<th>total emission annually [t]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Benzene</td>
<td>0.0410</td>
<td>676.5</td>
<td>479</td>
</tr>
<tr>
<td>Toluene</td>
<td>0.0776</td>
<td>1280.4</td>
<td>906</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>0.0175</td>
<td>288.75</td>
<td>204</td>
</tr>
<tr>
<td>m,p-xylene</td>
<td>0.0592</td>
<td>976.8</td>
<td>691</td>
</tr>
<tr>
<td>o-xylene</td>
<td>0.0194</td>
<td>320.1</td>
<td>226</td>
</tr>
</tbody>
</table>

4. Conclusion

The simulation in the field of IC engines and motor vehicles today represents a sophisticated world-recognized tool for solving complex problems in the area of defining emission characteristics. The modeling of the motor vehicle emissions via simulations significantly reduce the time that is normally needed for extensive experiments and prototypes, because these simulations can perform predictions of a large number of experiments. One such model can be used later for numerous studies where in many cases the high costs of engine testing can be avoided. It would be unrealistic to say that numerical calculation can completely replace test bench, but with validation, for example, of several working points and defining the motor model in accordance with the proven results, accurate results in other operating points can be expected. Experimental investigation, conducted within this paper, was used to define the most important engine operating points, where the engine works most of the time. In this way, the unnecessary experiments were avoided, i.e. setpoints that do not occur during engine exploitation of motor vehicles in urban driving conditions. In this way, the investigation which leads to the loss of valuable time on the analysis of toxicity of unnecessary operating points can be avoided.

The developed model enables the BTEX compound emissions to be predicted based on the exhaust gas analyses of different types of passenger cars at characteristic operating points of
the driving cycle. Besides that, contributory aspects like load, road gradient, gearshift strategies should be also included. Such a model shall be, thus, significantly more flexible than the existing approaches and would be especially useful for assessment of the local studies (i.e. the impact of traffic management schemes, the change of driving behavior, etc).

Acknowledgement:

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References


Dorić, J. 2012. Unapređenje efektivnosti motora SUS primenom nekonvencionalnog klipnog mehanizma. (Improving the efficiency of the IC engine by applying an unconventional piston mechanism), PhD Thesis, Faculty of Technical Sciences, University of Novi Sad, Serbia (in Serbian)


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