MATHEMATICAL MODEL OF THE EMISSIONS OF A SELECTED VEHICLE

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SHRNUTÍ

Článek se zabývá kvantifikací emisí z benzínových motorů během dynamických režimů. Hlavními sledovanými emisemi jsou oxid uhelnatý a oxid uhličitý. Výsledkem je matematický model popisující produkci jednotlivých složek emisí ve všech režimech (statických i dynamických). Článek popisuje také postup pro stanovení emisí z provozních parametrů motoru. Výsledky jsou porovnány s jinými možnými způsoby zjištění produkce emisí.

KLÍČOVÁ SLOVA: EMISE, DYNAMICKÝ REŽIM, NEPŘÍMÁ METODA, MÍRA TRANSIENTNOSTI

ABSTRACT

The article addresses the quantification of exhaust emissions from gasoline engines during transient operation. The main targeted emissions are carbon monoxide and carbon dioxide. The result is a mathematical model describing the production of individual emissions components in all modes (static and dynamic). It also describes the procedure for the determination of emissions from the engine's operating parameters. The result is compared with other possible methods of measuring emissions. The methodology is validated using the data from an on-road measurement. The mathematical model was created on the first route and validated on the second route.

KEYWORDS: EMISSIONS, TRANSIENT MODE, INDIRECT METHOD, TRANSIENT RATE

1. INTRODUCTION

The monitoring of the actual emissions of road vehicles during operation is important for reviewing the effectiveness of emissions control measures. One key control measure has been vehicle exhaust legislation. Legislated emission standards are defined over a synthetic laboratory driving cycle. However, real-world driving is more variable than that during the official New European Driving Cycle, with higher speeds and accelerations. [1]

The emissions and fuel consumption of light-duty vehicles have to be tested using prescribed cycles in order to be type-approved. This type-approval data is used to inform the customer and also serve as an input for models that predict the share of transportation in overall energy usage and production of emissions. However, several studies have shown that the type-approval data is not representative of real-world usage, because the current EU test cycles were not derived from real world in-use data and are not sufficiently dynamic. [2]

Nitrogen oxide emissions of modern light-duty diesel vehicles can be up to four times higher than type approval data [3, 4] and fuel consumption can be underestimated by up to 20% [5]. Variability in real-world tailpipe emissions for a given vehicle during its operation is associated with speed, acceleration, and road grade [6 – 8], which are used to determine the Vehicle Specific Power (VSP) [9 – 11]. The U.S. Environmental Protection Agency's Motor Vehicle Emission Simulator (MOVES) model uses second-by-second speed, acceleration, and road grade to calculate VSP [12]. Currently, there is no standard procedure for quantifying road grade on a second-by-second basis from a moving vehicle. [13]

There are two basic options for monitoring vehicle emissions under real-world driving conditions – a direct method, using a portable emissions analyser or remote optical sensing, and an indirect method, using engine operating parameters and measured emission maps.

Portable Emissions Measurement Systems (PEMS) are used to measure real-world tailpipe concentrations of carbon dioxide (CO₂), carbon monoxide (CO), hydrocarbons (HC), oxides of nitrogen (NO_x) and particulate matter (PM).

The indirect method uses measured emission maps on motor stands and engine speed and load, [14] but this method does not account for transients.

The main purpose of this article was to determine the relationship between the production of CO and CO₂ emissions and the operating parameters of the vehicle. The measurement was performed under laboratory conditions and a mathematical model has been presented from the measured values.

2. MATERIALS AND METHODS

Measurements were performed in the laboratory of the Department of Vehicles and Ground Transport of the Czech University of Life Sciences Prague. The measurement was performed on a three-cylinder gasoline engine, the basic characteristics of which are given in Table 1.

TABLE 1: Basic engine characteristics

TABULKA 1: Popis motoru

Engine code	AWY
Construction	Three cylinder in row
Compression ratio	10.3 : 1
Max power	40 kW @ 4750 1/min
Max torque	106 Nm @ 3000 1/min
ECU (engine control unit)	Simos 3PD (multipoint injector)
Fuel	Petrol

TABLE 2: Basic dynamometer characteristics.

TABULKA 2: Popis dynamometru.

Dynamometer	
Type	V125
RPM	300 – 2500 – 8000 1/min
Torque	134 – 478 – 149.5 Nm
Power	4.2 – 125 – 125 kW
Strain Gauge	
Nominal load	2 kN
Culminated error	0.5% of n.l.
Reproducibility	0.05%

The engine was connected to an eddy current dynamometer (technical parameters given in Table 2) on an engine test bench. The dynamometer allows simulation of different operating modes of the engine. Engine and dynamometer were connected and controlled using the Control Web software application (Moravian Instruments Inc.). This system allows remote control of the engine (simulation of accelerator pedal position to change the engine speed) and of the dynamometer (actuating current to change the engine load).

The instantaneous fuel consumption was measured by a WF005 in-line flow meter (Figure 1) with an output of 1800 pulses per liter of fuel.

The calculated production of CO₂ was checked using formula 1 for calculation of fuel consumption. Due to the unknown chemical composition of the fuel and its density, the fuel

FIGURE 1: Connecting the flow meter to the fuel system.

OBRÁZEK 1: Zapojení průtokoměru do palivového systému.

FIGURE 2: Fuel tank on scales.

OBRÁZEK 2: Palivová nádrž na plošinové váze.

consumption was further measured on a mass basis with a platform scale (SOEHNLE, see Figure 2) on which the fuel tank was placed. The scale precision of 2 g was not sufficient for determining the instantaneous fuel consumption, but acceptable for determining the total fuel consumption during the entire cycle.

$$mFUEL = \frac{mCO_2}{3,11} \quad (1)$$

where: $mFUEL$ weight of fuel consumed (g)
 mCO_2 mass production of CO_2 (g)
 3,11 ratio of molecular weights of CO_2 and fuel (gasoline commercial grade)

Engine speed, engine load, intake air temperature and intake air pressure, necessary for further calculations, were obtained from the ECU (Engine Control Unit) with a VAG-COM diagnostic system and VCDS software (Figure 3).

FIGURE 3: Software VCDS.

OBRÁZEK 3: Software VCDS.

Concentrations of hydrocarbons, carbon monoxide, carbon dioxide, nitrogen oxides and oxygen were measured by a PEMS emissions analyzer that evaluates emissions with a frequency of 1 Hz. This involves analysis of exhaust gases based on direct measurements of physical and chemical properties of the monitored emissions components (CO , CO_2 , HC – NDIR method, O_2 , NO_x – an electrochemical cell). Results are obtained on a volume basis (% , ppm). To obtain the mass production of emissions, a conversion is required (formulas 2 and 3) using values obtained from the ECU. [14]

$$Q_{mv} = \frac{28,96 \cdot \left(p_s - \frac{p_{atm}}{\epsilon} \right) \cdot V_z \cdot \eta_d \cdot n}{600 \cdot i \cdot R \cdot T_{vzd}} \quad (2)$$

where: Q_{mv} the amount of air aspirated by engine ($g \cdot s^{-1}$)
 28,96 molar mass of air ($g \cdot mol^{-1}$)
 p_s intake pressure (mbar)
 p_{atm} atmospheric pressure (mbar)
 ϵ engine compression ratio (1)
 V_z engine capacity (dm^3)
 η_d engine volumetric efficiency (1)
 n engine speed (min^{-1})
 600 constant conversion units (1)
 i constant depending on engine type, $i = 1$ for two-stroke engine, $i = 2$ for four-stroke engine (1)
 R universal gas constant ($J \cdot mol^{-1} \cdot K^{-1}$), for an ideal gas $R = 8,314$
 T_{vzd} intake air temperature (K)

$$M_i = \frac{\left(\frac{Q_{mv}}{28,96} + \frac{Q_{mp}}{14,17} \right) \cdot C_i}{100} \cdot Q_i \quad (3)$$

where: M_i mass production of components of emissions ($g \cdot s^{-1}$)
 Q_{mv} the amount of air aspirated by engine ($g \cdot s^{-1}$)
 Q_{mp} the amount of fuel supplied to the engine ($g \cdot s^{-1}$)
 C_i concentration of one emission component in exhaust gas (%)
 28,96 molar mass of air ($g \cdot mol^{-1}$)
 14,17 molar mass of fuel ($g \cdot mol^{-1}$), while the composition $C_{1,1,89}O_{0,016}$
 Q_i molecular weight of one emission component in exhaust gas ($g \cdot mol^{-1}$)

2.1 RATE OF TRANSIENT CO_2 EMISSION

This indirect method uses the relationships between the production of emissions and engine operating parameters (RPM, load, change of RPM, change of load). In addition to these parameters, the change in emissions is reflected during transient modes. However, it is necessary to determine the relationship between the engine operating parameters and emissions. For these engine operating parameters it is essential to find a single value which reflects the strength of influence of each engine parameter. This value will be referred to as a transient rate.

A transient rate is specified as a ratio of engine operating parameters (RPM and load) that correlates best with the mass production of one specific emission component. Besides the speed and engine load it is further vital to reflect the rate of change of these values. For all of these values (RPM, change of RPM, load, change of load) it is necessary to find such factors in which the correlation coefficient between the transient rate and mass production of emissions will be as close as possible to 1. These coefficients can be determined using an appropriate

software tool, e.g. MS Office with add-in Solver. Each emission component has different coefficients. The transient rate for CO₂ emission has been determined for the measured engine as:

$$MT = 2,23 \cdot n + 100 \cdot M_t + 1,4 \cdot (n_2 - n_1) + 119 \cdot (M_{t2} - M_{t1}) \quad (4)$$

where: MT transient rate (1)
 n instantaneous engine speed (min⁻¹)
 M_t instantaneous engine load (%)
 $(n_2 - n_1)$ changing of engine speed (min⁻¹)
 $(M_{t2} - M_{t1})$ change of engine load (%)
 2,23, 100, 1,4 and 119 coefficients calculated with add-in Solver (1)

The engine load level from the ECU has been used for the calculation of the transient rate. In this case (the engine on a test bench), the engine has been constantly loaded with the dynamometer's resistance. In addition, the engine was also loaded with the usual vehicle components such as an alternator, a coolant pump, etc. The total engine load is about 15 Nm.

To determine the instantaneous emissions during road operation it is sufficient to read engine speed and load from the ECU. With these values you can use formulas 2 and 3 to calculate the instantaneous mass of CO₂ emission.

Comparison of the two indirect methods was done during the same cycle, during which the data was recorded from the ECU. These data were used for the calculated mass of CO₂ emissions. To check the fuel flow meter (instantaneous fuel consumption), a PEMS analyzer (direct measuring method) and weight were used.

The relationship between the production of CO₂, which is ascertained by the direct method, and the transient rate, calculated according to formula 4, is shown in Figure 4. If these points are approximated, we get a bisector where formula 5 expresses the mathematical relationship between the transient rate and mass of CO₂ emission.

$$mCO_2 = 0,00049 \cdot MT - 1,6741 \quad (5)$$

where: mCO_2 mass production of CO₂ (g)
 MT transient rate (1)

2.2 TRANSIENT RATE FOR CO EMISSION

CO emissions are not produced (measured behind a catalyst) in all engine operation modes. Therefore, it is crucial to determine the conditions under which the CO production shall be calculated. These conditions are summarized in the formula as follows:

$$\frac{n \cdot M_t}{10\,000} < 20 \quad (6)$$

where: n instantaneous engine speed (min⁻¹)
 M_t instantaneous engine load (%)

In other cases it is possible to use the transient rate. For CO the formula with the most appropriate coefficients of transient rate is as follows:

$$MT = 0,75 \cdot n + 99,4 \cdot M_t - 0,6 \cdot (n_2 - n_1) + 30,8 \cdot (M_{t2} - M_{t1}) \quad (7)$$

Figure 5 shows the process of CO production (by direct method) and the transient rate during the cycle which satisfies the conditions outlined in formula 6.

Figure 6 represents a relationship between the CO production which has been determined by the direct method and the transient rate calculated according to formula 7.

This relationship is not linear and it is necessary to use 3 formulas to calculate mass of CO production. All formulas are shown in Table 3.

FIGURE 4: Relationship between mass production of CO₂ and transient rate for CO₂.

OBRÁZEK 4: Závislost hmotnostní produkce CO₂ na míře transientnosti CO₂.

FIGURE 5: Process of CO production and transient rate for CO.

OBRÁZEK 5: Průběh produkce emisí CO a míry transientnosti CO.

TABLE 3: Mathematical model of CO production.**TABULKA 3:** Matematický model produkce CO.

Transient rate (-)	CO production (g)
$\frac{n \cdot M_t}{10\,000} < 20; MT \leq 9\,600$	$mCO = 0$
$9\,600 < MT \leq 10\,300$	$mCO = 0,00001 \cdot MT - 0,09565$ *)
$10\,200 < MT < 11\,000$	$mCO = 0,001 \cdot MT - 10,15467$
$MT \geq 11\,000$	$mCO = 0,00026 \cdot MT - 1,92438$

*) For simplification can be used $mCO = 0,005$.

FIGURE 6: Relationship between mass production of CO and the transient rate for CO.**OBRÁZEK 6:** Závislost hmotnostní produkce CO na míře transientnosti CO. **FIGURE 7:** Comparison of production of CO emissions.**OBRÁZEK 7:** Porovnání produkce emisí CO. **FIGURE 8:** Comparison of production of CO₂ emissions.**OBRÁZEK 8:** Porovnání produkce emisí CO₂.

3. RESULTS

Calculation of emissions by transient rate was compared to the other methods of measuring emissions – both direct and indirect methods. This comparison allows us to evaluate the accuracy of this method.

3.1 COMPARISON OF CO EMISSIONS

The production of CO observed in various ways is shown in Figure 7.

As seen in Figure 7, the error from the estimation (calculation) of CO using emission characteristics determined at steady speeds (static emission map) has a greater magnitude (correlation coefficient 0.82) than the error from the calculation of CO production using the terms and equations set out in Table 3 (correlation coefficient 0.94).

As a result, the calculated CO production correlates fairly well with the values determined by the direct method of measurement.

If we take into consideration the total CO emissions during the entire cycle, the value obtained by calculation using the direct method is 25.52 grams. Using indirect methods for

FIGURE 10: A plot of engine speed and load.**OBRÁZEK 10:** Průběh otáček a zatížení motoru. **FIGURE 11:** CO₂ production as a function of the transient rate.**OBRÁZEK 11:** Závislost produkce emisí CO₂ na míře transientnosti.

FIGURE 9: The data collection route for creating a mathematical model.

OBRÁZEK 9: Trasa sběru dat pro vytvoření matematického modelu.

measuring emissions the summaries of total production are 31.65 g CO (calculated by the transient rate) and 38.74 g (reading from a static emission map).

3.2 COMPARISON OF CO₂ EMISSIONS

Applying the transient rate for calculation of CO₂ production presents more accurate results than using the static emission map. The correlation coefficient between the values determined by the direct method and indirect method by transient rate is 0.97. When comparing the values determined by the direct method and indirect method by static emission map correlation, the coefficient is only 0.81. The production of CO₂ observed in various ways is shown in Figure 8.

Total CO₂ emissions during the cycle calculated by the direct method was 1744 g. CO₂ emissions determined by an indirect method using the transient rate was 1756 g and by static emission map production of CO₂ was 2085 g.

To check the calculation of CO₂ emissions formula 1 can be used for the calculation of fuel consumption. These values detected in this manner can be compared with the value from the flowmeter in the fuel system. From the flowmeter the fuel consumption is 560 g. If the fuel consumption is calculated

(using formula 1) from CO₂ emissions, the results for fuel consumption is approximately 565 g (indirect method using the transient rate), 561 g (by direct method) and 670 g (indirect method using static emission map).

3.3 VERIFICATION OF THE METHODOLOGY DURING AN ON-ROAD TEST MEASUREMENT

The verification was performed on a Škoda Fabia 1.2 HTP car using the same diagnostic systems as in laboratory conditions, i.e. PEMS analyzer VMK, Flowmeter WF005 and diagnostic system VAG-COM.

The mathematical model was determined based on the data measured and collected on-road taking a route from Chýně to Zličín (Figure 9).

A sufficient number of data samples with different combinations of engine operating parameters were collected whilst driving this route. A plot of engine speed and load is shown in Figure 10.

The transient rate of this specific vehicle has been obtained from the collected data. The CO₂ emissions transient rate is as follows:

$$MT_{CO_2} = 2,8 \cdot n + 310 \cdot M + 2,1 \cdot (n_2 - n_1) + 76 \cdot (M_2 - M_1) \quad (8)$$

The immediate level of emissions and the intensity of the transient rate was calculated according to formulas 2 and 3 for each time moment during the measurement. The relationship between these values was plotted on a graph (Figure 11) and subsequently the conditions for calculating CO₂ emissions were determined using the indirect method.

TABLE 4: A mathematical model of CO₂ production for on-road operations.
TABULKA 4: Matematický model produkce emisí CO₂ pro silniční provoz.

Transient rate (-)	CO ₂ production (g)
$MT < 10\,000$	0,4 (for simplification)
$MT \geq 10\,000$	$0,00024 \cdot MT - 2,00741$

FIGURE 14: A comparison of CO₂ production on a verification route.
OBRÁZEK 14: Srovnání produkce emisí CO₂ na ověřovací trase.

FIGURE 15: A comparison of CO production on a verification route.
OBRÁZEK 15: Srovnání produkce emisí CO na ověřovací trase.

TABLE 5: Evaluation of different methods of measuring emissions.
TABULKA 5: Vyhodnocení produkce emisí různými metodami

Transient rate (-)	CO Production (g)
$MT < 10\,000$	0,01 (for simplification)
$10\,000 \leq MT < 15\,000$	$4 \cdot 10^{-6} \cdot MT - 0,03$
$MT \geq 15\,000$	$7 \cdot 10^{-6} \cdot MT - 0,0075$

A mathematical model of CO₂ emissions during the on-road operation is as follows:

The calculation of CO emissions was similarly processed and evaluated. A transient rate of CO emissions is the following:

$$MT_{CO} = 1,9 \cdot n + 225 \cdot M + 1,1 \cdot (n_2 - n_1) - 12 \cdot (M_2 - M_1) \quad (9)$$

The relationship between CO production and transient rate is shown in Figure 12. In this case a correlation coefficient of 0.68 has been achieved; a lower degree of accuracy can be assumed in the calculation of the CO emissions. The mathematical model of CO emissions is shown in Table 5.

The verification of these mathematical models was checked on route from Kralupy nad Vltavou to Praha-Dejvice (Figure 13). Driving time was 37 minutes and the distance 24.7 km.

The development of CO₂ and CO production over time is presented in Figures 14 and 15. A comparison of the results obtained by mathematical models and by the direct method is shown in Table 6.

FIGURE 12: CO emission production as a function of transient rate.
OBRÁZEK 12: Závislost produkce emisí CO na míře transienčnosti.

FIGURE 13: Route for verification of the mathematical model.

OBRAZÉK 13: Trasa pro ověření matematického modelu.

4. DISCUSSION

Currently, there are two basic principles for determining emissions volume during real-world driving. The first method is the direct measurement of emissions, which uses exhaust gas analysis and recording of the concentration of the individual emissions components. The major disadvantage of this measurement method is the necessity of using an analyzer (PEMS), which is very expensive and using this method of measurement is not suitable for all vehicles.

The second method of measurement (the indirect method) uses the measured emission characteristics (static emission maps) and according to engine operating parameters determines the output of the emission constituents. This method is easy in respect of the instrumentations and it is possible to use it on a larger scale. This method implicitly works with emission maps measured during static engine modes. A difference is assumed between the static and transient modes during emissions measurement with the static emission maps. Therefore, the results are not fully accurate. The above-presented methodology for creating a mathematical model cannot provide absolute accuracy of the calculation of the produced emissions, but it is sufficiently precise and works with

a limited number of parameters. Should more accurate results need to be obtained a more complex mathematical model would be developed and/or the monitoring and measurement of other parameters affecting the emission levels (e.g. engine temperature, catalyst temperature, the exact composition of the fuel etc.).

5. CONCLUSION

By the introduction and utilization of the transient rate, the change of speed and change of load is used together with the engine speed and engine load, which leads to more accurate results when using the indirect method of measurement, as shown in the Table 7.

Using the transient rate to calculate emissions production by the indirect method can achieve more accurate results compared to the indirect method without using the transient rate. Refinement can be up to 28% in CO emissions and up to 19% in CO₂ emissions (in our case).

For calculation of the transient rate it is important to have sufficiency of the measured and processed data and for calculation of CO to have correctly determined conditions for evaluation. It can be assumed that the coefficients are not generally applicable, but are only valid for the tested engine type. Moreover, it is likely that the coefficients will change with the technical state of the engine.

However, the indirect method of measuring emissions using transient rate includes many unknown parameters such as the engine operating temperature, air humidity, technical condition

TABLE 6: A comparison of CO₂ and CO total production and fuel consumption.

TABULKA 6: Porovnání celkové produkce emisí CO₂ a CO a spotřeby paliva.

	CO ₂ production (g)	CO production (g)	Fuel consumption (g)
Direct method	3723	49,9	1222
By transient rate	3674	34,7	1199
Flowmeter	–	–	1165

TABLE 7: Evaluation of different methods of measuring emissions (laboratory conditions).

TABULKA 7: Vyhodnocení produkce emisí různými metodami (laboratorní podmínky).

	Direct method	Indirect method (static emission map)	Indirect method (transient rate)	Refinement
CO	25,52 g	38,74 g	31,65 g	27,78 %
CO ₂	1744 g	2085 g	1756 g	18,86 %

of the engine, the chemical composition of the fuel, etc. Despite of these shortcomings, more accurate data are obtained compared to the alternative without use of the transient.

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