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A simple numerical model for monitoring the quantity of carbon monoxide in the air caused by the traffic pollution

ABSTRACT

Investigation of the quality of air includes a series of specific emission and immision measurements of pollutants and it is regulated by domestic and foreign laws. The urban traffic is considered one of the emitters of noxious matters in the air. The emission of exhaust gases from the internal combustion engines is the source of numerous pollutants: burned or partially burned hydrocarbon, carbon monoxide, nitrogen oxides, soot, etc. The paper presents a numerical model that enables prevention of carbon monoxide concentration in the air based on air parameters measured through forming algebraic polynomials by the least-squares method. The measurement of parameters was performed in the Republic Institute of Public Health, at the location near the National Theatre in the Mediana Municipality, the City of Niš. The numerical model was realized in the symbolic system of Mathematica. Based on the formed model, numerical results are given related to the monitoring of carbon monoxide in the air caused by the traffic pollution.

Keywords: air pollution, approximation, carbon monoxide.

1: INTRODUCTION

The combustion process is a chemical-physical process in which the chemical energy bonded in fuel gets transformed under the influence of high temperature. In chemical terms, combustion is oxidation, bonding of all fuel elements with oxygen, which is a tumultuous and fast process itself. The combustible elements of gaseous fuels are mainly hydrogen, carbon monoxide and hydrocarbons. The non-combustible elements of gaseous fuels are carbon dioxide, nitrogen and oxygen. Carbon monoxide is a highly toxic colorless, odorless and tasteless gas and it is lighter than air. It belongs to the group of chemical choking gases and it causes general hypoxia due to irreversible bonding with hemoglobin (Hb). The toxic CO effect develops quickly in small concentrations[1]. Carbon monoxide occurs in the process of incomplete oxidation of organic matter.

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The exhaust gas from the internal combustion engines is one of the most significant air pollution sources where its quantity may range from 1-14 vol %, while the metal industry is the next great air polluter. In the USA, exhaust gases from motor cars and other internal combustion engines make 58% of the total CO quantity emitted in the atmosphere. More than 50% of all fatal poisonings were caused by CO. Carbon monoxide is inhaled into and eliminated from the organism through lungs, while the ultimate toxic effect reflects in hypoxia caused by the formation of carbonyl compounds which inhibit oxygen (O₂) binding or its transport, delivery and utilization in the body tissues and cells. The binding of CO to Hb is somewhat slower than the O₂ binding, but the affinity between Hb and CO is 210-240 times stronger than the affinity between Hb and O₂ [2]. Therefore, CO has the advantage in binding to hemoglobin even if it is present in too small quantities compared to oxygen. The toxic effect of CO on the body also depends on the exposure duration and emphasizing factors, i.e. on respiratory minute volume, muscle output, individual resistance of each person, concentration of CO and intensity of hypoxia. The lethal dose for

humans is 1000-2000 ppm (0.1-0.2%) within the exposure of 30 minutes. With high CO concentrations in the inhaled air, 1-2 minutes of exposure may lead to death. Maximum allowed concentration (MAC) in industry amounts to 50 ppm (0.005%) within 8 hours of exposure, while the scuba-diving compressed air can contain 10 ppm (0.001%) at the most. The clinical picture of the poisoning is untypical. Nitrogen oxides emitted in the atmosphere in the combustion process are the pollutants that destroy the stratospheric ozone, increase the intensity of UV radiation, influence global climate changes, produce acid rains and photochemical smog. Formation of nitrogen oxides in burning of fossil fuels is a very complex process affected by chemism, fuel, thermal-mass exchange, as well as by the flow characteristics. Nitrogen oxides represent major polluting matters. Solid fuel appliances emit large quantities of nitrose (nitrogen) oxides. Formaldehyde is the simplest aldehyde. It is produced industrially by the hydrogenization of methanol. Its molecular formula is HCHO. The extensive effect on the environment is connected to human activities and unrestrained exploitation of natural resources [3].

we obtain:

$$S = \sum_{k=0}^n (f(x_k) - \sum_{i=0}^m a_i \varphi_i(x_k))^2 \Rightarrow \frac{\partial S}{\partial a_j} = \sum_{k=0}^n (f(x_k) - \sum_{i=0}^m a_i \varphi_i(x_k)) (\varphi_j(x_k)) = 0$$

The most important approximation is the approximation by algebraic polynomials, where space orthogonalization is carried out by some orthogonalization procedure (Graham-Schmidt procedure), in which the following system of algebraic equations is obtained for the discrete case:

$$\begin{aligned} a_0(\varphi_0, \varphi_0) + a_1(\varphi_1, \varphi_0) + \dots + a_m(\varphi_m, \varphi_0) &= (f, \varphi_0) \\ a_0(\varphi_0, \varphi_1) + a_1(\varphi_1, \varphi_1) + \dots + a_m(\varphi_m, \varphi_1) &= (f, \varphi_1) \\ \vdots & \\ a_0(\varphi_0, \varphi_m) + a_1(\varphi_1, \varphi_m) + \dots + a_m(\varphi_m, \varphi_m) &= (f, \varphi_m) \end{aligned}$$

where for the functions g and h we have

$$(g, h) = \sum_{k=0}^n g(x_k) h(x_k).$$

The error in the nodes to be minimized is

$$S = S(a_0, a_1, \dots, a_m) = \sum_{k=0}^n (f(x_k) - \varphi(x_k))^2 = \sum_{k=0}^n (f(x_k) - a_0 - a_1 x_k - \dots - a_m x_k^2)^2 \rightarrow \min$$

The realization of this model in the Mathematica programming system starts with the definition of data as arranged triplets of digits [6].

2. FORMATION OF ALGEBRAIC POLYNOMIALS BY THE LEAST-SQUARES METHOD (FOR A DISCRETE CASE)

Let f be a function defined on the discrete set of points X_0, X_1, \dots, X_n and let the approximated function for $n \geq m$ be $\varphi(x, a_0, a_1, \dots, a_m)$. The function φ is determined from the condition that the sum of squared difference between the function and the approximated function in nodes is minimal [4]:

$$S = \sum_{k=0}^n (f(x_k) - \varphi(x_k))^2 \rightarrow \min$$

The function S is interpreted as a function of unknown parameters $S = S(a_0, a_1, \dots, a_m)$. Since $S \geq 0$, regardless of parameters, the problem is reduced to the minimization of the function S as a function with several variables a_0, a_1, \dots, a_m .

From the conditions of extreme $\partial S / \partial a_k = 0$, $k = 0, 1, \dots, m$ and the approximated function of the form of [5]:

$$\varphi(x) = a_0 \varphi_0(x) + a_1 \varphi_1(x) + \dots + a_m \varphi_m(x)$$

3. IMPLEMENTATION IN THE EXAMPLE OF CARBON MONOXIDE APPROXIMATION

The measurements of exhaust gases from motor vehicles in the Municipality of Mediana made

Table 1. Approximation carbon monoxide

Tabela 1. Prikaz količine ugljen monoksida

Mediana – National Theater						
Number	Period	Nitrogen oxide Nox	Formaldexy de HCHO	Carbon monoxide CO measured	Carbon monoxide CO approximated	difference
1	June	13.500	6.600	0.900	0.93	0.03
2	July	13.700	6.600	4.100	4.13	0.03
3	August	5.200	6.600	3.600	3.61	0.01

near the National Theater in the period of June - July - August 2014 were used as an example. The measurements of exhaust gases from motor vehicles numerical show in Table 1.

Graphic representation of the results from Table 1. is shown in the chart Figure 1.

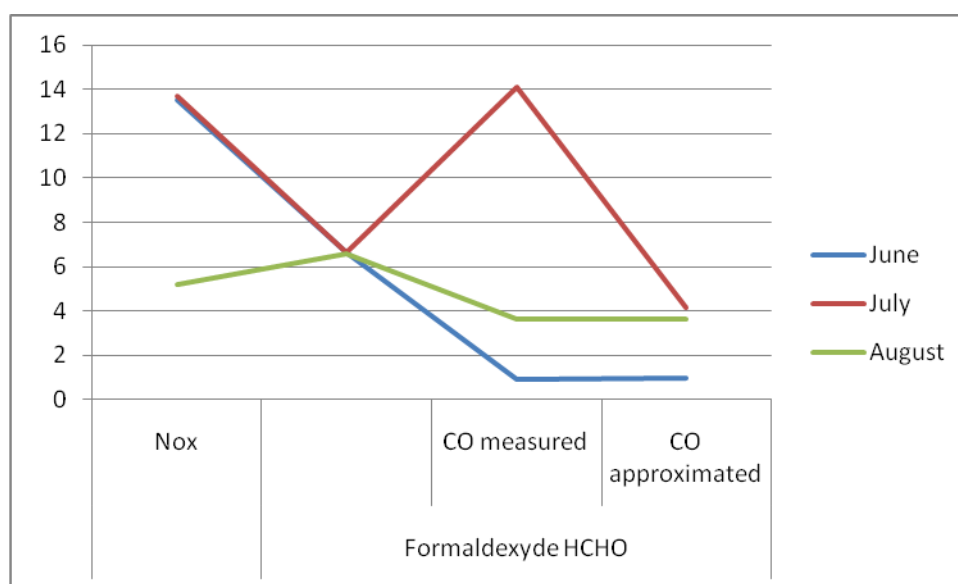


Figure 1. Graphical illustration of approximation carbon monoxide

Slika 1. Grafička ilustracija kolicine ugljen-monoksida

The above explained procedure in the Mathematica system was applied, with a tabular presentation of the results, Table 2. [7].

Table 2. Standard errors and confidence intervals for each coefficient separately

Tabela 2. Standardne greške i intervali poverenja za svaki koeficijent posebno

Parameter	Estimate	Std. Error	95% Confidence Interval	
			Lower Bound	Upper Bound
b0	,050	,218	-2,719	2,819
b1	1,000	,316	-3,018	5,018
b2	2,000	,316	-2,018	6,018
b3	-3,000	,447	-8,682	2,682

Dependence forms:

$$z = b_0 + b_1 \cdot x + b_2 \cdot y + b_3 \cdot x \cdot y.$$

The method of nonlinear regression:

$$z = 0.05 + x + 2y - 3xy$$

4. CONCLUSION

The applied model shows that it is possible to predict amounts of carbon monoxide in the air on the basis of other measured parameters. Since these measurements are precise, the least-squares method yields well fitted approximation functions, as may be seen in the Table, where the error is reduced. The application of such numerical methods is reasonable in cases where measuring costs should be reduced and where it is necessary to obtain needed data with sufficient accuracy in a simplified manner.

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IZVOD

JEDNOSTAVNI NUMERIČKI MODEL ZA MONITORING KVALITETA UGLJEN MONOKSIDA U VAZDUHU OD DRUMSKOG SAOBRAĆAJA

Kvalitet životne sredine, a samim tim i praćenje kvaliteta vazduha kao jednog od najvažnijeg faktora za živi svet sve više je u fokusu interesovanja naučnih krugova. U ovom radu je prikazan jednostavni matematički model kojim je moguće izvršiti predikciju količine ugljen monoksida u vazduhu, na osnovu drugih parametara koji se određuju merenjima. Aproksimacija količine ugljen monoksida ostvarena je formiranjem polinoma različitih stepena, metodom najmanjeg kvadrata i sa minimalnim brojem merenih podataka. Kao reprezentativni, prikazani su rezultati merenja parametara pokazatelja kvaliteta vazduha, u Nišu, opština Medijana kod Narodnog pozorišta. Na osnovu njih je izvršena predikcija ugljen monoksida a aproksimirani podaci su upoređeni sa merenim. Matematički model je realizovan u programu Mathematica®.

Ključne reči: aproksimacija, numerički model, kvalitet vazduha, ugljen monoksid.

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