Mathematical model of pollution compounds calculus in function of traffic capacity from urban areas

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Abstract: - The Brasov city is one of the biggest towns in Romania. In the central area of the Brasov city can be found the biggest concentration of the carbon monoxide, nitrogen oxides, the ozone and the volatile organic compounds. For intersection’s analysis there were collected data about the road traffic and data about the chemical pollution in the neighborhood of the road. In order to realize the model there were made tables with the traffic values and the values of the three pollutants, in function of the intersections of the analyzed route. For calculus were used the equations corresponding to the determined polynomial curves, for each pollutant, using the values obtained experimentally. The working page of the mathematical model was made grouping the four analyzed situations.

Key-Words: - Chemical, pollution, traffic, mathematical, model, etalon vehicle

1 Introduction
The human activity generates the emission of many gaseous pollutants into the atmosphere. The vehicles give many pollutants, and the studies made at international level allow quantification of the pollutants from the traffic flow. From all the primary pollutants made by the internal combustion engines, there are distinguished seven significant atmospheric pollutants, brought under regulation in Europe:

- sulphur dioxide (SO₂);
- particles (with a diameter <10 µm);
- lead (Pb);
- nitrogen oxide (NOₓ);
- carbon monoxide (CO);
- unburned hydrocarbons (HₙCₘ) – benzene;
- the ozone (O₃) from atmosphere, in concentrations of 0.5-10[ppm] [5].

A synthesis of the traffic flow development shows three significant travel phases:
- daily travels to and from work;
- afternoon travels to different centers (commercial, social-cultural, of individual or group meetings);
- going to and especially coming back from the week-end, generally outside the city, in order to relax.

The simple enunciation of these three main phases of travel present in city’s life can prove the variety of the urban traffic flow structure and intensity, where the vehicle has the main role, having the purpose to assure the maximum comfort of the travels, by its accessibility from “door to door”.

The essence of the problem is the mutual accommodation city-vehicle, its solution not being the sacrifice of one for the other.

If at the big traffic flow volume of the small vehicles we add the common transportation (which in many cities has the first place in order to satisfy the travel necessary of the habitants) and the transportation of goods and services, it can be said that the traffic flow needs two categories of measures in the urban areas:

- the adequate arrangement of a main road network, which can satisfy the traffic flow which is increasing continuously, but also which does not disturb the urban ambience;
- the organization, regulation and control of the traffic flow in intersections, which represents for the urban traffic real intake and exhaust valves, being for the streets network their strangulation points, the ones which determine the intrinsic capacity of the traffic flow [6].

The region of Brasov is situated in a mountainous area in the centre of Romania. In Brasov County there are 4 municipalities and 5 towns, 43 communes and 150 villages. The county population registered is 626499 inhabitants, from which in the urban environment 472620 inhabitants and in rural environment 153879 inhabitants.

In the central area of the Brasov City can be found the biggest concentration of the carbon monoxide, where the majority in traffic is composed by the vehicles equipped with gasoline engines, where the
traffic conditions are admitting their functioning frequently at uneconomical regimes, with partial loads, low engine speeds and uncompleted burnings of the fuel [4].

The nitrogen oxides, the ozone and the VOC are usually specific to the peripheral urban areas, where it can be noticed a high volume of heavy vehicles, which have diesel engines.

The following list describes the potential health risks associated with these emissions:
- Carbon Monoxide (CO): An odorless and colorless gas which is highly poisonous. CO can reduce the blood's ability to carry oxygen and can aggravate lung and heart disease. Exposure to high concentrations can cause headaches, fatigue and dizziness.
- Nitrogen Oxides (NO$_x$) and Nitrogen Dioxide (NO$_2$): These chemicals form the yellowish-brown haze seen over dirty cities. When combined with oxygen from the atmosphere, NO becomes NO$_2$, a poisonous gas that can damage lung tissue [2].
- Hydrocarbons (HC): This is a group of pollutants containing hydrogen and carbon. Hydrocarbons can react to form ozone. Some are carcinogenic and other can irritate mucous membranes. Hydrocarbons include: Volatile organic compounds (VOC); Volatile organic gases (VOG); Reactive organic gases (ROG); Reactive organic compounds (ROC); Non-methane hydrocarbons (NMHC); Non-methane organic gases (NMOG).
- Ozone (O$_3$): This is the white haze or smog seen over many cities. Ozone is formed in the lower atmosphere when NMOC and NO$_x$ react with heat and sunlight. Ozone can irritate the respiratory system, decrease lung function and aggravate chronic lung disease such as asthma [5].

2 The studied area

For the pollution level measurement it was chosen the Brasov’s historical center area. In this area there are many commercial, cultural and touring objectives: institutions (City Hall, Prefecture, University’s buildings, high schools and schools), shops, hotels, churches, museums, theatres, monuments and parks. These objectives bring on each day a high number of pedestrians which are exposed to the pollution caused by road traffic from this area.

The analyzed route was: Lungă Street, Eroilor Boulevard, 15 Noiembrie Street, Castanilor Street, Iuliu Maniu Street, Nicolae Iorga Street.

The objectives from this picture are: 1- The City Hall; 2- Prefect Hall; 3- Building N of the Transilvania University; 4- Unirea High School; 5- Capitol Hotel; 6- Aro Palace Hotel; 7- Casa Armatei Building; 8- Sica Alexandrescu Theatre; 9- Building M of the Transilvania University; 10- Comercial Area; 11- C.F.R. Hospital; 12- Lecture Room of the Transilvania University; 13- Mihail Eminescu Hospital; 14- Romano-Catholic Church; 15- Offices and Banks Area.

The route includes six intersections, from which four are with traffic lights and two are marked with traffic signs.

The six intersections are:
- Intersection 1 - Castanilor Street + Iuliu Maniu Street;
- Intersection 2 - Alexandru Ioan Cuza Street + Agrigelor Street + Iuliu Maniu Street;
- Intersection 3 - Nicolae Iorga Street + Lungă Street;
- Intersection 4 - Lungă Street + Eroilor Boulevard + Mureșenilor Street;
- Intersection 5 - Eroilor Boulevard + Vlad Țepeș Street + Nicolae Bălcescu Street + 15 Noiembrie Boulevard;
Intersection 6 - 15 Noiembrie Boulevard + Castanilor Street.

On three of those the access of the road traffic is made from the residential areas to the historical center (intersections 1, 2 and 3), and on the other three there is an opposed flux.

Fig. 3 Analyzed route: Iuliu Maniu Street, Nicolae Iorga Street, Lunga Street, Eroilor Boulevard, 15 Noiembrie Boulevard and Castanilor Street.

3 Road traffic and chemical pollution data measurement methodology

For intersection’s analysis there were collected data about the road traffic and data about the chemical pollution in the neighborhood of the road (the values of some pollutants resulted from the fuel combustion).

The most common and handy method is the manual collecting of the road traffic data, with the help of an observer team, each member of this team writing down a specific element of the road traffic.

For a certain input with variable time signals it is established the following data measurement in order to analyze the intersection: traffic volume, number of vehicles which are passing the stop line, for each traffic direction (forward, left, right), for each vehicle category. In the figure above it is presented a regular intersection with four phases, with observers placed so that to obtain a minimum number of them. In this case, with special turning moves there are necessary more persons, the maximum number being of 5: one for each entrance and the 5th one to measure the time interval [4], [5].

The volume of the traffic flow was determined by counting the total number of the vehicles, which passed through the intersection during one hour (8.00-9.00 and 15.00-16.00) in all ways.

The volumes of the traffic flows from the studied intersections are presented in the next picture:

<table>
<thead>
<tr>
<th>Intersection number</th>
<th>Bus &amp; Coach Vehicles</th>
<th>Light vehicles</th>
<th>Trucks</th>
<th>Buses and Troleys</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>2569</td>
<td>2428</td>
<td>30</td>
<td>113</td>
</tr>
<tr>
<td>8</td>
<td>3245</td>
<td>2776</td>
<td>27</td>
<td>127</td>
</tr>
<tr>
<td>9</td>
<td>3657</td>
<td>3075</td>
<td>28</td>
<td>151</td>
</tr>
<tr>
<td>3</td>
<td>4678</td>
<td>4773</td>
<td>36</td>
<td>119</td>
</tr>
<tr>
<td>2</td>
<td>4505</td>
<td>4471</td>
<td>13</td>
<td>124</td>
</tr>
<tr>
<td>1</td>
<td>5451</td>
<td>4679</td>
<td>69</td>
<td>182</td>
</tr>
</tbody>
</table>

Fig. 5 The registered values for the 8.00-9.00 hour interval, for one intersection

For measuring the concentration of the chemical pollutants from the studied area it will be used a team of two persons. The two persons will use the necessary equipment (portable gas analyzer) and will write the specific values of the measurement points [7].

The MX21 Plus is a portable multi-gas monitor which can detect up to four gasses simultaneously and includes features such as: data logging, interchangeable pre-calibrated sensor blocks, instantaneous, STEL and TWA alarms. The unit is programmable via serial link from a PC or via a user-friendly menu interface and is approved for use in hazardous areas. By the use of intelligent plug-in sensor modules the device has one of the largest range of toxic sensors (20 plus) including CO₂, CO, H₂S, SO₂, CL₂, NO, NO₂, HCN, HF, PH₃, O₃, H₂, solvents etc.

Another unique feature of the MX21 Plus is the ability to measure CH₄ in percentage volume as well percentage LEL with a library of 32 pre-programmed flammable gasses to allow for more accurate monitoring of specific flammable gasses by
simply selecting the target gas CH₄, H₂, butane, petrol vapors etc., from a menu.

![Image](92x152 to 283x351)

The measurement cells:
- Oxygen and toxic gases measurement cells;
- Anemometric cell;
- Carbon dioxide measurement cell;
- Explosive gases measurement cell.

![Image](318x162 to 537x335)

Advantages:
- Simple to use. The MX 21 PLUS incorporates a self-diagnostic function, which indicates any irregularities in its operation thereby providing complete confidence measurement.
- Clear messages. Without having to calibrate the MX 21 PLUS, you can select the gas you wish to measure from any of the 16 preprogrammed flammable gases or vapors from its international library, thereby ensuring a direct reading in % LEL. If the concentration exceeds the LEL range, the instrument will display over range in compliance with "non-ambiguity readout"
- Reliable oxygen measurement. The oxygen sensor manufactured in OLDHAM's modern laboratories provides accurate and reliable measurement [8]. The user can carry the MX21 PLUS apparatus in housing. The apparatus is designed so that the measurement cells are oriented to exterior. This fact makes that the holes for the measurement cells are visible during measurements. The MX21 PLUS apparatus must be put in vertical position, with the battery downwards. Depending on the gas types that are measured, the apparatus must be placed:
  - on ground, for heavy gases measurement (H₂S, CO);
  - on medium height (about 1 meter above the ground) or at the exhaust of some ventilation tubes from the industrial zone (for the general measurement of the maximum number of gases or for oxygen supervise).

![Image](283x151)

Next is presented as an example the scheme of an intersection, with the chosen measurement points in order to make the measurements.
The measurements were made for each of the 6 intersections of the route. Simultaneously there were taken the values of traffic flow and the values of main chemical compounds pollutants. The four distinct situations, in function of season and time interval in which the measurement was made are:

- cold season (winter), morning rush hour (8.00-9.00);
- cold season (winter), evening rush hour (15.00-16.00);
- warm season (summer), morning rush hour (8.00-9.00);
- warm season (summer), evening rush hour (15.00-16.00).

From the six pollutants for which were made measurements, there were analyzed only three and these are: carbon monoxide (CO), volatile organic compounds (VOC) and ozone (O₃). The rest of the pollutants were not analyzed for the following reasons:

- Nitrogen monoxide (NO) – the values of the NO concentration are for most of the intersections minimum (1 [ppm])
- Sulphuretted hydrogen (H₂S) – the values of the H₂S concentration varies very little from one season to another, and is not specific to vehicles.
- Nitrogen dioxide (NO₂) – the values of the NO₂ concentration varies depending on the season and on the time interval when the measurements were made. The values are between 0.1 and 0.2 [ppm] for most of the cases. Though, it could not be established a dependency of the NO₂ concentration in function of the etalon vehicle number. The values measured varies randomly in function of the weight of different categories of vehicles from the road traffic, but also in function of geometrical parameters of each intersection. For exemplification it was chosen the route 2, in the summer, for the evening rush hour.

![Fig. 9 The points where the measurements were done](image1)

![Fig. 10 The concentration variation of NO₂ [ppm] for one intersection](image2)

The concentration variation of three chemical pollutants (CO [ppm], VOC [ppm], O₃ [ppm]), specific to the areas near the road infrastructure for the two analyzed time intervals is presented in the next graphics (for one intersection):

![Fig. 11 The concentration variation of CO [ppm] for Intersection 5 - Eroilor Boulevard + V. Țepeș Street + N. Bălcescu Street + 15 Noiembrie Blvd.](image3)
pollutant it will be established an average value, expressed in the corresponding measuring unit. The average will be a rounded arithmetical mean, which will contain all the values obtained in the measurement points, but without the maximum and the minimum value.

\[
X_{\text{medie}} = \frac{\sum_{i=1}^{n} p_i - \min(p_i) - \max(p_i)}{n - 2}
\]

where: \(X_{\text{average}}\) = the average value of the analyzed pollutant; \(p_i\) = the value of the pollutant in each of the analyzed points; \(n\) = the number of analyzed points for each intersection.

In order to realize the model there were made tables with the traffic values and the values of the three pollutants, in function of the intersections of the analyzed route. For calculus were used the equations corresponding to the determined polynomial curves, for each pollutant, using the values obtained experimentally.

**Fig. 14** Tables with the chemical pollutant values for one intersection

The working page of the mathematical model was made grouping the four analyzed situations, for each of the analyzed route. For each of these situations, the intersections were sorted increasingly by the number of etalon vehicles. For each of the studied pollutants there were determined their variations in function of the etalon vehicles number.

The taken values vary randomly in function of weight of the different vehicles’ categories from the road traffic, but also in function of the geometrical parameters of each intersection.

For each of the four situations, the intersections were arranged increasingly after the number of etalon
vehicles. Next to each intersection there were written the average values of the two pollutants, to represent in a chart the dependence between these two and the number of etalon vehicles. The obtained curves were calculated for each representation of the experimental values (obtained from measurements), obtaining a theoretical curve given by a polynomial equation. It was wished to obtain a theoretical curve very closed to the curves obtained with the experimental values. For each situation, the resulted theoretical curves will be described through polynomial equations of 2nd and 3rd degree [1], [3]. Next it will be presented the resulted curves and equations from the analysis, for each of the three studied pollutants, for a single situation. For exemplification there will be presented the variation curves for CO, VOC and O3 in the warm season, at the morning rush hour.

![Image of CO concentration variation](image1.png)

**Fig. 15** The variation of the CO concentration in function of the etalon vehicles number

![Image of VOC concentration variation](image2.png)

**Fig. 16** The variation of the VOC concentration in function of the etalon vehicles number

![Image of O3 concentration variation](image3.png)

**Fig. 17** The variation of the O3 concentration in function of the etalon vehicles number

For this analyzed chemical compounds, in order to realize a unitary mathematical model, it can be written equations of pollution concentration variation depending on etalon vehicles number measured in one hour time interval.

\[
\text{CO}_{\text{theoretical}} = 2.32428 + 1.09063 \cdot 10^{-4} \cdot V_E + \\
+ 9.27022 \cdot 10^{-8} \cdot V_E^2 \tag{2}
\]

\[
\text{VOC}_{\text{theoretical}} = -15.45515 + 0.01672 \cdot V_E - \\
- 4.3480 \cdot 10^{-6} \cdot V_E^2 + 3.9856 \cdot 10^{-10} \cdot V_E^3 \tag{3}
\]

\[
\text{O}_3_{\text{theoretical}} = 0.01179 - 2.2649 \cdot 10^{-6} \cdot V_E + \\
+ 6.65935 \cdot 10^{-10} \cdot V_E^2 \tag{4}
\]

Where: \(\text{CO}_{\text{theoretical}}\), \(\text{VOC}_{\text{theoretical}}\) and \(\text{O}_3_{\text{theoretical}}\) = the theoretical values of the CO, VOC and O3 concentrations which describes the variations of the mathematical model curves; \(V_E\) = The number of etalon vehicles;

These equations can be generalized, using for all situations representative constants.

\[
\text{CO}_{\text{theoretical}} = A_{CO} + B_{CO} \cdot V_E + C_{CO} \cdot V_E^2 + \\
+ D_{CO} \cdot V_E^3 \tag{5}
\]

\[
\text{VOC}_{\text{theoretical}} = A_{VOC} + B_{VOC} \cdot V_E + \\
+ C_{VOC} \cdot V_E^2 + D_{VOC} \cdot V_E^3 \tag{6}
\]

\[
\text{O}_3_{\text{theoretical}} = A_{O3} + B_{O3} \cdot V_E + C_{O3} \cdot V_E^2 + \\
+ D_{O3} \cdot V_E^3 \tag{7}
\]

Where: \(A_{VOC}, B_{VOC}, C_{VOC}, D_{VOC}, A_{CO}, B_{CO}, C_{CO}, D_{CO}, A_{O3}, B_{O3}\) and \(C_{O3}\) = Representative constants for
each analyzed situation.
After the introduction of the formulas and the graphical representation of the three pollutants, result the theoretical curves corresponding to the used equations.
In figure 18 are presented the table and the corresponding diagrams for route, in the warm season and the morning rush hour (8:00-9:00). In the table are presented: the corresponding number for each intersection, the traffic values (etalon vehicles), the average values for the chemical pollutants concentration (determined using the data obtained experimentally) and the pollutants’ values obtained through calculus, using the polynomial equation of each pollutant compound.
The three diagrams represent the variation of the three pollutants in function of the measured traffic volumes in the route’s intersections. The blue spots represents the values determined experimentally, from the measurements and corresponds to the values from the table (written also in blue), from columns C, E and G. The red curves represent the pollutants variations with the etalon vehicle number, using the values obtained mathematically using the polynomial equations corresponding to each pollutant. These values are written in red and they are situated in columns D, F and H of the table.

Fig. 18 Presentation of mathematical model results for one of the four situations, for the analyzed route

Exemplification are presented the variation curves of the carbon monoxide (CO), for the four studied situations. In the four figures it can be noticed the visible differences of the etalon vehicles number from the intersections for the measurement time interval, but also of the variation curves’ shape.

Fig. 19 The variation of the CO concentration for the 8.00-9.00 hour interval and for the winter season

Fig. 20 The variation of the CO concentration for the 15.00-16.00 hour interval and for the winter season
Fig. 21 The variation of the CO concentration for the 8.00-9.00 hour interval and for the summer season

Fig. 22 The variation of the CO concentration for the 15.00-16.00 hour interval and for the summer season

4 Conclusion

The mathematical model can be used for different routes and situations and introducing a number of etalon vehicles for an intersection can be estimated the pollution level for three chemical pollutants.

In the case of the cold season (winter), on the morning rush hour (8.00-9.00), the CO and VOC concentration variations are after two ascending curves, given by the 2\textsuperscript{nd} degree polynomial equations. For CO the curve is convex and for VOC the curve is concave.

In the case of the cold season (winter), on the evening rush hour (15.00-16.00), the CO concentration variation is after one ascending curve, given by the 3\textsuperscript{rd} degree polynomial equation and the VOC concentration variation is after one ascending concave curve given by the 2\textsuperscript{nd} degree polynomial equation.

In the case of the hot season (summer), on the morning rush hour (8.00-9.00), the CO and O\textsubscript{3} concentration variations are after ascending convex curves given by the 2\textsuperscript{nd} degree polynomial equations, and the VOC concentration variation is after an ascending curve given by a 3\textsuperscript{rd} degree polynomial equation. For all three pollutant compounds, their concentration variation in function of the etalon vehicle number is similar.

In the case of the hot season (summer), on the evening rush hour (15.00-16.00), the CO and O\textsubscript{3} concentration variations are after concave ascending curves given by 2\textsuperscript{nd} degree polynomial equations, and the VOC concentration variation is after an ascending curve given by the 3\textsuperscript{rd} degree polynomial equation. For all three pollutant compounds, their concentration variation in function of the etalon vehicle number is, as in the case of the morning rush hour, similar.

From this study which as realized on the base of the data obtained experimentally can be observed some characteristics of the pollution made by traffic flow:
• Substantial increments of the chemical compounds concentrations resulted from the fossil fuels burning are in the case of transitory functioning of internal combustion engines.
• The time interval and the season influence visibly the chemical pollutant compounds.
• The meteorological conditions (temperature, wind’s speed and direction, humidity, air pressure) influence the pollutants’ values.
• The traffic’s flow composition (cars, trucks, buses, trolleybuses) but also the traffic volume values (expressed by the Traffic capacity = etalon vehicles / hour) have a determinant role over the city’s pollution level.
• Intersection’s and main street’s geometry on which is developing the city’s transitory traffic influences significantly the pollution level.
• The biggest impact over the air quality, from the areas designated to pedestrians, is given by the traffic road; the pollutant emissions from the vehicles being maximal near the roads, at the height of the human respiratory organs.

The main contributions given by this research about the chemical pollution from the road traffic are the following:
• There were identified the major problems about the organization of the road traffic from Brasov District which contributes to the chemical and noise pollution from the urban areas.
• There were made road traffic and environment measurements, aiming to locate the levels of chemical and noise pollution from the traffic road.
• There was analyzed the local vehicles park, its structure, perspectives, the level of pollutant emissions from this one and the causes of the pollutant emissions generation.
• It was realized a complex data base, which includes the values of the traffic road, the chemical pollutants and the noise levels. The data base will be updated with the values measured in the next years.
• It was identified the current and the future international and the national legislation regarding the maximum allowed levels of the chemical and noise pollution caused by road traffic.
• It was realized a mathematical model of estimation of the chemical and noise pollution levels in function of the time interval for the two routes studied.

References:
[8] OLDHAM MX 21 PLUS, Technical Documentation