Prediction model of chemical pollutants produced by the road vehicles

STELIAN TARULESCU, CORNELIU COFARU
Department of Mechanical Engineering
Transilvania University of Brasov
Eroilor Boulevard, No 29, Brasov
ROMANIA
ccornel@unitbv.ro, starulescu@unitbv.ro

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 intersections’ analysis there were collected data about road traffic and air pollution in the neighborhood of the road. After collecting the data, made tables with the traffic values and the values of the three pollutants were made, according to the intersections from the analyzed route (nine intersections). 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 prediction model was made by grouping the four analyzed situations (depending on season and hour interval).

Key-Words: - Pollution, vehicles, prediction, measurement, traffic.

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 (SO\textsubscript{2}); particles (with a diameter <10 µm); lead (Pb); nitrogen oxide (NO\textsubscript{x}); carbon monoxide (CO); unburned hydrocarbons (H\textsubscript{n}C\textsubscript{m}) – benzene; the ozone (O\textsubscript{3}) from atmosphere, in concentrations of 0.5-10[ppm] [3].

The combustion process results in emissions of VOC, NO\textsubscript{x}, PM, and CO, which are released from the tailpipe while a vehicle is operating. VOC also escape into the air through fuel evaporation. Despite evaporative emissions controls, evaporative losses can still account, on hot days, for a majority of the total VOC pollution from current model cars. VOC and CO emissions rates typically drop as speed increases [7].

NO\textsubscript{x} emissions rates turn up at higher speeds. Emissions rates at all speeds have been falling over time as newer, more controlled vehicles enter the fleet. Emissions rates are higher during stop-and-go, congested traffic conditions than free flow conditions operating at the same average speed.

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 weekend, 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 [7].

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 communities and 150 villages. The registered county population is of 626499 inhabitants, from which 472620 inhabitants in the urban environment and 153879 inhabitants in rural environment.
In the central area of the city of Brasov the biggest concentration of the carbon monoxide can be found, 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 [3].

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

- 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\textsubscript{x}) and Nitrogen Dioxide (NO\textsubscript{2}): These chemicals form the yellowish-brown haze seen over dirty cities. When combined with oxygen from the atmosphere, NO becomes NO\textsubscript{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); Reactive organic gases (ROG); Reactive organic compounds (ROC); Non-methane hydrocarbons (NMHC); Non-methane organic gases (NMOG).
- Ozone (O\textsubscript{3}): This is the white haze or smog seen over many cities. Ozone is formed in the lower atmosphere when NMOG and NO\textsubscript{x} react with heat and sunlight. Ozone can irritate the respiratory system, decrease lung function and aggravate chronic lung disease such as asthma [3].

2 The analyzed 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 (STAR Shopping Centre);
  - hotels (Aro Palace Hotel, Capitol Hotel);
  - churches (Romano-Catholic Church, Saint Nicholas Church);
  - museums (Brasov Art Museum, First Romanian school)
  - theatres (Sica Alexandrescu Theatre)
  - monuments (The mayor’s former office building, The Rope Street, Ecaterina Gate, Schei Gate)
  - parks (Nicolaie Titulescu Park).

These objectives bring on each day a high number of pedestrians which are exposed to the pollution caused by road traffic from this area.
Intersection 4 - 15 Noiembrie Boulevard + Nicolae Balcescu Street + Vlad Tepes Street;  
Intersection 5 - Nicolae Balcescu Street + Dobrogeanu Gherea Street;  
Intersection 6 - Prundului Street + Beethoven Street + Gheorghe Bălăușescu Street;  
Intersection 7 - Muresenilor Street + Beethoven Street + Gheorghe Dima Street + Cibinului Street;  
Intersection 8 – Eroilor Boulevard + Lunga Street + Muresenilor Street;  
Intersection 9 - Nicolae Iorga Street + Lunga Street.  
Intersection 4 - Lunga Street + Eroilor Boulevard + Muresenilor Street;  

3 Road traffic and chemical pollution data measurement methodology  
For intersection’s analysis 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) were collected.  
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.

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.  
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>Binal Vehicles</th>
<th>Light vehicles</th>
<th>Trucks</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>2969</td>
<td>2428</td>
<td>50</td>
</tr>
<tr>
<td>8</td>
<td>3245</td>
<td>2776</td>
<td>27</td>
</tr>
<tr>
<td>9</td>
<td>3657</td>
<td>3075</td>
<td>28</td>
</tr>
<tr>
<td>3</td>
<td>4678</td>
<td>4173</td>
<td>36</td>
</tr>
<tr>
<td>2</td>
<td>4905</td>
<td>4471</td>
<td>13</td>
</tr>
<tr>
<td>1</td>
<td>5431</td>
<td>4629</td>
<td>69</td>
</tr>
</tbody>
</table>

Fig. 4 The registered values for the 8.00-9.00 hour interval, for several intersections

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, H₃, 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.
Fig. 5 The OLDHAM MX21 Plus portable multi-gas detector

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

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].

Fig. 6 The OLDHAM MX21 measurement cells

Fig. 8 Measurement with the OLDHAM MX21 Plus portable multi-gas detector

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).
Next is presented as an example the scheme of an intersection, with the chosen measurement points in order to make the measurements.
For measuring the concentration of the chemical pollutant from the studied area, a team of two persons was used. The two persons used the necessary equipment (portable gas analyzer) and wrote the specific values of the measurement points [1].

In order to determine the pollution degree of this area, an OLDHAM MX21 Plus portable multi-gas detector was used. The MX21 Plus is a portable multi-gas monitor which can detect up to four gasses simultaneously [5]. The measurements were made for each of the 9 intersections of the route. Simultaneously, the values of traffic flow were taken. The four distinct situations, depending on season and time interval in which the measurement was made are:
- cold season, morning rush hour (8.00-9.00);
- cold season, evening rush hour (15.00-16.00);
- warm season, morning rush hour (8.00-9.00);
- warm season, evening rush hour (15.00-16.00).

An example the scheme of an intersection, with the chosen measurement points in order to make the measurements will be presented in the next part of the paper.

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 shown in the next graphics (for one intersection):

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 vary 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. 10 The concentration variation of NO₂ [ppm] for one intersection

Fig. 11 The concentration variation of CO [ppm] for Intersection 4 - Eroilor Boulevard + Vlad Tepes Street + Nicolae Balcescu Street + 15 Noiembrie Boulevard
Fig. 12 The concentration variation of VOC [ppm] for Intersection 5 - Eroilor Boulevard + Vlad Tepes Street + Nicolae Balcescu Street + 15 Noiembrie Boulevard

Fig. 13 The concentration variation of O₃ [ppm] for Intersection 4 - Eroilor Boulevard + Vlad Tepes Street + Nicolae Balcescu Street + 15 Noiembrie Boulevard

4 Prediction model for the pollutant concentrations

Using the measured data from the intersections, an average pollution level for each of these ones can be established. For each intersection, only the points which are near the road were analyzed, excluding the points far from the road or placed after green areas or other objectives. For each pollutant an average value, was established expressed in the corresponding measuring unit. The average was a rounded arithmetical mean, which contained all the values obtained in the measurement points, but without the maximum and the minimum value.

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

(1)

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.

<table>
<thead>
<tr>
<th>Season</th>
<th>Interval</th>
<th>The average value CO [ppm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>winter</td>
<td>08:00-9:00</td>
<td>5.4286</td>
</tr>
<tr>
<td></td>
<td>15:00-16:00</td>
<td>4.3429</td>
</tr>
<tr>
<td>summer</td>
<td>08:00-9:00</td>
<td>4.0000</td>
</tr>
<tr>
<td></td>
<td>15:00-16:00</td>
<td>4.2857</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Season</th>
<th>Interval</th>
<th>The average value VOC [ppm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>winter</td>
<td>08:00-9:00</td>
<td>4.2857</td>
</tr>
<tr>
<td></td>
<td>15:00-16:00</td>
<td>3.7143</td>
</tr>
<tr>
<td>summer</td>
<td>08:00-9:00</td>
<td>7.4286</td>
</tr>
<tr>
<td></td>
<td>15:00-16:00</td>
<td>4.8571</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Season</th>
<th>Interval</th>
<th>The average value NO₂ [ppm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>winter</td>
<td>08:00-9:00</td>
<td>0.1000</td>
</tr>
<tr>
<td></td>
<td>15:00-16:00</td>
<td>0.1000</td>
</tr>
<tr>
<td>summer</td>
<td>08:00-9:00</td>
<td>0.0000</td>
</tr>
<tr>
<td></td>
<td>15:00-16:00</td>
<td>0.1000</td>
</tr>
</tbody>
</table>

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

In order to realize the model, tables with the traffic values and the values of the three pollutants were made, depending on the intersections of the analyzed route. The equations corresponding to the determined exponential regression curves were used, for calculus for each pollutant, using the values obtained experimentally. The working page of the mathematical model was made by grouping the four analyzed situations, for 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 their variations were determined according to the etalon vehicles number.

The taken values vary randomly depending on the weight of the different vehicles’ categories from the road traffic, but depending on 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 the average values of the two pollutants were written, in a chart the dependence between these two and the number of etalon vehicles.
vehicles to be represented. The obtained curves were calculated for each representation of the experimental values (obtained from measurements), obtaining a theoretical curve given by a regression 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 were described through exponential regression equations [2], [4], [6]. The resulted curves and equations from the analysis will be presented, for each of the three studied pollutants, for a single situation. For exemplification, the CO, VOC and O₃ variations for warm season, at the morning and evening rush hour will be presented.

For the morning rush hour, the data are presented in the following graphics: Fig. 15, Fig. 16 and Fig. 17. The equation regarding this three variations are presented in the (2), (3) and (4) formulas.

\[
CO_{\text{theoretical}} = -5,1953 \cdot e^{-4149,48 \cdot V_E} + 6,55853 \quad (2)
\]

\[
VOC_{\text{theoretical}} = 1595742,22 \cdot e^{\frac{V_E}{1326706569,54}} - 1595742,29 \quad (3)
\]

\[
O_3_{\text{theoretical}} = 2985,20621 \cdot e^{\frac{V_E}{726916471,38}} - 2985,208 \quad (4)
\]

Where:

- \(CO_{\text{theoretical}}\), \(VOC_{\text{theoretical}}\) and \(O_3_{\text{theoretical}}\) = the theoretical values of the CO, VOC and O₃ concentrations describing the variations of the mathematical model curves;
- \(V_E\) = the number of etalon vehicles.

For the evening rush hour, the data are presented in the next three graphics: Fig. 18, Fig. 19 and Fig. 20. The equation regarding this three variations are presented in the (5), (6) and (7) formulas.

\[
CO_{\text{theoretical}} = 2,84345 \cdot e^{\frac{V_E}{5186,97}} - 2,18811 \quad (5)
\]

\[
VOC_{\text{theoretical}} = 578135,49 \cdot e^{\frac{V_E}{202352151,94}} - 578133,97 \quad (6)
\]

\[
O_3_{\text{theoretical}} = 3064,69423 \cdot e^{\frac{V_E}{404910338,81}} - 3064,69984 \quad (7)
\]
For this analyzed chemical compounds, in order to realize a unitary mathematical model, equations of pollution concentration variation depending on etalon vehicles number measured in one hour time interval can be written.

After the introduction of the formulas and the graphical representation of the three pollutants, the result is the theoretical curves corresponding to the used equations. In figure 21 the table and the corresponding diagrams for route 1, in the warm season and the evening rush hour (15.00-16.00) 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 equation of each pollutant compound in the table are presented.
5 Conclusion

The prediction model can be used to approximate the air pollution level in urban areas. The values of CO, VOC and O₃ concentrations regarding to the number of etalon vehicles in one hour interval (for morning or evening rush hour) can be determined.

From this study realized on the base of the data obtained experimentally some characteristics of the pollution made by traffic flow can be observed:
- 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 and main street’s geometry on which is developed 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.

For accomplish the mathematical model of pollutant approximation it can be used the following methodology:
Step 1 – Choosing the area that will be analyzed (Choosing the routes; Choosing the intersections; Assignation of the measurement points; Determination of the time intervals for the measurements; Choosing the time for measurements (season, month, week, day)).
Step 2 – Accomplish the chemical pollution measurements (Traffic flow measurements; Chemical pollution measurements).
Step 3 – Data centralization (Accomplishment or creation of a data base for traffic and chemical pollution values).
Step 4 – Data analysis (Data centralization using Microsoft Excel; Identify the chemical pollution level for each intersection; Pollutant analysis regarding accomplishment of the mathematical model).
Step 5 – Obtain the curves of chemical pollutants variation in function of the traffic flow (Assignation of the approximation method for each pollutant; Making the work pages using the analyzed data, with the OriginPro software; Obtaining the variation chemical pollutants curves).
Step 6 – Establish of the work pages for the mathematical model (Accomplishment of the tables from the final work pages; Accomplishment of the graphics for each studied route).
Step 7 – Verification of the mathematical model (Accomplishment of the verification measurements in similar condition with initial measurements; Including of...
this data in the work pages; Analysis of the obtained graphics).
Step 8 – Using the mathematical model (Using the work pages for chemical pollution approximation for different traffic flow values).
The resulted levels of air pollutant concentrations are relatively high for the analyzed area. To reduce the pollution in the historical center of Brasov, we propose several measures:
- road traffic limitation in the historical center of the city;
- optimization of road traffic in the entire city;
- creation of a data base that would include traffic volumes and air pollutant concentrations, for all crowded areas in the city;
- traffic flows analysis and prediction using simulation and modeling software;
- fleet modernization for all vehicle categories from Brasov city;
- reparation and modernization of roads and common transportation lines;
- making bicycle lanes and modern bicycle transportation systems;
- drawing of pollution maps for Brasov city.

References: