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APPLICATION OF POLLUTION DISTRIBUTION MODELING IN AIR QUALITY MANAGEMENT SYSTEM - CHALLENGES AND POSSIBILITIES

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Abstract: Direct measurements represent the most reliable way of ambient air quality assessment. However, the measuring scope is quite often limited by purchase expenses, appliance and maintenance of analyzers. Therefore, in some cases, the application of different dispersion models can provide reliable and necessary information. The possibility of modelling in the air quality management system through the simulation of nitrogen oxide (NO_x) dispersion at a busy road in Zrenjanin is presented in this paper. The modelling was conducted using ADMS-Urban software. To assess the quality of modelled concentrations, a comparative analysis of the modelled measured and NO_x concentrations was performed using sets of quality indicators which showed that in addition to certain limitations in the input data, the deviation error was within the legally prescribed limits.

Keywords: ambient air quality, dispersion models, DMS-Urban software, NO_x concentrations

1. INTRODUCTION

Air pollution has been a major problem in recent decades, having a serious toxicological impact on human health and the environment. Sources of pollution can vary from a single cigarette to volcanic activity or large amounts of emissions from motor vehicles or industrial activities. The long-term effects of air pollution have a major impact on the occurrence of diseases such as respiratory infections and inflammation, cardiovascular dysfunction, and cancer. Therefore, air pollution globally is associated with millions of deaths each year. A recent study showed an association between male infertility and air pollution. Air pollution is currently also present in developing countries because of industrial activities and increasing emissions from inadequate vehicles [1].

Concentrations of certain pollutants such as sulphur dioxide (SO₂), particulate matter (PM₁₀ and PM_{2.5}), ozone (O₃), carbon monoxide (CO), nitrogen oxides (NO_x that make up: NO, NO₂, N₂O) are rising in many cities and in many cases, they are already beyond the standards defined by the World Health Organization. Poor air quality is responsible for the deaths of as many as 3 million people each year and is a problem for millions of people suffering from asthma, acute respiratory diseases, cardiovascular diseases, and lung cancer. The World Health Organization (WHO) has estimated that more than 530 000 premature deaths in Asia are caused by urban pollution. If adequate measures are not taken to reduce emissions from motor vehicles, urban air quality will continue to deteriorate [2].

— Traffic-Related Air Pollution

Transport is a very important and necessary part of modern society, but some of its side effects have also been recognized. From the aspect of environmental protection, a significant negative impact of transport is air pollution. Combustion of one litre of fossil fuels produces approximately 100 grams of carbon monoxide (CO), 20 grams of volatile organic compounds (non-methane volatile organic compounds (NMVOC)), 30 grams of nitrogen oxides (NO_x), 2.5 kilograms carbon dioxide (CO₂) and many other harmful substances. All these substances lead to some degree of air pollution, either by direct impact on health or by global impact, for example causing greenhouse effects and global warming.

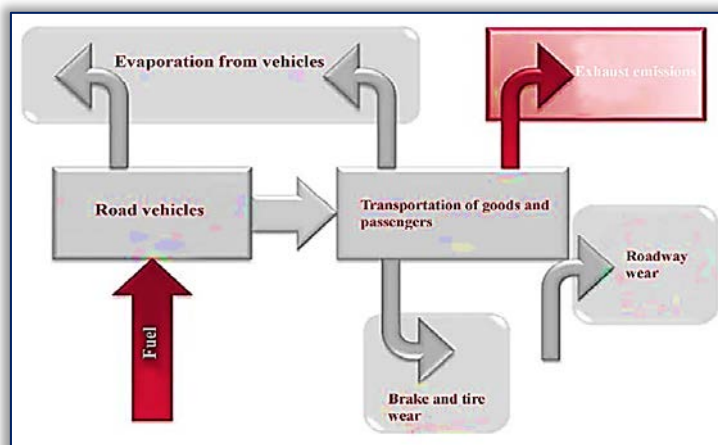


Figure 1. Road traffic emissions flow [3]

In road traffic, exhaust gas emissions are caused by the combustion of fuels (petrol, diesel, liquefied petroleum gas and natural gas) in internal combustion engines. The mixture of air and fuel is ignited by spark (Otto engines) or compression (autoignition in diesel engines) [3]. Emissions from road traffic are shown in Figure 1. The most important pollutants emitted by road vehicles are ozone precursors (CO, NO_x NMVOC), greenhouse gases (CO₂, CH₄, N₂O), acidic compounds (NH₃, SO₂), carcinogenic compounds (polycyclic aromatic hydrocarbons (PAH) and persistent organic compounds (POPs)), toxic substances (dioxins and furans), as well as heavy metals. Figure 2 shows the composition of exhaust gases in diesel and gasoline engines.

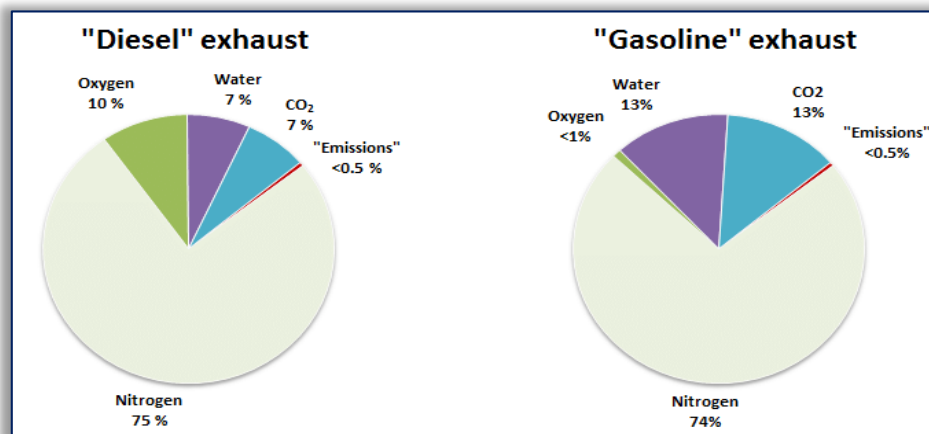


Figure 2. Graphical representation of exhaust gas components from diesel and gasoline engines [4]

Considering that most of the exhaust gases of internal combustion engines are nitrogen oxides, a simulation of this pollutant distribution, at the traffic intersection in Zrenjanin, was performed. The simulation performed in this paper can be an effective tool to supplement regular air quality monitoring and air quality management.

— Pollution distribution modelling

Monitoring certainly represents one of the activities for successful air quality management. The air quality monitoring system establishes local and state measuring station networks and immovable measuring spots on the territory of the Republic of Serbia. The state network includes 40 automatic stations for air quality monitoring. (AQMS-Air quality monitoring station). On the territory of APV in 2005, a network of 7 AQMS was established. One of them which is 15 years old and was out of function for a certain period is currently located in Zrenjanin. Also, on the territory of Zrenjanin, the air quality is monitored at three immovable measuring stations using manual methods (conducted by the Institute of Public Health of Zrenjanin) which calculate the average 24-hour concentration values for the previous day which is adequate if the goal is only to follow the monitoring trends and mere concentration recording. However, these data cannot be used in cases of emergency, when only episodic pollution occurs, cannot identify pollution sources as well as key problems connected to the concentration peaks.

Therefore, considering the size of the city and the present industrial activities, it would be necessary to develop a special, more comprehensive local monitoring network in Zrenjanin that would give more reliable information about air quality.

In such situations, when the data are not available or there are no measurements conducted, the Law on Air Protection [5], as well as the EU Air Quality Directive [6], define the possibility of air quality assessment using modelling. Based on the knowledge about physical, chemical, and thermodynamic laws on fluid transfer in the atmosphere, models of atmospheric dispersion aim to predict the concentration of pollutants at any location and time for familiar parameters of pollutant emissions.

There are numerous models that are used for air pollution dispersion modeling. There variety of models could be expressed for example in resolution (ranking from resolution of 20km to 5000km and global models), equations that are used for dispersion calculation (e.g., mathematical, physics models) etc. Although it is not the state of the art anymore, Gaussian dispersion model is the most used one because of its simplicity [7] (Figure 3).

Gaussian model dispersion is expressed with following equation:

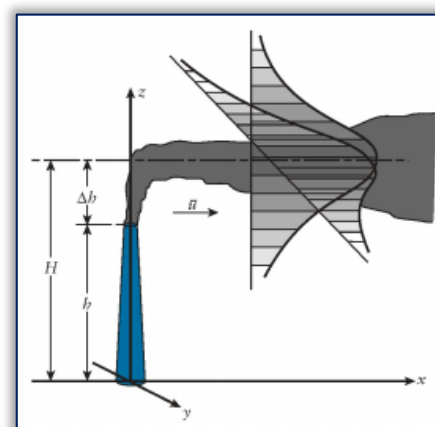


Figure 3. Gaussian dispersion model [7]

$$c(x, y, z) = \frac{Q}{\pi u \sigma_y \sigma_z} \exp\left(-\frac{1}{2}\left[\frac{y^2}{\sigma_y^2} + \frac{(z-H)^2}{\sigma_z^2}\right]\right) \quad (1)$$

where: Q – continual emission from point source (g/m³), by and σz – dispersion coefficients (m), y- average wind speed (m/s), H – point souece height (m).

2. METHODOLOGY

In this research work, ADMS-Urban was used to estimate NOx concentration levels on a busy road, and the quality assessment of the modeled concentrations was performed through a set of quality indicators.

— **ADMS-Urban software**

ADMS Urban is an advanced Gaussian dispersion model developed by Cambridge Environmental Research Consultants, which can simulate air pollution dispersion. To define the boundary layer structure, the model uses the Monin - Obukhov length and boundary layer height. Besides defining the type of the pollution sources (road, point, linear) and pollution intensity (in this case emission rate), a series of additional parameters which include information used to define the areas for modelling (modelling domain definition, surface roughness, road geometry, elevation, and width etc.) were used [8].

— **Vehicle emission assessment**

One of the basic input parameters for ADMS-Urban is the degree of emission caused by vehicles (g/km/s) which programme user can define by himself/herself or with the help of ADMS-Urban software itself which calculates the degree of emission caused by pollutants based on the vehicle composition and traffic flow for the given area.

Traffic flow estimation methods are different, but they all come down to counting vehicles that pass a certain traffic section for a certain time interval. The method type that would be used depends on different factors such as available workforce, budget, instruments etc. Generally, the counting methods are divided into two groups: manual and automatic [9].

For the purposes of this paper and with the aim to assess the pollutant emission degree, manual traffic counting has been performed.

The manual counting method of the traffic volume involves a group of people counting the vehicles passing at a predetermined location using the counting labels in charts (Figure 4). This method of data collecting could be expensive because of the workforce but in most cases it is necessary.

— **Quality indicators**

The estimation of the accuracy of modelled NO₂ concentration was performed using classical statistical indicators. To assess hourly values of the modelled NO₂ concentration, Mean Absolute percentage error (MAPE) was used. Index of Agreement (IA) and Mean Bias Error (MBE) were used for the overall evaluation of the performances of modelled concentrations of NOx.

Index of agreement is a measure how the model will represent the pattern of perturbation about the mean values. Values may range from 0-1 (the ideal is 1) [10].

$$IA = 1 - \frac{\sum_{i=1}^n (O_i - P_i)}{\sum_{i=1}^n (|P_i - \bar{O}| + |O_i - \bar{O}|)} \quad (2)$$

Mean absolute percentage error (MAPE) is a measure of the accuracy of the predicted values compared to the measured ones and it is expressed in percentages [11].

$$MAPE = \frac{100}{n} \sum_{i=1}^n \frac{|O_i - P_i|}{|O_i|} \quad (3)$$

Mean bias error (MBE) – defines if the modeleed concentrationa are overestimated (positive MBE value) or underestimaten (negative MBE value) in comparasion to the measured one [12].

$$MBE = \bar{P} - \bar{O} \quad (4)$$

where: O_i- Observed (mesured) NOx concentration (µg/m³), P_i – Modeled NOx concentration (µg/m³), n – Number of mesurment, \bar{O} - Average value of measured NOx concentration (µg/m³), \bar{P} – Average value of modeled NOx concentration (µg/m³).

Date		Weather conditions		
		1	2	3
Time	1	Temperature		
	2	Humidity and Wind speed		
	3	air pressure and direction		
1				Σ for 10 min
Light vehicles (10 min)				
Heavy vehicles (10 min)				
2				Σ for 10 min
Light vehicles (10 min)				
Heavy vehicles (10 min)				
3				Σ for 10 min
Light vehicles (10 min)				
Heavy vehicles (10 min)				

Figure 4. The manual vehicle counting method

3. RESULTS AND DISCUSSION

— Research domain

In Zrenjanin city, that is located in central part of Banat Region in Republic of Serbia, a numerous industry facilities are located. Industry and location of Zrenjanin, that connects two big cities Novi Sad and the capital, Belgrade, as well as the fact that transit road is not relocated from the city center, contribute to the very intensive traffic. Figure 5 represents location of the Zrenjanin city, as well as the location of the research domain. Close to the busy street, elementary school and student dormitory are located.



Figure 5. Research domain

Using ADMS Mapper software, 3D environment of research domain is defined, creating effect of real surrounding. (Figure 6).

In order to obtain most reliable data, besides 3d environment, the additional input parameters were defined: Surface roughness factor that is defined for urban areas (0,5), Surface albedo for surfaces that are not covered with snow (0.23) and minimum reciprocal Monin-Obukhov length for medium sized cities of 30m.

— Emission factors for NO_x

During the research, the manual method of traffic counting was conducted in three intervals during a single day. The duration of one interval was 10 minutes. The intervals included morning hours, peak hours (from 2 pm to 5 pm) and evening hours when the traffic was not dense. Light vehicles i.e. passenger vehicles, trucks and public transport vehicles were all included while counting. The highest number of light vehicles per hour was 1224 and of trucks was 168. Figure 7 shows the ratio between light and heavy vehicles for data collected in intervals of 10 minutes.

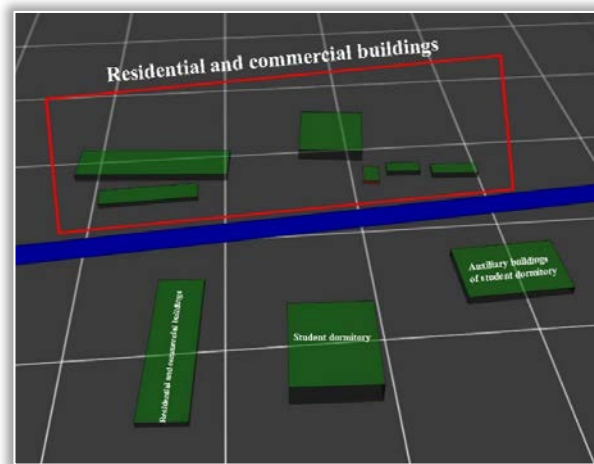


Figure 6. 3D model of the research domain (busy crossroad)

The highest number of light vehicles per hour was 1224 and of trucks was 168. Figure 7 shows the ratio between light and heavy vehicles for data collected in intervals of 10 minutes.

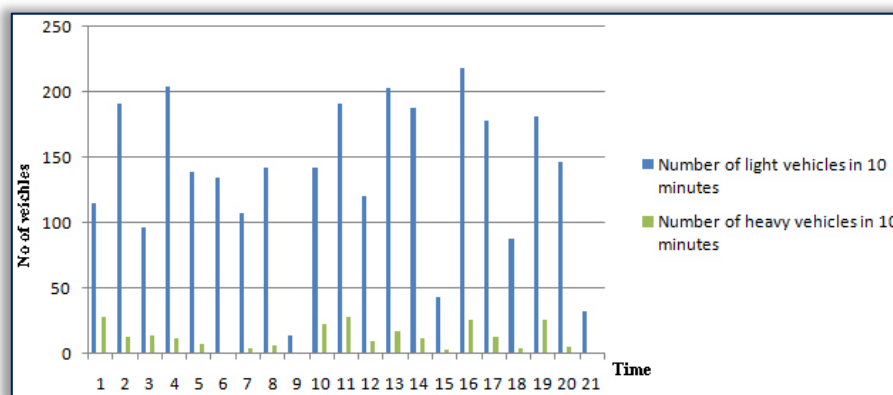


Figure 7. Number of light and heavy vehicles in time of 10 minutes

— Meteorological data and measured NO_x concentrations

In the immediate vicinity of the road that is the subject of the study, there is an automatic air quality monitoring station. The station is used for monitoring the pollution level indicators in the residential business zone, which mainly comes from traffic, but it does not exclude other sources of pollution. At the automatic

station, in addition to pollutants (sulfur dioxide, nitrogen oxides, benzene, toluene, ethylbenzene and xylene), meteorological parameters (temperature, atmospheric pressure, relative humidity, wind direction and speed) are also monitored.

For comparison and quality assessment of data obtained by modeling, data from this automatic station were used for the day when the traffic flow measurement was performed (February 19, 2021).

Meteorological data (wind speed (m/s) and wind direction (°), air temperature (° C), relative air humidity (%), air pressure), were also taken from the automatic air quality monitoring station. During the day 19.2.2021. year, the northwest wind was predominant, with a maximum speed of 2.44 m/s, and the atmospheric temperature ranged from 2.6 to 11.5 ° C. The day was relatively sunny with an average cloud cover of 2 octas.

— Modelled NOx concentrations

After meteorological data processing and 3D modeling of area surrounding, NOx concentration modelling was performed according to all necessary input data. Visual representation of modeled concentration is presented in Figure 8.

According to the data of performed modelling the maximal concentration was 43.6 µg/m³, average modeled NOx concentration was 33.4 µg/m³, and 98.th percentile, C98, was 56.3 µg/m³.

— Comparative analysis of modelled and measured NOx concentration

Analysis were performed by comparative analysis of statistical data of both groups of NOx concentration (Table 1 and Figure 9). Overall performances of modeled concentration are additionally accessed using quality indicators: IA (Index of agreement), MAPE (Mean absolute percentage error) and MBE (Mean bias error).

Comparative analysis results have showed that value of IA was 0.5. Values for this quality indicator could be in range of 0 to 1, and values closer to 1 are considered as a better results (smaller error).

Values for Mean absolute percentage error, MAPE, were 39%. Since MAPE is usually expressed in percentage (0-100%) values closer to 0% are consider better.

Mean bias error, MBE, shows if the modelled values are underestimated (negative MBE values) or overestimated (positive MBE values) in comparison to the measured concentrations. In our case, MBE value were -6,9 µg/m³, that indicates that modelled concentration was slightly under measured concentration. Negative MBE value, in this case, could be interpreted with the fact that the modeling was performed using just traffic influence. Neglecting all the other emission sources that could be significant especially in wintertime when households heating is one of the dominant pollutants in urban areas leads to negative MBE values.

One of the factors that could affect better values of quality indicators are more accurate input data (type of vehicles, fuels, age). Also, hourly NOx emission data would be providing better quality indicators. Although, statistical data and quality indicators have showed some extent of deviation from ideal and expected value, EU Directive on air quality (6) allows 50% deviation for hourly modeled concentrations and 30% for daily modeled concentration that lead us to the conclusion that in this case modeled NOx concentrations are acceptable.



Figure 8. Modelling results

Table 1. Comparative presentation on statistical data on NOx concentration (µg/m³)

NOx concentration	Maximal	Minimal	Average	C98
Modeled	43,6	21,5	33,4	56,23
Measured	60,4	15,6	40,3	60,2

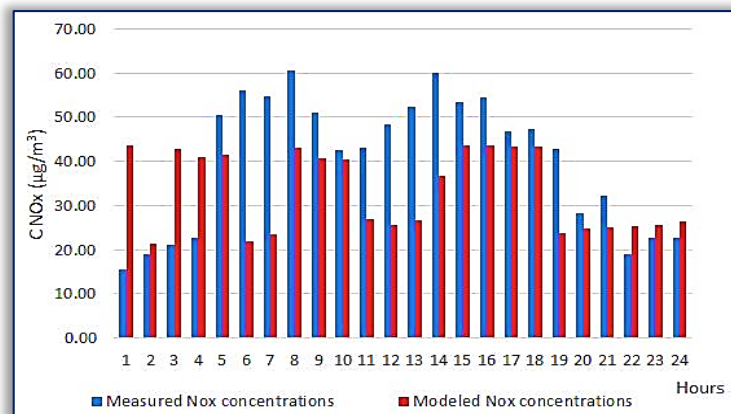


Figure 9. Comparative presentation on statistical data on NOx concentration (µg/m³)

4. CONCLUSIONS

Considering the location and the size of the city of Zrenjanin, the traffic intensity, present industry and the fact that new factories are being opened as well as the fact that Zrenjanin has only one automatic station for measuring pollution concentration that provides real-time data and several measuring stations where the concentration of pollutants is determined by manual measuring methods and which show information on the average concentration of pollutants for the last 24 hours, it could be concluded that the available information on air quality in this town are not satisfactory.

Therefore, to perceive the possibility of performance of pollution dispersion modelling from traffic within the air quality management system, this paper includes conducted modelling which aimed to evaluate the traffic impact on NO_x concentration levels in ambient air. For modelling purposes, ADMS-Urban software was used. The quality evaluation of modelled concentrations was conducted with the help of the following quality indicators: Index of Agreement (IA), Mean absolute percentage (MAPE) and Mean bias error (MBE). The results showed that the obtained modelled concentrations in relation to the measured ones were within the error limits defined by the EU Directive.

As the models for air pollution dispersion simulation are implemented in the legislation of most European countries, based on the research conducted in this paper, it can be concluded that the application of this type of pollution assessment is an essential tool for optimization, air quality improvement strategies and that it supports local, regional and global air protection organizations.

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