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**MATHEMATICAL MODELLING OF ODORANT GASES AND PARTICULATE MATTER
FROM AREA SOURCES IN URBAN ENVIRONMENTS USING AERMOD - WASTEWATER
TREATMENT PLANTS AND TRAFFIC ROADS**

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Abstract: The air quality in urban areas is a major concern of environmental regulation. In developing countries, the urban population increases every year without any planning or management, becoming worse the amount of air quality patterns trespassing events. The several existent forms of land use and occupation also directly influence the dispersion of pollutants. Additionally, recent surveys noticed a large percentage of the population disturbed by odorous gases concentration above the detection limit. The present paper aims to carry out mathematical modelling of gaseous pollutants (odorant and not odorant) dispersion using the AERMOD software. The study intends to calculate concentrations, to understand and discuss two main air pollution problems found in great urban centers in Brazil: odorous gases from wastewater treatment plants and emissions from vehicles. Vehicles have complex calculation of emission rates issuing very dependently on the current fleet and the emission factor. First results of the modelling of hydrogen sulphide gas (H₂S) dispersion proved to be in good agreement with what is routinely felt by the population in the same region of study.

Key words: *Air pollution – Odour emissions – Gaussian modelling – Wastewater treatment – Vehicles emissions*

INTRODUCTION

Highly populated urban areas have a common list of sources of air pollution. Two among the main sources of air pollution are requiring special attention from environmental agencies and the disturbed population: (i) odorant gases emissions from wastewater treatment plants and (ii) particulate matter and gases from vehicles. Odorant gases emission rates and concentration are increasing and many countries do not have any legislation for the maximum concentration allowed in the atmosphere. Vehicles are a special problem in urban centers due to the huge amount of traffic which emits daily tones of particulate matter, carbon dioxide and nitrogen oxide. The environmental agency from the region concerned by the present paper published a technical note informing that 65% of the complaints are due to the air pollution.

Odour emissions from wastewater treatment plants (WWTP) are normally caused by volatilization of organic compounds on water surface or biodegradation of sewage, which its main cause of formation is anaerobic degradation (CAPELLI, 2009). The main odorant compound is the hydrogen sulphide (H₂S). The main impact of H₂S in atmosphere is the annoyance caused to people due to the considerable emission rate and low olfactive perception limit - about 0.5 ppb (SÁ, 2011). The H₂S emission or any material discharged in atmosphere are carried by winds and diluted by turbulence. The dispersion plume of this material follows the mathematical model from Gaussian equation, forming a cone shaped plume. So, in areas nearby the WWTPs there will be higher H₂S concentrations. The Gaussian model can not predict hourly concentration and it does not contain a representative scale of odors, so it is necessary to predict the higher H₂S concentration and analyse if these few seconds of peak have a big impact on human perception (LATOS, 2011).

The absence of public policies for mass transportation and the growing fleet of individual cars strengthen the air pollution indices of this origin. Unfortunately, this reality is not restricted to the transport of people, but also of cargo. The lack of plurality in the transportation of cargo in Brazil, due to the

historical characteristics implanted in the country, reflects in a logistics dependence, in large part, trucks traveling great distances reflect inefficiently, mainly in the aspect of fuel consumption (MMA, 2015). When it comes to air pollutants emitted by vehicles, the concentration depends on several factors such as the type of engine, its regulation, the way of driving and the maintenance of the car. In regions of major traffic congestion, vehicle traffic can account for approximately 90% of CO emissions, 80 to 90% of NO_x, particulate and hydrocarbon pollution, which can cause serious damage to human health, especially respiratory diseases. A form of study of atmospheric dispersion of pollutants in urban centers is the use of the mathematical modelling mechanism to evaluate the efficiency of techniques and strategies proposed for the control of emissions and possible environmental impacts, determination of new measures against the levels of pollution found and, in addition, planning of territorial occupation (concerning the position of stabilization ponds) and the management of vehicles traffic. Recently, many authors have focused on the study of atmospheric dispersion through mathematical modelling, such as the simulated PM₁₀ dispersion in India, as a way of analyzing its concentration on the urban center (KESARKAR, 2007).

The present study used the USEPA software AERMOD, in order to obtain a modelling of the dispersion plume. To approximate the theoretical values to the real one, it is necessary to input some specific data about boundary in AERMOD. This information consists in: terrain model, the roughness, pollutant emission rate, wind magnitude and direction, geographic position of sources. It's necessary to look closer how a WWTP works for H₂S measurement. The preliminary treatment is made by a grit chamber, that retains large particles and remove sand protecting others WWTPs equipments as pumps and pipes. This part of the processes is responsible to emit the biggest part of H₂S, since the sludge is so raw. The mathematical dispersion modelling uses these data as input (PAINE et al., 2016).

METHODOLOGY

Meteorology and computational domain

Atmospheric pollutants are released in the atmosphere and noticed by receptors as a nuisance and presenting health impacts. Information is necessary to obtain specific data about atmosphere and ground occupation, as the studied topography, wind direction, frequency and magnitude, terrain roughness and elevation. The basic input data for AERMOD includes sources location and configuration and local meteorology. In order to obtain meteorological data, AERMET is used, in which a file obtains surface scalar values and contours. To analyze terrain elevation, AERMAP is used before AERMOD. For AERMET, meteorological data of the year of 2015 was acquired from the National Oceanic and Atmospheric Administration (NOAA), creating a Wind Rose (Figure 1(a)) using the *WRPlot* (Lakes Environment) as a tool. *WRPLOT* generates wind rose statistics and plots for several meteorological data formats. Wind rose determines how the wind influences the dispersion of the pollutants and depicts the frequency of occurrence of winds in each of the specified wind direction sectors and wind speed classes for a given location and time period.

Specifically, the wind rose shown in Figure 1, is an average of 1-year data. Evidently, the predominate wind is in the North and the Northeast directions. The magnitude was higher, but it does not happen very often in the Southeast-South and the South-Southwest directions. The meteorological station is located in the middle of the studied region. The selected region is located in the State of Espírito Santo, in Brazil. The analyzed sources are in the district Jardim Camburi, in Vitória and the others in the city of Serra. In order to obtain more details about the terrain, the domain was divided by 4 sectors, characterized with same land use and occupation: Low Intensity Residential, Open Water, High Intensity Residential and Mixed Forests. Each sector presented different values for Albedo and Bowen, used as input data for AERMET, as the AERSURFACE manual of USEPA recommends. Is it worth to say that each modelling (WWTP and traffic roads) was performed in the same region. However, sectors and grid are quite different. For odour emissions modelling, the computational domain was established as 20,4 km x 25,8 km, with 1 km in each axis for the grid, 60 receptors interspaced every 395 meters in horizontal axis and 60 receptors every 310 meters for vertical axis. On the other hand, for vehicles emission we simulated a domain of 24 km x 22 km, where the horizontal axis had 61 receptors and vertical axis 55 receptors. The AERMAP terrain preprocessor, which uses U.S. Geological Survey (USGS) Digital Elevation Model (DEM) data as

an input, may also be used to generate the terrain elevations for the receptor locations. It is helpful to determine and analyze the topography of the region. The AERMAP program generates an output file that contains the receptor pathway data for AERMOD, along with the AERMET file. Data about the emissions is input in the AERMOD file. The AERMOD model produces a main output print file of model results. This file is used in the Surfer tool to generate the dispersion plume of H₂S.

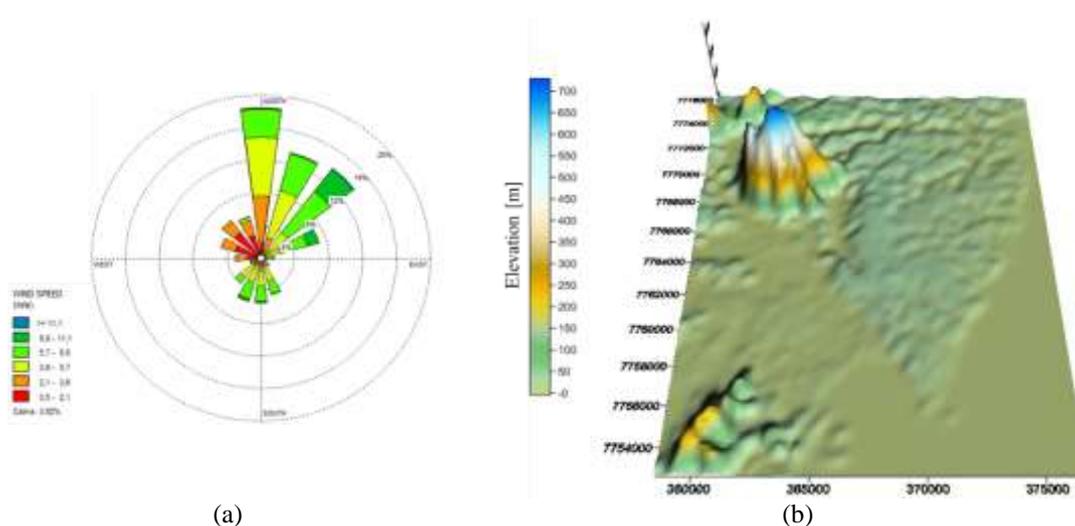


Figure 1 – (a) Wind rose: data represent an annual average; (b) Digital elevation model of the studied region

Emission rate quantification

Odour emission rate quantification from wastewater treatment plants

A very important point about the atmospheric dispersion modelling procedure is the correct quantification of its emission. Several parameters from the sources are defined in this step and if it is not taken in the characteristics, the simulation will have a huge chance of obtaining a result that does not describe correctly the situation (GOMES, 2012). In wastewater treatment plants (specifically stabilization ponds) the odour emissions can be influenced by different factors as the components of the wastewater, the methods and the conditions of the treatment (like Reynolds number, temperature, pH, time of hydraulic detention). The emissions factors allow to quickly and easily estimate the general emissions from a wastewater treatment industry (CAPELLI et al, 2009), the calculus of the emission factor is given by Equation 1,

$$\text{OEF} = \text{OER} / \text{C} \quad (1)$$

where OEF is the emission factor in ou/m³ and OER is the emission rate in ou/year and C is the early treatment capacity in m³/year. The OEF represents the quantity of emitted odour related to the wastewater volume unit, i.e., it is expressed in odour units per cubic meter of treated sewage. The OEF must be evaluated separately for each part of the treatment and for each odour source, considering that each odour source is represented by the single treatment phases of the depuration cycle. The odour sources considered for this study are: Wastewater arrival, Pre-treatments and Secondary sedimentation.

Emission rate of vehicles air pollution

Identifying the proper share of cars' contribution to air pollution becomes complex, as several factors, such as engine type, fuel, maintenance and age of the fleet, interfere with the estimation of pollutants. For example, trucks and buses that use diesel as fuel are responsible for the higher fraction of emissions of NO_x and SO_x, while light vehicles using alcohol or gasoline are responsible for most of the emissions of carbon monoxide (CO) and hydrocarbons. In addition, there are other references such as Paine et al (1998), Hanna et al. (2001)) and Perry et al (2005). In this study, the first part of the present study aims to

estimate the emission rate of the pollutants Carbon Monoxide (CO) and Nitrogen Oxides (NO_x) and evaluate the use of the AERMOD air quality model to model the dispersion of atmospheric emissions, as well as to quantify the contribution of several avenues with large traffic in the city of Vitoria, concerning its emission and dispersion of pollutants. The software used, AERMOD, is a modelling system for the dispersion of pollutants in the atmosphere based on turbulence concepts in the planetary boundary layer, and includes the treatment of both surface and elevated sources, and simple and complex terrain. The input data for the calculation of emission rates was obtained in the national inventory for vehicles air pollution.

RESULTS

Hydrogen sulphide concentration plume and perception limits

As a result of computational combinations and using the Software Surfer as a tool, the dispersion plume of H₂S was created as shown in Figure 2. The colormap shows the results of odour concentration in OU/m³ as the emission rate input in AERMOD software was OU/s. Two regions are highlighted in the image: Jardim Camburi district (south of the computational domain) and Serra (north of the computational domain). In Jardim Camburi, one WWTP with three stabilization ponds are responsible for the pollution. In Serra, at least twenty ponds were considered. It is worth to observe how serious is the odourant gases dispersion problem. The highly concentrated lines of same concentration are the worst case where the H₂S concentration is certainly above the perception limit. The odour concentration was calculated as a 5-minutes average following the methodology presented by Dourado et al. (2012).

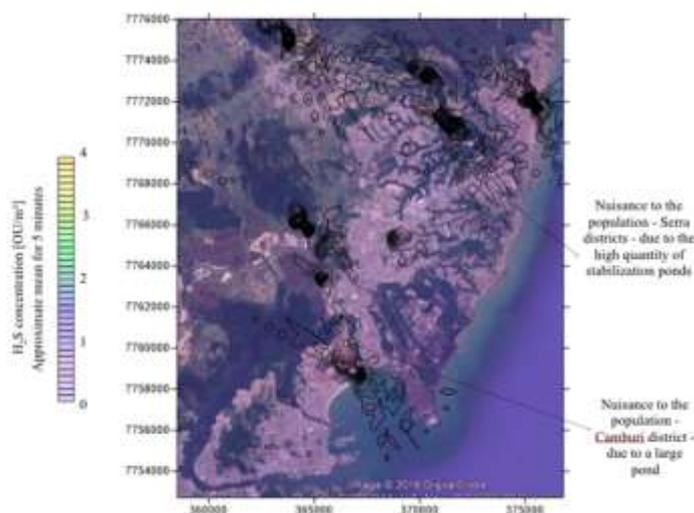


Figure 2 – H₂S dispersion modelling plume

The odour concentration can be multiplied by the air flow rate, cubic meters per second, resulting in a pseudo-dimension of “odour units per second,” analogous to grams per second. Because “odour concentrations” from 7 different source types cannot be “added” nor can they be “averaged,” odour modelling must be conducted with caution. The resulting “odour concentration” value of “1”, calculated by a dispersion model, represents the odour detection threshold that was determined using the “best estimate criteria.” A value of less than 1 represents “no odour” or “sub-threshold.” A value of greater than 1 represents “odour” at a “supra-threshold” level (MCGINLEY, 2000). The unit used in this study is odour unit per second or OU/s.

CO and NO_x dispersion from vehicles emissions

Vehicles emits several types of pollutants. In the present extended abstract two pollutants (CO and NO_x) were chosen to be modelled as the emission factors were more faithful. Particulate matter will be modelled for a second part of the present study. The modelling of line sources (avenues) as area sources

worked well in the AERMOD software. For CO and NO_x the concentration did not trespass the limit established by the local air quality regulation. The concentration peaks of pollution from vehicles are located on the highest elevations. The concentration presented in Figure 3 is a 8-hour average for both dispersion plumes (this is the reason for the same shape of plumes in each plot).

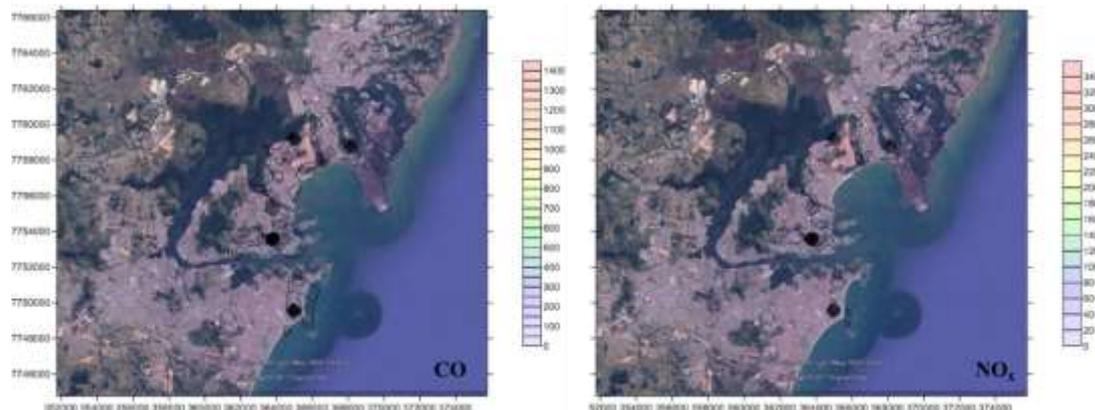


Figure 3 – Dispersion of CO and NO_x emitted from vehicles. Concentration values are in µg/m³.

CONCLUSION

The prediction of pollutants concentration in urban regions faces great challenges. Since experimental analysis of field can be costly, execution is difficult, and applications are limited, the mathematical modelling is presented as an alternative, especially the gaussian model, which presents low computational cost and is applicable for a large computational domain representing a metropolitan region. In addition, the sources investigated still represents a major challenge for air pollution modelers: odorous gases and vehicles. The several existent forms of land use and occupation also directly influence the dispersion of pollutants. This is because the process of urbanization is determinant for the emergence of industries, volume of traffic of vehicles and commercial and residential buildings. These structures tend to behave as obstacles to the dispersion of atmospheric pollutants, including roughness on the natural surface of the terrain. The present paper carried out mathematical modelling of gaseous dispersion using the AERMOD software. The study intended to calculate concentrations, to understand and discuss about two main air pollution problems found in great urban centers in Brazil: odorous gases from wastewater treatment plants and emissions from vehicles. Vehicles have complex calculation of emission rates issuing very dependently on the current fleet and the emission factor. First results of the modelling of hydrogen sulphide gas (H₂S) dispersion proved to be well suited as the average modelled concentrations are in good agreement with what is routinely felt by the population in the same region of study.

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