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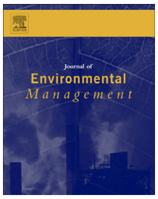

Mathematical modeling of sulfur dioxide concentration in the western part of Romania

Alina Barbulescu [a, b], Lucica Barbes [a, *]

[a] Ovidius University of Constanta, 124 Mamaia Blvd., 900527, Constanta, Romania
[b] Higher Colleges of Technology, University City, P.O. Box 7947, Sharjah, United Arab Emirates

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ABSTRACT

Nowadays air pollution is a major issue, due to its effect on the human health and environment. Therefore, in this article, we analyze the evolution of sulfur dioxide (SO_2) concentration for eight months (November 2015–June 2016) at three monitoring stations in Timisoara, Romania. The results indicate that the legal limits have been exceeded only a few times and the pollutants' distribution is strongly influenced by the relative atmospheric calm in the County. We also propose a new model for the SO_2 dissipation, which takes into account the individual data series, as well as the specific atmospheric conditions.

1. Introduction

Air pollution has significant negative effects on the human health and environment. Therefore, particular attention must be given to monitoring and improving the air quality, which is strongly influenced by emissions from stationary sources (thermal power plants, industrial facilities etc.), pollution from diffuse and mobile sources (traffic) and the pollutants' transport at long distances (Bauduin et al., 2014; Meraz et al., 2015).

One of the gases with atmospheric acidifying effect is the sulfur dioxide (SO_2), which is a highly reactive gas, flammable, with a pungent odor, which irritates the eyes and the respiratory system. It appears mainly from burning sulfur fossil fuels (coal, oil) and the exhaust of vehicles' engines. The value of anthropogenic emissions of sulfur in the atmosphere, generated by burning coal and sulfur-rich smelting, is estimated at 80 Tg/year, the plants with large combustion capacity being the main source of pollution (about 67%). In Romania, the total sulfur oxides emissions (SO_x) in SO_2 equivalent are 241,864 t/year (EEA, 2015), the largest contribution being that of the energetic sector, as follows: approximately 97% of power stations and other combustion plants and approximately 2.04% of oil and gas refineries.

SO_2 transformation processes in the air can lead to the atmosphere acidification and the apparition of acid rain. SO_2 can persist in the atmosphere for a few hours or a few days and can be transported at hundreds of kilometers. The topography of the human settlements and the climatic conditions of atmospheric calm or thermal inversion can prevent the pollutants' spread, leading to their accumulation for short periods of time.

For monitoring and reducing the air pollution, in 2011 Romania adopted the Law no. 104 concerning the ambient air quality, which is in concordance with the Directives 2004/107/EC and 2008/50/EC of the European Parliament on the ambient air quality for cleaner air in Europe. Accordingly, the admissible limits of the SO_2 concentrations in the ambient air are the following. The hourly limit value for the human health protection is 350 $\mu g/m^3$, and must not be exceeded more than 24 times/year. The daily limit value for the human health protection is 125 $\mu g/m^3$, and must not be exceeded more than three times in a year. The upper evaluation threshold for the human health protection is 75 $\mu g/m^3$, and must not be exceeded more than three times in a year. The maximum alert threshold for SO_2 is 500 $\mu g/m^3$, measured three consecutive hours at the monitoring stations situated in an area of 100 km^2 or for an entire zone or town (M.O., 2011).

Observing the anthropogenic sources is an essential component of atmospheric global models (Crippa et al., 2016). Big data sets of emissions from geographic regions with a multitude of main

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* Corresponding author.
E-mail addresses: emma.barbulescu@yahoo.com (A. Barbulescu), lucille.barbes2009@gmail.com (L. Barbes).

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pollution sources are usually estimated using complex algorithms (Elkamel et al., 2008; Yim et al., 2010; Li and Xie, 2016), whose input data may include parameters such as the fuel consumption in the area of the monitoring stations of traffic type and the efficiency of the systems of removal the pollutants' emissions (Streets et al., 2003; Carn et al., 2007).

Different mathematical techniques, like statistics, artificial intelligence (Barbes et al., 2009), remote sensing (Gibson et al., 2013; Koukouli et al., 2016), etc. can be used for analyzing the pollutants' series of the spatial variation of the models' parameters that could be updated in real time (Adams and Kanaroglou, 2016). Descriptive statistics provide indicators related to the measures of central tendency, dispersion and correlation of pollutants series (Pedrero et al., 2009; Barbulescu and Barbes, 2013, 2014, 2016). Statistical methods are used for establishing correlations between meteorological variables and pollutants' concentrations in the atmosphere (Barbulescu and Barbes, 2014; Gao and Washington, 2009; Hosseiniebalam and Ghaffarpasand, 2015; Zannetti, 1990). Fast Fourier Transform or Continuous and Discrete Wavelets Transforms proved to be efficient tools for analyzing the cycles of contaminant series (Rodriguez et al., 2008).

In this context, our research aims at studying the distribution of mean SO_2 concentration in Timisoara, to compare the characteristics of the pollutants series collected at different monitoring stations and to determine a common model for the concentration series function of the atmospheric temperature and humidity and the wind speed.

2. Data and methods

2.1. Site description and data

Timisoara is located in Romania, at the confluence of Timis and Bega Rivers, at 45°44′ northern latitude and 21°13′ eastern longitude. Timisoara benefits from a moderate continental climate, characterized by diversity and irregularity of atmospheric processes. Being under the influence of the maritime air masses from the north-west, Timisoara receives a higher amount of precipitation than the cities situated in the Romanian Plain (RO, 2012). The annual precipitation average of about 650 l/m^2 is achieved mainly due to the high amount of precipitation recorded in May–July and, respectively, in November–December, when a secondary maximum is registered. The winds' distribution (from the north-western and western part) affects to some extent the air quality in Timisoara because the pollutants emitted by the industrial plants situated in the western and southern part of the town are driven towards the city. The predominant atmospheric calm facilitates the persistence of the pollutants over the city.

The dynamics of the economic development the last 10–15 years makes Timisoara the best business city in the Western Romania. With a population of over 300,000 inhabitants (INSE, 2015), the urban concentration spans over a total area of 485.9 ha, with 15.85 m^2/inhabitant green space and only 88 ha of recreational areas. The main pollution sources in Timisoara are the two district heating plants (CHP Center and CET - South), a tire factory (S.C. Continental Automotive Products SRL) and two factories that use chemical reagents (S.C. Detergents S.A and S.C. Azur S.A.).

In Timis County, the air quality is continuously monitored through seven automatic measuring stations belonging to the National Network for Monitoring Air Quality (RNMCA), equipped with physicochemical analyzers that measure the concentrations of sulfur dioxide, nitrogen oxides, carbon monoxide, volatile organic compounds, ozone, particulate matter (PM_{10} and $PM_{2.5}$) in the ambient.

In Timisoara city, there are two stations of type traffic – **TM1**-Calea Sagului (45°43′40.22″ N; 21°12′17.36″ E; 87 m altitude; intense traffic > 10.000 vehicles/day), **TM5 -** Calea Aradului (45°46′35.28″ N; 21°13′14.84″ E; 91 m altitude; intense traffic > 10.000 vehicles/day) and one station of urban type - **TM2** – C. D. Loga Blvd. (45°45′16.88″ N; 21°14′05.91″ E; 92 m altitude; traffic of 2.000–10.000 vehicles/day).

For studying the extent of the SO_2 pollution in Timisoara, the hourly concentrations recorded at TM1, TM2 and TM5 have been downloaded daily from the site of Romanian National Environmental Monitoring Center (http://www.calitateaer.ro/) from 1st of November 2015 till 20th of June 2016. They are reliable data, with no gap.

2.2. Mathematical methodology

The steps of our study are the following:

(1) Statistical analysis of the hourly and daily average data.
(2) Analysis of the evolution of the maximum daily concentrations and comparison with those stipulated in the legislation.
(3) Testing the null hypothesis that the series collected at TM1, TM2 and TM5 come from the same population, against the hypothesis that they come from populations with different distributions. For this aim, the two - sample Kolmogorov-Smirnov test was used (Marsaglia et al., 2003). If the p-value associated with the test statistic is less than the significance level, then, the null hypothesis can be rejected. Alternatively, the null hypothesis is rejected if the value of the test statistic is greater than the critical value given in the table of two-sample Kolmogorov-Smirnov test.
(4) Study of the autocorrelation of pollutants' data at the stations, and in the case of the correlation existence, predicting the evolution of the series using the simple exponential smoothing, given by the formula:

$$\hat{y}_{t+1} = \hat{y}_t + \alpha(y_t - \hat{y}_t), \tag{1}$$

where: $\alpha \in (0, 1)$ is the smoothing parameter, that must be determined, y_t is the recorded value at the moment t and $\hat{y}_t$, $\hat{y}_{t+1}$ are the values evaluated respectively at the moment t and $t+1$ (Brown, 1956).

The parameter α is estimated by minimizing the prediction errors. The mean absolute deviation (MAD) and the mean standard deviation (MSD) have been used to estimate the estimation accuracy.

(5) Modeling the dependence between the SO_2 concentration, humidity and temperature of the air and the wind speed.

Starting from the remark that there is a dependence between the SO_2 concentration and the humidity and an inverse relationship between the concentration and the wind speed, we tested two models. The first one has the equation:

$$c \times v = A_i \times H^{\alpha_1} \times e^{\alpha_2 T} \times \eta, \tag{2}$$

where v is the wind speed, H is the humidity, T - the temperature, η is the random variable, A_i is a constant term (that differs function of the monitoring site), α_1, α_2 are coefficients to be computed.

Taking logarithm in (2), it results the equivalent form:

$$\ln(c \times v) = k_i + \alpha_1 \ln H + \alpha_2 T + \varepsilon, \tag{3}$$

where $k_i = \ln A_i$, $\varepsilon = \ln \eta$.

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