Investigation of the dynamic variability in the amount of contaminants in urbanized atmosphere

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Abstract. The dynamic variability in the amount of contaminants in urban atmosphere and the mathematical models which allow describing the given variability have been analyzed. The models of the seasonal variation in the amount of solid particles in the atmosphere of Volgograd were developed based on Fourier series. The seasonal index was determined. A dynamic equation characterizing the seasonal variability in the amount of solid particles in the atmosphere of Volgograd was obtained applying the method of analytical seasonal adjustment.

Nomenclature
C - annual average concentration of dust, μg/m³,
Ci - calculated value of annual average concentration, μg/m³,
c - average dust concentration in the considered month within the period under investigation, μg/m³.

Introduction
The parameters of urban atmosphere pollution are determined by variations in emissions from industrial enterprises and transport infrastructure as well as in climatic factors and show a significant temporal variability [1, 2, 5-11].

The article [8] describes the conducted investigations into the variation in the concentration of fine dust (PM_{10}), carbon oxide, carbon dioxide and nitrogen dioxide during the warm and cold periods of a year in the atmospheric air of St. Petersburg, which allowed concluding on the seasonal variations in the concentration of contaminants. In the cold period, the concentrations of all the pollutants are higher, and a more close relationship is observed between contaminants concentration and meteorological factors than in the warm period of a year.

Climatic parameters exert different influence on the contaminants concentration depending on the season of a year. Thus, air humidity does not significantly influence the concentration of harmful substances in the cold period, while in the warm period the level of carbon oxide and nitrogen dioxide increases by 2-3 times and the level of nitrogen oxide increases by 5 times with the growth of humidity values. The amount of harmful substances in the atmosphere increases when the temperature is lower than -25°C, and a sharp rise in the concentrations of carbon oxide and suspended particles is observed when the temperature exceeds +30°C.
The investigations of the seasonal variations in the ecological conditions of the air environment in Tambov applying the Air Pollution Index (API) showed that the seasonal variations of the index are insignificant throughout the territory of the city. In spring-summer period, the level of API is higher and amounts to 3.84, on the average. In autumn-winter season, the level of API decreases and reaches the value of 3.32 [6].

The results of the multiannual investigations analyzed in the paper [11] also allow drawing a conclusion on the seasonal variability of air pollution with fine particles. Winter period is characterized by a steady level of the content of particles PM$_{10}$, and quite the opposite, the parameter varies within a wide range in spring period. Cases of considerable exceedance over the hygiene standards are registered, especially when the temperature fluctuates and the air humidity decreases.

S.V. Mikhaylyuta carried out investigations applying a mobile laboratory and revealed the specific features of the spatial and temporal variability in pollutants concentration in the atmosphere of Krasnoyarsk [10]. The spatial and temporal distribution of the concentrations of harmful substances in the atmosphere is determined by the dynamics of traffic flows, by the non-uniformity of the landscape and temperature levels in the city. The temperature non-uniformity in the territory in the winter period leads to a 1.5 times increase in the level of pollution with carbon oxide and nitrogen oxide in the central part of the city. Such an increase for sulphur dioxide is of higher significance.

In summer, the atmospheric circulation and the city landscape induce an increase in the pollution level by four times or higher.

A considerable seasonal variation in contaminants in the atmosphere is registered in the paper [9].

The investigations into the atmospheric pollution with particulate matter PM$_{10}$ in the city of Vladivostok revealed a seasonal variability [5]. The winter period is characterized by a steady amount of particulate matter PM$_{10}$, in spring this parameter varies within a wide range and the cases of considerable exceedance over the standard values are registered, especially in the case of fluctuations in temperature and an increase in humidity.

**Review**

The dynamic processes in ecology are studied in variety of ways [3, 12]. Among them, modeling is the most promising method.

Additive and multiplicative models are known [12]. In the additive model, the seasonality is expressed through a certain number which is added to or subtracted from the trend value, while in the multiplicative model it is expressed as percentage of the trend value. Both models use either integral or seasonal average indexes as the initial data.

The paper [12] suggests a formula for the periodic process approximation with a trigonometric polynomial according to the least square method in the interval (0;2$\pi$):

\[ Y = \tilde{\lambda}_0 + \sum_{k=1}^{m} (\tilde{\lambda}_k \cos kx + \tilde{\mu}_k \sin kx) \]  

(1)

At the equidistant argument values $x_i$, the estimations of the coefficients $\lambda_k$ and $\mu_k$ are determined according to Bessel’s formulas at k=1,2,3…….m:

\[ \tilde{\lambda}_0 = \frac{1}{n + 1} \sum_{i=1}^{n} y_i \]  

(2)

\[ \tilde{\lambda}_k = \frac{2}{n + 1} \sum_{i=1}^{n} y_i \cos kx_i \]  

(3)
\[ \tilde{\mu}_k = \frac{2}{n+1} \sum_{i=1}^{n} y_i \sin kx \]  

The computation according to the given formulas is rather laborious. There exists a method for the periodic process approximation applying Fourier series [3, 12]:

\[ y_1 = a_0 + \sum_{k=1}^{m} (a_k \cos kt + b_k \sin kt) \]  

The coefficients are calculated according to the equation (6), (7), (8):

\[ a_0 = \frac{1}{n} \sum_{k=1}^{n} y_k \]  

\[ a_k = \frac{2}{n} \sum_{k=1}^{n} y_k \cos kt \]  

\[ b_k = \frac{2}{n} \sum_{k=1}^{n} y_k \sin t \]  

The approximation obtained applying one or two harmonics is considered to be a rather good one. For the purpose of the investigation of seasonality, \( n \) is often assumed to be equal to the number of months in a year. Then the first harmonic has the form:

\[ y_1 = a_0 + a_1 \cos t + b_1 \sin t \]  

Then:

\[ a_0 = \frac{1}{12} \sum_{k=1}^{12} y_k \]  

\[ a_k = \frac{1}{6} \sum_{i=1}^{12} y_k \cos t \]  

\[ b_k = \frac{1}{6} \sum_{i=1}^{12} y_k \sin t \]  

In the case of such approximation, the trend of the process stays constant and equals to \( a_0 \).

In order to describe the seasonal variations in the concentration of a harmful substance in the air, we assume \( n=12 \) (equal to the number of months in a year), then the equation (5) will have the form:

\[ C = a_0 + a_1 \cos t + b_1 \sin t \]  

The amount of solid particles in the air of Volgograd in the period from 2006 to 20017 was analyzed to reveal the seasonal variations. The data were based on the “State reports on the environmental conditions in the city of Volgograd” [4]. Table 1 presents the analysis of the seasonality of variations in dust concentration in the air of Volgograd (c, mg/m³).

The equation of the seasonal model will have the form:
\[ c = 5.62 - 0.05 \cos t - 0.22 \sin t \quad (14) \]

“\( c \)” is the average dust concentration in the considered month within the period under investigation, \( \mu g /m^3 \).

**Table 1.** Analysis of the seasonality of variations in dust concentration in the air of urbanized territory.

| Month     | t     | c    | \( \cos t \) | \( \sin t \) | \( c\cos t \) | \( c\sin t \) | \( y_t \) |
|-----------|-------|------|--------------|--------------|---------------|---------------|-----------|
| January   | 0     | 4.87 | 1.000        | 0            | 4.87          | 0             | 4.62      |
| February  | \( \pi/6 \) | 5.52 | 0.866        | 0.5          | 4.78          | 2.76          | 4.78      |
| March     | \( \pi/3 \) | 6.08 | 0.500        | 0.866        | 3.04          | 5.27          | 4.31      |
| April     | \( \pi/2 \) | 6.24 | 0.000        | 1            | 0             | 6.24          | 6.99      |
| May       | 2\( \pi/3 \) | 4.77 | -0.500       | 0.866        | -2.39         | 4.13          | 4.83      |
| June      | 5\( \pi/6 \) | 5.01 | -0.866       | 0.5          | -4.34         | 2.51          | 5.35      |
| July      | \( \pi \) | 6.18 | -1.000       | 0            | -6.18         | 0             | 6.00      |
| August    | 7\( \pi/6 \) | 5.46 | -0.866       | -0.5         | -4.73         | -2.73         | 6.46      |
| September | 4\( \pi/3 \) | 4.14 | -0.500       | -0.866       | -2.07         | -3.59         | 6.25      |
| October   | 3\( \pi/2 \) | 8.86 | 0.000        | -1           | 0             | -8.86         | 7.56      |
| November  | 5\( \pi/3 \) | 5.46 | 0.500        | -0.866       | 2.73          | -4.73         | 6.56      |
| December  | 11\( \pi/6 \) | 4.62 | 0.866        | -0.5         | 4.00          | -2.31         | 5.92      |
| Total     | -     | 67.75 | -           | -            | -2.38         | -0.3          | -1.32     |

The seasonal index, i.e. the ratio of the average value of the actual levels for similarly-named months to the average value of the adjusted levels for the same months [3], is presented in Table 2:

\[ I_{\text{seasonal}} = \frac{y_i \text{ actual}}{y_i \text{ average}} \quad (15) \]

The mean-square deviation of the seasonal index from 100% serves to show the degree of the time series variability due to the seasonal nature of the process:

\[ \sigma = \frac{\sqrt{(i - 100)^2}}{12} \quad (16) \]

The obtained values are given in Table 2.

**Table 2.** Seasonal index and the mean-square deviation of the seasonal index from 100%.

| January | February | March | April | May | June | July | August | September | October | November | December |
|---------|----------|-------|-------|-----|------|------|--------|-----------|---------|----------|----------|
| 1.01    | 1.15     | 1.41  | 0.89  | 0.99| 0.94 | 1.03 | 0.85   | 0.67      | 1.10    | 0.83     | 0.78     |
| 0.83    | 1.25     | 3.41  | 1.2   | 0.75| 0.5  | 0.25 | 1.25   | 2.75      | 0.83    | 1.42     | 1.83     |

A method of periodic process approximation by a function is known:

\[ y = a + bx \cos \frac{2\pi t}{T} \quad (17) \]
In this case, the trend of the process remains constant, which reduces the accuracy of the computations if it is actually growing or decreasing.

In order to reveal the main trends of ecological processes development, seasonal adjustment methods are used, among which analytical seasonal adjustment is an efficient one [3]. The essence of the analytical seasonal adjustment method is to choose a theoretical curve for the given time series which reflects the main features of the actual dynamics. For this purpose, the least square method is often used.

According to the least square method, we have a system of normal equations:

\[ \sum_{t} a_{0} + a_{1} \sum_{t} t = \sum_{t} y, \]
\[ a_{0} \sum_{t} t + a_{1} \sum_{t} t^2 = \sum_{t} ty \]

\( n \) - the number of members of the time series.

The system of equations simplifies if the zero-time reference is transferred to the middle of the period under consideration.

Then the coefficients can be found according to the following equations (19), (20):

\[ a_{0} = \frac{\sum_{t} y}{n}, \]
\[ a_{1} = \frac{\sum_{t} ty}{\sum_{t} t^2}. \]

In order to reveal the seasonal variations, the amount of solid particles in the air of Volgograd in the period from 2006 to 2017 was analyzed. The data were based on the “State reports on the environmental conditions in the city of Volgograd” [4].

The calculated values for determining the dynamics equation are given in Table 3.

| Year | Level, \( t \) | \( C_{i} \), \( \mu g/m^3 \) | \( t^2 \) | \( C_{ti} \) | \( C_{ai} \), \( \mu g/m^3 \) |
|------|----------------|-----------------|--------|---------------|-----------------|
| 2006 | -6             | 121             | 36     | -726          | 120.928         |
| 2007 | -5             | 124             | 25     | -620          | 119.120         |
| 2008 | -4             | 120             | 16     | -480          | 117.312         |
| 2009 | -3             | 113             | 9      | -339          | 115.504         |
| 2010 | -2             | 108             | 4      | -216          | 113.696         |
| 2011 | -1             | 108             | 1      | -108          | 111.888         |
| 2012 | +1             | 111             | 1      | 111           | 108.272         |
| 2013 | +2             | 110             | 4      | 220           | 106.463         |
| 2014 | +3             | 101             | 9      | 303           | 104.654         |
| 2015 | +4             | 101             | 16     | 404           | 102.845         |
| 2016 | +5             | 102             | 25     | 510           | 101.0365        |
| 2017 | +6             | 102             | 36     | 612           | 99.227          |
| Total| 0              | 1321            | 182    |               | -329            |

“\( C \)” is the annual average concentration of dust, \( \mu g/m^3 \). “\( C_{i} \)” is the calculated value of annual average concentration, \( \mu g/m^3 \).

The dynamics equation has the form:

\[ C = 110.08 - 1.8087t \]
The mean square of the deviations of the actual levels of time series from the variable levels computed according to the trend on the basis of the data from Table 3 $\sigma_i^2 = 8.86$ serves as the measure of variability of the time series level. The relative measure of variability is determined by the equation (22):

$$V_i = \frac{\sigma_i}{n}$$  \hspace{1cm} (22)

In the present case, $V_i = 0.08 = 8\%$. This quantity serves as the criterion of the accuracy of the choice of trend equation.

There also exists a method called the periodogram analysis [12]. It develops the application of Fourier series for the analysis of seasonal processes. The principle of the method is to find the period of a fluctuating process ($T = \frac{2\pi}{\alpha}$) in Fourier series:

$$f(x) = A_0 + A_1 \sin(\alpha t + \beta) + A_2 \sin(2\alpha t + \beta) + \ldots$$  \hspace{1cm} (23)

The computation procedure is rather laborious and the possible changes in the trend are not taken into account.

A way to investigate a periodic process through functions is suggested [12]:

$$y = at + b + c \sin \left( \frac{2\pi}{T} t \right)$$  \hspace{1cm} (24)

or

$$y = at + b + c \cos \left( \frac{2\pi}{T} t \right).$$  \hspace{1cm} (25)

In this case, the part of the function $at+b$ shows the trend of the process, and the sine curve models the periodic process developing around the trend.

The least square method and Cramer theorem are used to obtain the coefficients [3, 12].

Mathematical models have been developed, which allow obtaining the values of future time series based on their previous values [104, 125]. The autoregressive moving-average model is referred to this group of models; it can also be used in the case of nonstationary time series characterized by a polynomial trend [12].

The paper [7] suggests that cognitive modeling is used to investigate seasonal variations in climate. A model based on cognitive maps of the mechanisms of chemical pollution of an urban ecosystem in summer and winter periods has been developed. The use of cognitive technologies with map development as the basis for further modeling of various scenarios of the investigated processes allows both forecasting the possibility of occurrence of some ecological situation and taking a series of measures aimed at reducing the environmental risk degree. Based on the investigation of the seasonal variation in the form of pollution, the author suggests the development and use of the seasonal values of the MPC of polluting substances [7].

2. Conclusions

1. The authors carried out the analysis of the dynamic variability in the amount of contaminants in urban atmosphere as well as of the mathematical models which allow describing the given variability.
2. The models of the seasonal variation in the amount of solid particles in the atmosphere of Volgograd were built applying Fourier series. The seasonal index was determined.
3. Applying the analytical seasonal adjustment method, the dynamics equation was obtained, which characterizes the seasonal variability in the amount of solid particles in the atmosphere of Volgograd.
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