ECOLOGY

Розглянуто використання оцінки значень функції невизначеності щодо виявлення небезпечних станів для довільного вектора атмосферних забруднень. При цьому оцінку функції невизначеності пропонується проводити в рухомому по траєкторії вектора станів вікні фіксованої ширини. Це дозволяє не тільки виявляти моменти виникнення небезпечних станів атмосферних забруднень, але і одночасно визначати їх радіальну швидкість щодо поста контролю. Нульова радіальна швидкість небезпечних станів атмосферних забруднень дозволятиме виявляти поточні стани атмосфери, у яких відсутнє розсіювання забруднень у повітрі. Саме такі стани виявляються особливо небезпечними, оскільки призводять до накопичення забруднень та зростання їх концентрації в атмосфері. Верифікація можливості використання функції невизначеності щодо виявлення небезпечних станів вектора атмосферних забруднень проводилася на прикладі експериментальних даних. При цьому в якості небезпечних складових вектора станів атмосферних забруднень розглядалися: формальдегід, аміак і оксид вуглецю. Результати верифікації в цілому свідчать про можливість використання функції невизначеності для виявлення небезпечних станів вектора атмосферних забруднень. Встановлено, що використання функції невизначеності виявляється інваріантним по відношенню до нерегулярності реєстрації атмосферних забруднень на стаціонарних постах контролю. Показано, що застосування функції невизначеності забезпечує виявлення небезпечних станів, що характеризуються не тільки перевищенням граничних допустимих концентрацій, а також нульовою радіальною швидкістю їх переміщення щодо пункту контролю. Експериментально встановлено, що для виявлення небезпечних станів забруднення атмосфери протяжність вікна повина становити від 4 до 8 відліків реєстрації

Ключові слова: атмосферні забруднення, концентрація забруднень, функція невизначеності, радіальна швидкість, вектор стану

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USE OF UNCERTAINTY FUNCTION FOR IDENTIFICATION OF HAZARDOUS STATES OF ATMOSPHERIC POLLUTION VECTOR

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1. Introduction

The current situation with atmospheric pollution (AP) in the world can be described as a crisis. This situation has been formed for a rather long period due to neglect of the objective laws of development and reconstruction of the natural and resource complex. The current situation is characterized by high levels of AP. The major

anthropogenic source of AP is large industrial conglomerates, including motor transport [1]. Fires also lead to air pollution [2]. At the same time, landscape fires [3] and fires at oil and gas industry facilities [4] usually lead to environmental disasters. The most severe forms of AP are observed at industrial sites and adjacent territories. It is here that the highest concentrations of harmful substances in atmospheric air arise, exceeding the maximum permissible concentrations (MPC) by two to five and often more times. On a global scale, AP leads to the greenhouse effect, acid rain [5] and pollution of aquifers [6]. In this regard, the problem of identifying AP-hazardous cities with the most concentrated population, transport and industry becomes especially acute.

2. Literature review and problem statement

The influence of meteorological conditions on AP is complex and uncertain. The relationship between AP concentrations and meteorological conditions for different cities is similar. This is due to the similarity of the AP emission structure and characteristics of urban infrastructure. The importance of meteorological conditions lies in the fact that they contribute to the accumulation or dispersal of AP impurities in atmospheric air. The meteorological parameters of the conditions that most affect AP are wind (speed and direction), air temperature, as well as precipitation and fog. To assess the state of AP, identify its hazardous states and then make management decisions, networks of AP monitoring posts are arranged on the territory of cities, which allow tracking the dynamics of the content of harmful substances. Changes in meteorological conditions specific for a particular territory can increase the adverse effect of AR on the human body. Thus, an increase in the number of temperature anomalies, calm phenomena and temperature inversions may ultimately have a significant impact on primary morbidity, exacerbation and mortality. This is due to the fact that under such conditions there is an increased accumulation of toxic substances in the air (at the same intensity of AP).

The transfer and dispersion of AP are generally a rather complex nonlinear system. The principle of linearity for such systems is usually not fulfilled [7], which in turn leads to an incorrect representation of real physical processes of AR. At the same time, the identification of the dynamics of hazardous HE states is of paramount importance to prevent them [8]. In this regard, nonlinear dynamics methods become an active area of research [9]. Methods based on correlation dimension, Lyapunov exponents and entropy are becoming the most popular in the study of various complex systems [10]. However, the application of these methods is based on rather long series of observational data, which cannot always be obtained for real natural systems. Incorrect application of such methods, especially to natural systems, often leads to false results [11]. In order to successfully investigate a complex system like AP, it is better to use non-linear tools that are independent of a priori statistical data distributions and allow using a short data set taking into account noise, transients and artifacts [12]. Such tools are based on the fundamental property of dissipative dynamic systems – state recurrence. This property is expressed in the fact that even the smallest disturbance of the system, causing an exponential increase in its state, after some time tends to return to the state close to the previous one, while having a similar dynamics. Such recurrent behavior of complex systems is proposed to be displayed as corresponding recurrence plots (RP) [13]. RP-based methods have been successfully applied to the study of various biological systems [14], as well as in Earth sciences [15]. However, these methods need additional research, taking into account the features of environmental monitoring [8]. It should be noted that the application of the methods of the theory of deterministic and stochastic dynamic systems to the analysis of various ecosystems, including AP, is being actively developed [16, 17]. The model under study is described by a system of deterministic or stochastic differential equations, and the more complex the system, the more equations must be used to adequately describe it. In particular, various systems can be analyzed from the standpoint of the theory of dynamic systems and fractal sets [17]. For example, experimental study of the dynamics of air pollution by hazardous factors of indoor fire is carried out in [18]. In [18, 19], it is experimentally confirmed that the dynamics of AP states is complex and unsteady. In conditions of unsteady dynamics of air pollution states during fires, it is proposed to increase the speed of control sensors. The solution of this problem is addressed in [20]. To overcome the a priori uncertainty in the dynamics of air pollution states in a room, it is proposed to use self-adjusting sensors [21]. In [22], only the dynamics of threshold self-adjustment and probability of detecting hazardous events by sensors is analyzed. The analysis of the possibility of using the recurrence property of air pollution states is not considered. The analysis of correlation dimension of the air state in the advance ignition of materials is the subject of [23]. However, the possibilities of using the uncertainty function (UF) to identify hazardous AP states are not studied. The work [24] is devoted to the experimental study of time autocorrelations for the main hazardous AP during fires. The paper notes that indicators of their structural interactions are important for identifying hazardous AP states. The methods proposed in [25] are based on a stationary approach, which allows revealing only the average energy distribution for hazardous states. In this case, the time-frequency structure of hazardous states is not taken into account. The work [26] is devoted to the review of methods of time and frequency resolution. At the same time, the problem of frequency and time localization of hazardous states remains unresolved. Known methods are difficult to implement and unsuitable for identifying hazardous states.

In [27], the method for the rapid detection of AP-hazardous cities based on the calculation of the proposed state recurrence measures is analyzed. It is noted that in conditions of a priori uncertainty, an adaptive approach should be taken. The application of this approach to the calculation of AP RP is the subject of [28]. At the same time, the possibilities of using UF for identifying hazardous AP states are not discussed. In [29], timing analysis of nonstationary states based on the Fourier transform for stationary fragments of the state trajectory is considered. However, early identification of hazardous states is usually accompanied by non-stationary segments of observed data. The work [30] is devoted to the study of using state increments as signs of early detection of hazardous states in local ecosystems. However, the results presented in this paper are limited to the analysis of the statistics of increments of the main states of the gaseous medium. Features of the structural dynamics of state increments based on the UF for a trajectory fragment in multidimensional space are not reviewed. General methods of time-frequency representation and identification of nonlinear systems based on the short-term Fourier transform are examined in [31, 32]. The application of the short-term Fourier transform to the analysis of real observations is addressed

in [33]. It is noted that the methods [31–33] are quite difficult to implement and cannot be regarded as constructive for identifying hazardous states in complex dynamic systems. Other methods based on the UF and non-Fourier approaches are not analyzed. At the same time, additional studies are required to identify hazardous AP states based on the UF. In [34], the application of the known time-frequency approach and its modification to the study of the dynamics of hazardous states of the gas medium is considered. The overall complexity of these approaches is noted.

Thus, it follows that at present one of the constructive and developed methods for identifying hazardous AP states are the methods of RP of state recurrence measures. In general, these methods make it possible to identify various structural features of the dynamics of states of complex systems of any nature that cannot be detected on the basis of known classical methods. However, the methods of RP and recurrence measures remain quite complex and do not fully allow adequate identification of hazardous AP states. It is known that the UF is widely used in various radio applications of radar and optimal reception and allows simultaneous localization of the received signal by time and radial velocity. However, the use of the UF for the detection of hazardous AP states according to the data of pollutants concentration has its own characteristics and specifics. Therefore, an important and unresolved part of the problem of identifying hazardous AP states is the study of the possibility and features of using the UF for current concentrations of pollutants and excess of MPC.

3. The aim and objectives of the study

The aim of the work is to study the possibilities of using the uncertainty function to identify hazardous states of the polluted atmosphere based on recording current concentrations and excess of the maximum permissible concentrations.

To achieve this aim, the following objectives were set:

– to consider the theoretical features of determining the uncertainty function for current concentrations of atmospheric pollution;

– to verify the possibility of using the uncertainty function to identify hazardous states of atmospheric pollution using the example of experimental current excess of the maximum permissible concentrations of atmospheric pollution for a typical urban infrastructure.

4. Theoretical features of determining the uncertainty function for current concentrations of atmospheric pollution

The modern theory of turbulent diffusion shows that the propagation of AP as concentrations of certain substances occurs due to their transfer by the cross flow and diffusion caused by turbulent fluctuations in the cross flow velocity. In this case, the molecular flow due to the thermal motion of molecules can be neglected. In the process of transfer, the pollutant may undergo changes, entering into physical and chemical interaction with environmental particles and other impurities that alter the mechanical, physical and chemical properties of the pollutants.

Turbulent transfer and dispersion of AP are among the most complex problems of modern science, which has not yet been fully solved. This is due to the complexity and diversity of the processes that occur in a real atmosphere during AP with emissions. It is known that hazardous AP states generally depend both on the power of the polluting emission, and on the characteristics of atmospheric transport, and above all on the wind speed and current stability of the atmosphere. At present, however, there is no generally accepted criterion for determining categories of atmospheric stability, and therefore, the vertical temperature gradient (Pasquill) classification is more often used. This classification for identifying hazardous AP states is rather rough and does not take into account specific current conditions.

In general, AP emissions are produced at random times without taking into account the meteorological parameters of the atmosphere. At the same time, AP concentrations recorded by city monitoring posts take into account all factors of current turbulent transfer and dispersion of pollution. In [35], it is noted that when studying the dynamics of AP concentrations in cities as a sanitary and hygienic standard, it is advisable to use average daily MPC, which are specifically developed for populated areas and do not cause negative effects on the human body for an unlimited period of exposure. Therefore, we will assume that the set of recorded AP concentrations is determined by the vector $\mathbf{X}$, which, due to the random nature of turbulent transfer and dispersion in the atmosphere, has both time and frequency shifts. In this case, the frequency shift is due to the radial velocity of AP in the direction of the monitoring post. Let the operator Φ_τ determine the time shift of the vector $\mathbf{X}$ of the initial AP concentrations by the value of τ, and the operator Φ_ϕ – its frequency shift by the value of ϕ, due to the radial velocity V of concentrations $\mathbf{X}$. Then, for the current vector $\mathbf{X}$ of recorded AP concentrations, the operator representation $\Phi_\phi(\Phi_\tau(\mathbf{X}))$ will be valid. The energy of the standard deviation between the vector $\mathbf{X}$ and the vector $\Phi_\phi(\Phi_\tau(\mathbf{X}))$ in the space with the scalar product will be determined by

$$\varepsilon^2 = \left\|\mathbf{X} - \Phi_\phi\left(\Phi_\tau(\mathbf{X})\right)\right\|^2 = \\ = \left\|\mathbf{X}\right\|^2 + \left\|\Phi_\phi\left(\Phi_\tau(\mathbf{X})\right)\right\|^2 - 2\left\langle \mathbf{X}, \Phi_\phi\left(\Phi_\tau(\mathbf{X})\right)\right\rangle,$$

where $\|\mathbf{X}\|^2$ is the energy E_x of the recorded vector $\mathbf{X}$. If the time τ and frequency ϕ shifts are small, then $\|\mathbf{X}\|^2=\|\Phi_\phi(\Phi_\tau(\mathbf{X}))\|^2=E_x$. It follows that $\varepsilon^2 = 2E_{\mathbf{X}} - 2\left\langle \mathbf{X}, \Phi_\phi\left(\Phi_\tau(\mathbf{X})\right)\right\rangle$. The scalar product $\left\langle \mathbf{X}, \Phi_\phi\left(\Phi_\tau(\mathbf{X})\right)\right\rangle$ in this expression will determine the known UF $\Psi(\tau,\phi)=\left\langle \mathbf{X}, \Phi_\phi\left(\Phi_\tau(\mathbf{X})\right)\right\rangle$ for the vector $\mathbf{X}$ of AP concentrations.

It should be noted that the UF $\Psi(\tau,\phi)=\left\langle \mathbf{X}, \Phi_\phi\left(\Phi_\tau(\mathbf{X})\right)\right\rangle$ generalizes the concept of the correlation function for the vector $\mathbf{X}$ of AP concentrations in the case of time and frequency shifts due to turbulence and dispersion in the atmosphere. The UF $\Psi(\tau,\phi)$ has a number of useful properties. For example, the UF value at the origin $\Psi(0,0)=E_x$ is maximum and equal to the energy of the vector of recorded AP concentrations. It is also known that the two-dimensional Fourier transform of the UF determines the instantaneous spectrum or the time-frequency energy density of the AP vector for current time and frequency values. It can be shown that the square of the UF modulus is invariant with respect to the double Fourier transform. This property makes it possible to determine the square of the instantaneous spectrum modulus or the square of the time-frequency current energy density modulus for arbitrary AP concentration vectors using the UF.

Let us consider the operator Φ_ϕ of the frequency shift determined by the radial velocity V of the vector $\mathbf{X}$ of AP concentrations in more detail. The indicated frequency shift is generally caused by the Doppler-Fizeau effect. With respect to AP, this effect is manifested as changes in the time

scale in the time representation for each of AP. If the set of AP is recorded as the vector $\mathbf{X}(t)$ in continuous time t, then the change in the time scale for AP will be determined by the vector $\mathbf{X}(tk)$, where k is the time scale determined by

$$k = 1 - \frac{2V}{V_0},$$

V is the radial velocity of the vector $\mathbf{X}(t)$, and V_0 is the propagation velocity of the vector $\mathbf{X}(t)$ in the atmosphere. The indicated value of the time scale is valid if

$$\frac{V}{V_0} << 1 \cdot$$

With this in mind, the UF for the vector of AP concentrations recorded in continuous time will be determined by the relation

$$\Psi(\tau, k) = \langle \mathbf{X}(t), \mathbf{X}(tk - \tau) \rangle. \quad (1)$$

In the case of recording the vector $\mathbf{X}(t)$ at discrete time instants t_i, where i=0,1,2,... . The vector $\mathbf{X}(t_i)$=$\mathbf{X}_i$. Then the UF, following (1), will be determined by

$$\Psi(\tau, k) = \langle \mathbf{X}_i, \mathbf{X}_{tk-\tau} \rangle. \quad (2)$$

In the relation (2), the value i=0,1,2,... determines the discrete recording moments for the vector of AP concentrations. This means that the time scale k and delay τ in (2) can take only the corresponding discrete values. Given that in practice, the operation (2) is usually performed for a finite width of the averaging window and, passing from energy to average power, we can represent a discrete UF for the vector of recorded AP concentrations

$$\Psi'(\tau, k) = \frac{1}{M} \sum_{v=0}^{M-1} \mathbf{X}_{N-v}, \mathbf{X}_{N-vk-\tau}. \quad (3)$$

In the relation (3), the value M determines the number of readings of the averaging window, and N – the number of the discrete moment of recording corresponding to the final current discrete moment of the averaging window. This allows using only the data of recording the vector of AP concentrations available at a discrete moment N for the calculation of UF (3). When implementing (3), it is necessary to observe the condition that $N \geq M + Mk + \tau$. Given this condition, we can present a modified procedure for calculating the discrete UF for arbitrary values of N, M, k and τ as follows:

$$\Psi^{\mu}(N, \tau, k, M) = if \left\{ \begin{matrix} N < M + (M-1)k + \\ +\tau, 0, \frac{1}{M} \sum_{v=0}^{M-1} \mathbf{X}_{N-v}, \mathbf{X}_{N-vk-\tau} \end{matrix} \right\}. \quad (4)$$

The theoretical basis and features of determining the UF for current AP concentrations recorded in continuous and discrete time (3) and (4) are described. These ratios are valid for an arbitrary number and type of components of the vector of AP concentrations. In addition, they remain true even if the components of the vector are MPC excesses by AP. At the same time, the UF (3) and (4) make it possible to identify hazardous states in the polluted atmosphere by time and radial velocity of pollution without taking into account meteorological parameters and its stability.

5. Verification of the use of uncertainty function to identify hazardous states of atmospheric pollution

For verification, the real results of recording the MPC excess by typical AP of cities were used. As AP, formaldehyde, ammonia, and carbon monoxide were considered. The possibilities of using the UF to identify hazardous AP states were evaluated according to the recorded concentrations of AP for a typical urban infrastructure. The method of experimental measurements and characteristics of the equipment used are given in [27]. For verification, the data on AP concentration were normalized relative to the corresponding average daily MPC. Therefore, the data on the excess of the corresponding average daily MPC by AP were used as components of the initial HA vector. For verification, data on AP concentration for a limited interval from 490 readings to 520 readings were selected. The choice of this interval for verification is associated with the reliable presence of a hazardous AP state on it (region of 506 readings). Fig. 1, *a*, *b* shows the results of calculating the UF (3) in the time-delay plane for a different number of readings in the averaging window defined by 8 readings (two days) and 4 readings (one day), respectively.

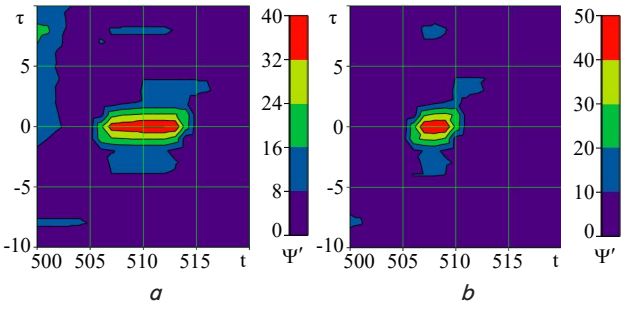

Fig. 1. Effect of the averaging window size when calculating the UF (3) in the time-delay plane: *a* – 8 readings; *b* – 4 readings

Similar results in the time-time scale plane are shown in Fig. 2. Fig. 3, *a*, *b* shows the results of calculating the UF (3) in the delay-time scale plane for a different number of readings in the averaging window for a fixed discrete time i=506.

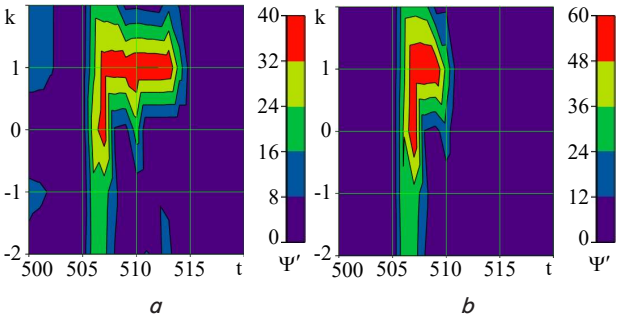

Fig. 2. Effect of the averaging window size when calculating the UF (3) in the time-time scale plane: *a* – 8 readings; *b* – 4 readings

Illustration of the UF dynamics determined by (4) in the current time-delay and current time-time scale coordinates with a fixed averaging window for one day (4 readings) for various parameters characterized by zero radial velocity V of AP (k=1) and zero delay is shown in Fig. 4, *a*, *b*, respectively.

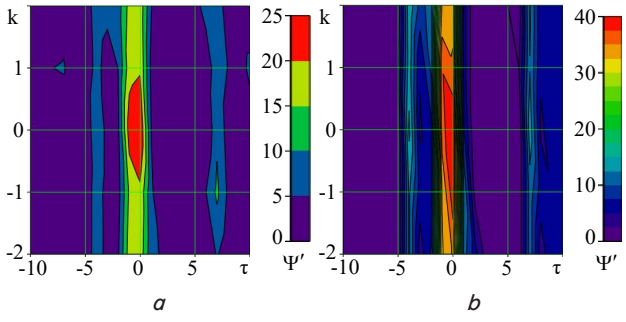

Fig. 3. Effect of the averaging window size when calculating the UF (3) in the delay-time scale plane: *a* – 8 readings; *b* – 4 readings

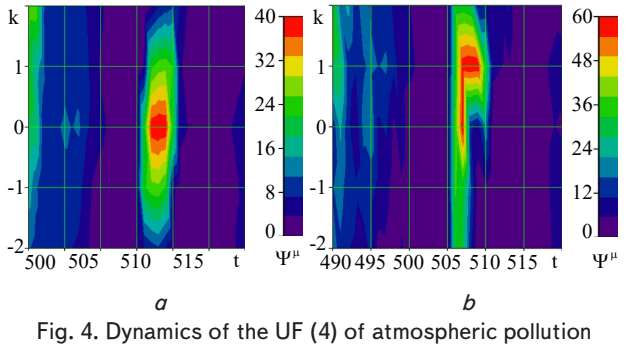

Fig. 4. Dynamics of the UF (4) of atmospheric pollution states with an averaging window of 4 readings for various parameters: *a* – zero radial velocity *V* of pollution (*k*=1); *b* – zero delay

Fig. 5 shows the current UF (4) in traditional delay-time scale coordinates for a fixed discrete time *i*=506 for different values of the averaging window, determined by two days (8 readings) and one day (4 readings), respectively.

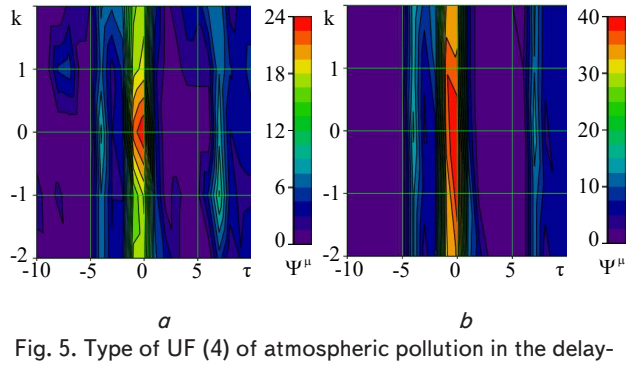

Fig. 5. Type of UF (4) of atmospheric pollution in the delay-time scale coordinates for a fixed discrete time *i*=506 for the averaging window values: *a* – 8 readings; *b* – 4 readings

From Fig. 5, it follows that when determining the UF of AP in the delay-time scale coordinates for a fixed discrete time, there are some advantages of choosing wide averaging windows.

6. Discussion of the results of verification of the use of uncertainty function to identify atmospheric pollution

The results shown in Fig. 1 generally demonstrate the presence of the effect of the width of the averaging window used when calculating the UF (3) on the identification and localization of hazardous AP. For the best time localization of hazardous AP states on the basis of UF, it is necessary to use narrow windows whose duration does not exceed one day. If the duration of the averaging window is two days, the UF section expands and shifts toward the previous points in time. In this case, the optimum values of time localization are achieved for zero delay in the UF. Similar requirements for the window width remain valid for calculation (3) and for using the time scale for identifying hazardous AP states (Fig. 2). The magnitude of the time scale in this case not only ensures time localization of hazardous AP states, but also makes it possible to identify their causes due to the radial velocities of pollution in an inhomogeneous atmosphere. From the analysis of the data shown in Fig. 3, it follows that the UF (3) for a discrete time *i*=506 in the delay-time scale plane weakly depends on the delay for a different number of readings in the averaging window. However, its value along the time scale axis substantially depends on the width of the averaging window. At the same time, for the window width of 8 readings, localization of hazardous AP along the time scale axis turns out to be twice as good as the window width of 4 readings. Illustration of the UF dynamics determined by (4) in the current time-delay and current time-time scale coordinates with a fixed averaging window of 4 readings for various parameters characterized by zero radial velocity *V* of AP and zero delay (Fig. 4) indicate the advantages of using the UF in the identification of hazardous AP. The indicated advantages consist in the possibility of using energy and velocity parameters to identify hazardous AP. At the same time, meteorological information about the current state of the atmosphere is not used. The type of AP UF (4) shown in Fig. 5 in the delay-time coordinates for a fixed discrete time *i*=506 shows some advantages of choosing wide averaging windows. These conclusions do not contradict the possibilities presented in Fig. 3.

The results of the study can be recommended for prompt and reliable identification of hazardous AP states. At the same time, current information on meteorological conditions in the area of the stationary monitoring post is not required. In practice, these results can significantly improve the efficiency of identifying hazardous states in atmospheric air pollution, regardless of the specific urban configuration and weather conditions. The results obtained can be a basis for modernizing existing methods for pollution assessment, which are based on calculating only average annual MPC. Average MPC are known to be a rather rough estimate of AP. Often in practice, the use of average MPC does not allow the identification of hazardous AP, which causes a negative impact on humans and the environment. In the everyday life of an environmental practitioner, the use of uncertainty function will allow identifying hazardous AP for any set of pollutants for the current MPC of stationary monitoring posts. The calculation of uncertainty function for MPC is not particularly difficult. Calculations using the following algorithms can be performed on any PC. The possibility of simultaneous identification of laminar states in the atmosphere allows predicting an increase in MPC. At the same time, it is advisable to limit the level of pollution emissions into the atmosphere in order to prevent the accumulation of pollution and prevent hazardous AP.

The limitations of the considered results include a rather large interval of discrete recording of pollution concentration data, determined by 6 hours. This somewhat narrows the possibility of identifying hazardous states by the radial velocity of pollution.

9. Conclusions

1. Theoretical features of determining the uncertainty function for current concentrations of atmospheric pollution recorded in continuous and discrete time are considered. It is noted that these ratios are valid for an arbitrary number and type of components of the recorded vector of atmospheric pollution concentration. It is shown that the ratios remain valid even when the components of the vector are MPC excesses by pollutants. Moreover, the uncertainty functions (3) and (4) make it possible to identify hazardous states in a polluted atmosphere by time and radial velocity of pollution, without taking into account current meteorological parameters and stability of the atmosphere.

2. Verification of the possibility of using the uncertainty function to identify hazardous states of atmospheric pollution was made using the example of experimental current excesses of the maximum permissible concentrations by the considered atmospheric pollution for a typical urban infrastructure. The presented verification results demonstrate sufficient advantages of using the uncertainty function for recorded concentrations of atmospheric pollution in order to identify hazardous states of pollution by their energy and velocity characteristics together. It was found that the width of the averaging window for recorded concentrations of pollutants should be from 4 to 8 readings, which corresponds to from one day to two days.

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