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NEW APPROACH AND MICROSYSTEM TECHNOLOGY OF ADVANCED ANALYSIS AND FORECASTING THE AIR POLLUTANT CONCENTRATION TEMPORAL DYNAMICS IN ATMOSPHERE OF THE INDUSTRIAL CITIES

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Abstract. We present the results of an advanced analysis, modeling and forecasting a temporal dynamics of the air pollutant (dioxide of nitrogen) concentrations in an atmosphere of the industrial city (Odessa, Ukraine; Gdansk, Polland) using comlex of new models and microsystem technology. An advanced non-linear analysis technique and modern chaos theory and dynamical systems methods have been applied. In order to analyse a measured time histories for the nitrogen dioxide concentrations in the Gdansk region the phase space of the system had been reconstructed by delay embedding. The mutual information approach, correlation integral analysis, false nearest neighbour algorithm, Lyapunov's exponent's analysis, and surrogate data method are used for comprehensive characterization. The correlation dimension method provided a low fractal-dimensional attractor thus suggesting a possibility of the existence of chaotic behavior. Statistical significance of the results was confirmed by testing for a surrogate data. A chaotic behavior in the nitrogen dioxide concentration time series at several sites in the Gdansk city is numerically investigated and the Lyapunov's exponents, the Kaplan-Yorke dimension and Kolmogorov entropy are precisely computed. An advanced computing has confirmed an existence of a low-D chaos in the cited system and given the improved short-terminal forecast of the atmospheric pollutants fluctuations dynamics.

Keywords: new mathematical models, new microsystem technologies, anthropogenic factor, atmospheric pollutants fluctuations, time series analysis and prediction

НОВИЙ ПІДХІД І МІКРОСИСТЕМНА ТЕХНОЛОГІЯ ВДОСКОНАЛЕНОГО АНАЛІЗУ І ПРОГНОЗУ ЧАСОВОЇ ДИНАМІКИ КОНЦЕНТРАЦІЙ ЗАБРУДНЮЮЧИХ РЕЧОВИН В АТМОСФЕРІ ПРОМИСЛОВИХ МІСТ

Ю. Я. Бунякова, О. В. Глушков, О. Ю. Хецеліус, Г. В. Ігнатенко, Н. Биковщенко, В. В. Буяджи

Анотація. Представлені результати вдосконаленого аналізу, моделювання і прогнозування часової динаміки концентрацій забруднюючих речовин (двоокису азоту) в атмосфері промислових міст (Одеса, Україна, Гданськ, Польща) з використанням комплексу нових моделей і нової мікросистемної технології. Застосовані методика нелінійного аналізу, теорія хаосу і методи теорії динамічних систем. Для аналізу виміряних часових періодів концентрацій діоксиду азоту фазовий простір системи було реконструйовано методом затримок. З метою виконання удосконаленого аналізу використовуються метод взаємної інформації, алгоритм кореляційного інтеграла, алгоритм помилкових найближчих сусідів, аналіз на основі показників Ляпунова і метод сурогатних даних. Метод кореляційної розмірності дозволив виявити дивний атрактор з низькою фрактальної розмірністю. Статистична значимість результатів була підтверджена тестуванням сурогатних даних. В рамках вдосконаленого підходу чисельно досліджена хаотична поведінка часових рядів концентрації двоокису азоту на декількох сайтах в містах Одеса (Україна) і Гданськ (Польща), розраховані показники Ляпунова, розмірності Каплана-Йорка і ентропія Колмогорова. Вдосконалений підхід природно підтвердив існування детерміністичного хаосу в досліджуваній системі. Запропоновано новий ефективний метод коротко-і середньотермінового прогнозування часової динаміки флуктуацій концентрацій забруднюючих атмосферу речовин на прикладі двоокису азоту

Ключові слова: нові математичні моделі, нові мікросистемні технології, антропогенний вплив, флуктуації атмосферних забруднювачів, аналіз та прогнозування часових рядів

НОВЫЙ ПОДХОД И МИКРОСИСТЕМНАЯ ТЕХНОЛОГИЯ УСОВЕРШЕНСТВОВАННОГО АНАЛИЗА И ПРОГНОЗА ВРЕМЕННОЙ ДИНАМИКИ КОНЦЕНТРАЦИЙ ЗАГРЯЗНЯЮЩИХ ВЕЩЕСТВ В АТМОСФЕРЕ ПРОМЫШЛЕННЫХ ГОРОДОВ

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Аннотация. Представлены результаты усовершенствованного анализа, моделирования и прогнозирования временной динамики концентраций загрязняющих веществ (двуокиси азота) в атмосфере промышленных городов (Одесса, Украина, Гданьск, Польша) с использованием комплекса новых моделей и микросистемных технологий. Применены методика нелинейного анализа, теория современного хаоса и методы динамических систем. Для анализа измеренных временных периодов концентраций диоксида азота фазовое пространство системы было реконструировано методом задержек. С целью выполнения усовершенствованного анализа используются метод взаимной информации, алгоритм корреляционного интеграла, алгоритм ложных ближайших соседей, анализ на основе показателей Ляпунова и метод суррогатных данных. Метод корреляционной размерности позволил выявить странный аттрактор с низкой фрактальной размерностью. Статистическая значимость результатов была подтверждена тестированием суррогатных данных. В рамках усовершенствованного подхода численно исследовано хаотическое поведение временных рядов концентрации двуокиси азота на нескольких сайтах в городах Одесса (Украина) и Гданьск (Польша), рассчитаны показатели Ляпунова, размерности Каплана-Йорка и энтропия Колмогорова. Усовершенствованный подход естественно подтвердил существование детерминистического хаоса в исследуемой системе. Предложен новый эффективный метод коротко-и средне-срочного прогнозирования временной динамики флуктуаций концентраций загрязняющих атмосферу веществ на примере двуокиси азота.

Ключевые слова: новые математические модели, новые микросистемные технологии, антропогенные воздействия, флуктуации атмосферных загрязнителей, анализ и прогнозирование временных рядов

1. Introduction

At the present time one of the most actual, important and fundamental problems of modern applied ecology, environmental protection is a problem of the quantitative treating pollution dynamics in the industrial cities and at whole regions and a search of new mathematical tools for analysis, modelling and forecasting a temporal dynamics of the air pollutant (dioxide of nitrogen) concentrations in an atmosphere of the industrial cities and regions [1-20]. It is well known that the most models, that are currently used to estimate the air pollution level, are either deterministic or statistical, but their skilfulness are still limited due to both inability for describing non-linearities in pollutant time series and lack of understanding involved physical and/or chemical processes. In Ref. [6] there is an analysis of the CO, O_3 concentrations time series. Also, it was shown that O_3 concentrations in Cincinnati (Ohio) and Istanbul are evidently chaotic, and non-linear approach provides satisfactory results [6]. In ref. [1-3] there is an analysis of the SO_2, CO, O_3 concentrations time series in a few industrial cities and it has been definitely received an evidence of chaos. More over it has been given a preliminary short-range forecasting atmospheric pollutants dynamics using the non-linear prediction method. These studies show that chaos theory methodology can be applied and the short-range forecast by the non-linear prediction method can be satisfactory.

In this paper we present the results of an advanced analysis, modeling and forecasting a temporal dynamics of the air pollutant (dioxide of nitrogen) concentrations in an atmosphere of the industrial city (Odessa, Ukraine and Gdansk, Polland) using a complex of new models and microsystem technology. An advanced non-linear analysis technique and modern chaos theory and dynamical systems methods have been applied (in versions [1-3,14-22]). An advanced computing has confirmed an existence of a low-D chaos in the pollutant dynamics and given the accurate short-terminal forecast of the atmospheric pollutants fluctuations. All calculations are performed with using "Geomath", "Superatom" and "Quantum Chaos" computational codes [14-78].

2. Technique of analysis and computing atmospheric pollutants fluctuations temporal dynamics

The key elements of the technique of computing atmospheric pollutants fluctuations dynamics are described in details in Refs. [1-3,14-22]. Here we are limited only by the key aspects. Let us consider scalar measurements:

$$s(n)=s(t_0+ n\Delta t) = s(n), \quad (1)$$

where t_0 is a start time, Δt is time step, and n is number of the measurements. In our case $s(n)$ is the time series of the atmospheric pollutants concentration. As processes resulting in a chaotic behaviour are fundamentally multivariate, one needs to reconstruct phase space using as well as possible information contained in $s(n)$. The main idea is that direct use of lagged variables $s(n+\tau)$, where τ is some integer to be defined, results in a coordinate system where a structure of orbits in phase space can be captured. Using a collection of time lags to create a vector in d dimensions,

$$\mathbf{y}(n)=[s(n),s(n + \tau),s(n + 2\tau),..,s(n +(d-1)\tau)], \quad (2)$$

the required coordinates are provided.

The dimension d is the embedding dimension, d_E. The goal of the embedding dimension determination is to reconstruct a Euclidean space R^d large enough so that the set of points d_A can be unfolded without ambiguity. The embedding dimension, d_E, must be greater, or at least equal, than a dimension of attractor, d_A, i.e. $d_E > d_A$. So, to analyse a measured time histories for the nitrogen dioxide concentrations, the phase space of the system had been reconstructed by the delay embedding.

Further the advanced versions of the mutual information approach, correlation integral analysis, false nearest neighbour algorithm, Lyapunov's exponent's analysis, and surrogate data method are used for comprehensive characterization [7-15]. The correlation dimension method provides a fractal-dimensional attractor. Statistical significance of the results was confirmed by testing for a surrogate data. The choice of proper time lag is important for the subsequent reconstruction of phase space. First approach is to compute the linear autocorrelation function $C_L(\delta)$ and to look for that time lag where $C_L(\delta)$ first passes through 0. This gives a good hint of choice for τ at that $s(n+j\tau)$ and $s(n+(j+1)\tau)$ are linearly independent. Alternative approach is given by a nonlinear concept of independence, e.g. an average mutual information [8] (see [14,15 too).

In order to compute an attractor dimension one should use the correlation integral analysis, which is one of the widely used techniques to investigate the signatures of chaos in a time series. According to [9], one must compute the correlation integral $C(r)$. If the time series is characterized by an attractor, then the correlation integral $C(r)$ is related to the radius r as [9]

$$d = \lim_{\substack{r\to 0 \\ N\to\infty}} \frac{\log C(r)}{\log r}, \quad (3)$$

where d is correlation exponent. If the correlation exponent attains saturation with an increase in the embedding dimension, then the system is generally considered to exhibit chaotic dynamics. The saturation value of correlation exponent is defined as the correlation dimension (d_2) of the attractor (see details in refs. [1,9]).

Further let us note that the spectrum of the Lyapunov's exponents is one of dynamical invariants for non-linear system with chaotic behaviour. The limited predictability of the chaos is quantified by the local and the global Lyapunov's exponents, which can be determined from measurements.

The Lyapunov's exponents are related to the eigenvalues of the linearized dynamics across the attractor. Negative values show stable behaviour while positive values show local unstable behaviour. The predictability can be estimated by the Kolmogorov entropy, which is proportional to a sum of the positive Lyapunov's exponents. For chaotic systems, being both stable and unstable, the Lyapunov's exponents indicate the complexity of the dynamics. The largest positive value determines some average prediction limit. Since the Lyapunov's exponents are defined as asymptotic average rates, they are independent of the initial conditions, and hence the choice of trajectory, and they do comprise an invariant measure of the attractor. An estimate of this measure is a sum of the positive Lyapunov's exponents. The estimate of the attractor dimension is provided by the conjecture d_L and the Lyapunov's exponents are taken in descending order. To compute Lyapunov's exponents, we use a method with linear fitted map [2], although the maps with higher order polynomials can be used too.

The principally important topic is development of an advanced approach to prediction of chaotic properties of complex systems. Our key idea is in the using the traditional concept of a compact geometric attractor in which evolves the measurement data, plus the implementation of neural network algorithms. The existing so far in the theory of chaos prediction models are based on the concept of an attractor. The meaning of the concept is in fact a study of the evolution of the attractor in the phase space of the system and, in a sense, modelling ("guessing") time-variable evolution.. From a mathematical point of view, it is a fact that in the phase space of the system an orbit continuously rolled on itself due to the action of dissipative forces and the nonlinear part of the dynamics, so it is possible to stay in the neighborhood of any point of the orbit *y (n)* other points of the orbit $y^r(n)$, $r = 1, 2, \ldots, N_B$, which come in the neighborhood *y (n)* in a completely different times than *n*. Of course, then one could try to build different types of interpolation functions that take into account all the neighborhoods of the phase space and at the same time explain how the neighborhood evolve from *y (n)* to a whole family of points about *y (n+1)*. Use of the information about the phase space in the simulation of the evolution of some geophysical (environmental, etc.) of the process in time can be regarded as a fundamental element in the simulation of random processes. In terms of the modern theory of neural systems, and neuro-informatics (e.g. [16,17]), the process of modelling the evolution of the system can be generalized to describe some evolutionary dynamic neuro-equations (miemo-dynamic equations). Imitating the further evolution of a complex system as the evolution of a neural network with the corresponding elements of the self-study, self- adaptation, etc., it becomes possible to significantly improve the prediction of evolutionary dynamics of a chaotic system.

Considering the neural network (in this case, the appropriate term "geophysical" neural network) with a certain number of neurons, as usual, we can introduce the operators S_{ij} synaptic neuron to neuron u_i u_j, while the corresponding synaptic matrix is reduced to a numerical matrix strength of synaptic connections: $W = || w_{ij} ||$.

The operator is described by the standard activation neuro-equation determining the evolution of a neural network in time: $s_i' = sign(\sum_{j=1}^{N} w_{ij} s_j - \theta_i)$, where 1< i <N. From the point of view of the theory of chaotic dynamical systems, the state of the neuron (the chaos-geometric interpretation of the forces of synaptic interactions, etc.) can be represented by currents in the phase space of the system and its the topological structure is obviously determined by the number and position of attractors.

These idea have been used in order to make more advanced the wide spread prediction model which is based on the constructing a parameterized nonlinear function F (x, a), which transform y (n) to y (n + 1) = F (y (n), a), and then using different criteria for determining the parameters a. As it is shown by Schreiber [13], the most common form of the local model is very simple :

$$s(n+\Delta n) = a_0^{(n)} + \sum_{j=1}^{d_A} a_j^{(n)} s(n-(j-1)\tau) \,, \quad (4)$$

where Δ n - the time period for which a forecast.

The coefficients $a_j^{(k)}$, may be determined by a least-squares procedure, involving only points $s(k)$ within a small neighbourhood around the reference point. Thus, the coefficients will vary throughout phase space. The fit procedure amounts to solving (d_A + 1) linear equations for the (d_A + 1) unknowns. Further, since there is the notion of local neighborhoods, one could create a model of the process occurring in the neighborhood, at the neighborhood and by combining together these local models to construct a global nonlinear model that describes most of the structure of the attractor. In order to get more advanced prediction of chaotic dynamics we have applied the polynomial model with using the neural network algorithm [16].

3. The advanced data for the nitrogen dioxide concentrations time series of the industrial cities and conclusions

In our study, we used the nitrogen dioxide concentration data observed at several sites of the Gdansk on 2003-2004, namely, the multi year hourly concentrations (one year total of 20x8760 data points) and the Odessa on 2001-2006, namely, the multi year hourly concentrations (one year total of 20x6570 data points). The temporal series of concentrations (in mg/m³) of the NO_2 are presented in figure 1 (for two sites). Let us note that in the Gdansk region, the Agency of Regional Air Quality Monitoring (ARMAAG) provides presently the 24-h forecasts of air quality levels using the model called CALMET/CALPUFF (CALPUFF) (see [1-4] and ref. therein).

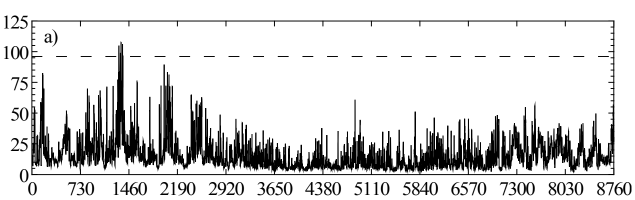

Figure 1a. The temporal series of concentrations (in mg/m³) of the of the NO_2 (cite 1; see text).

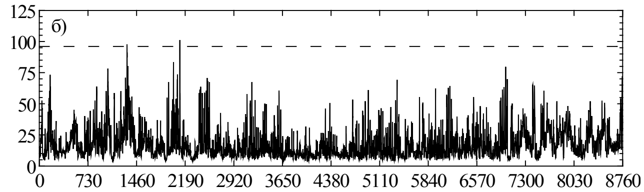

Figure 1b. The temporal series of concentrations (in mg/m³) of the of the NO_2 (cite 2; see text).

In Figure 2 we list the computed Fourier spectrum for the studied NO_2 time series. Having regard to the irregular nature of the changes of concentration it is not surprising that these spectra look the same as in a random process. In figure 3 we list the computed dependence of the correlation integral *C(r)* of radius r for different embedding dimensions *d* for the NO_2 at one of the sites of the Gdansk during 2003.

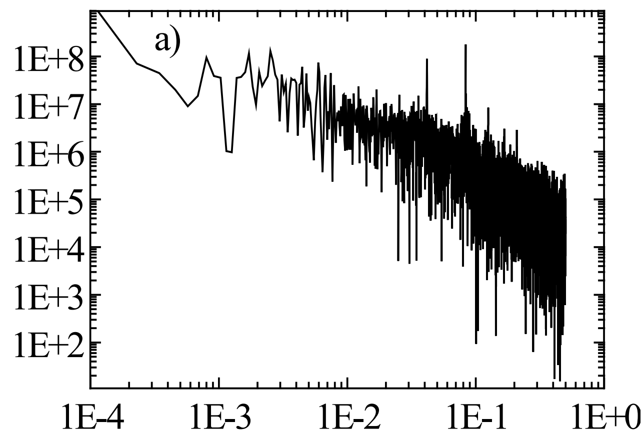

Figure 2. The Fourier spectrum for the NO_2 concentration series in the Gdansk region: X – frequency, Y - energy (see text).

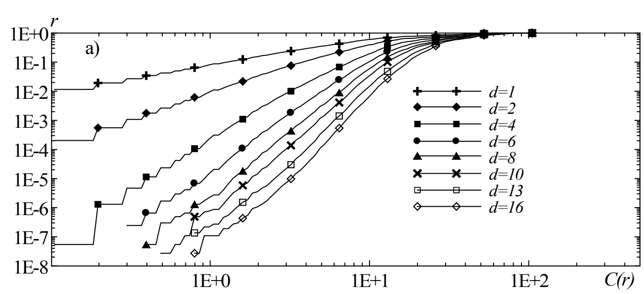

Figure 3. The dependence of the correlation integral C (r) of radius r for different embedding dimensions d for NO_2 (b) at the site 6 of the Gdansk during 2003.

In the Table 1 we list the data for the time lag calculated for first 103 values of time series. The autocorrelation function for all time series remains positive. In the Table 2 we present our advanced data on the correlation dimension (d_2), embedding dimension (d_E), Kaplan-Yorke dimension (d_L), two Lyapunov's exponents (λ_1,λ_2), the Kaplan-Yorke dimension (d_L), and average limit of predictability (Pr_{max}, hours) for time series of the NO_2 at sites of the Gdansk (during 2003 year).

Table 1

Time lags (hours) subject to different values of C_L, and first minima of average mutual information,I_{min1}, for the time series of NO_2 at the sites of Gdansk

	$C_L = 0$	$C_L = 0,1$	$C_L = 0,5$	I_{min1}
	Site 1			
SO_2	–	138	7	10
	Site 2			
SO_2	103	55	5	9

From the table 2 it can be noted that the Kaplan-Yorke dimensions, which are also the attractor dimensions, are smaller than the dimensions obtained by the algorithm of false nearest neighbours.

Firstly, one should note that the presence of the two (from six) positive λ_i suggests the system broadens in the line of two axes and converges along four axes that in the six-dimensional space. The time series of the NO_2 at the site 2 have the highest predictability (more than 2 days), and other time series have the predictabilities slightly less than 2 days. The concrete example is presented in Figure 4, where the empirical (solid line 1) and theoretical forecasting (solid line 2 by the Schreiber-type prediction algorithm with neural networks block and dotted line 3 by the standard Schreiber-type algorithm) concentration lines NO_2 (for the one hundred points) are presented.

In whole an analysis shows that almost all the peaks on the actual curve repeated on the prognostic difference between the forecast and the actual data in the event of high concentrations of the ingredients can be quite large. The prediction line 2 looks more exact in comparison with actual data. More detailed analysis of this fact will be presented in another paper.

Table 2

The correlation dimension (d_2), embedding dimension (d_E), first two Lyapunov's exponents, E(λ_1, λ_2), Kaplan-Yorke dimension (d_L), and average limit of predictability (Pr_{max}, hours) for time series of NO_2 at the Gdansk sites (during 2003)

	τ	d_2	d_E	λ_1	λ_2	d_L	Pr_{max}	K
	Site 1							
NO_2	9	5,31	6	0,0185	0,0060	4,11	41	0,68
	Site 2							
NO_2	8	5,31	6	0,0188	0,0052	3,85	42	0,66

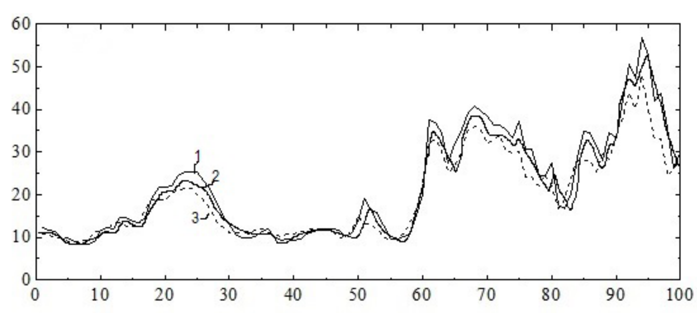

Figure 4. The empirical (solid line 1) and forecasting (solid line 2 and dotted line 3) NO_2 concentration lines for the last one hundred points (see text).

Here we only note that the results of our computational forecasting can be considered quite satisfactory.

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NEW APPROACH AND MICROSYSTEM TECHNOLOGY OF ADVANCED ANALYSIS AND FORECASTING THE AIR POLLUTANT CONCENTRATION TEMPORAL DYNAMICS IN ATMOSPHERE OF THE INDUSTRIAL CITIES

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Summary

The aim of the work is to develop and present a new approach and correspondingly a new microsystem technology for advanced analysis, modelling and forecasting the air pollutant concentration temporal dynamics in atmosphere of the industrial cities and apply it to studying a temporal dynamics of the air pollutant concentrations for the concrete large industrial cities We present the results of an advanced analysis, modelling and forecasting air pollutant (on the example of the dioxide of nitrogen) concentrations in an atmosphere of the Odessa (Ukraine) and Gdansk (Polland) using a group of new models and new microsystem technology.

An advanced non-linear analysis technique and modern chaos theory and dynamical systems methods have been applied. In order to analyse a measured time histories for the nitrogen dioxide concentrations in the Gdansk region the phase space of the system had been reconstructed by delay embedding. The mutual information approach, correlation integral analysis, false nearest neighbour algorithm, Lyapunov's exponent's analysis, and surrogate data method are used for comprehensive characterization. The correlation dimension method provided a low fractal-dimensional attractor thus suggesting a possibility of the existence of chaotic behaviour. Statistical significance of the results was confirmed by testing for a surrogate data.

A chaotic behaviour in the nitrogen dioxide concentration time series at several sites in the Gdansk and Odessa cities is numerically investigated. Different topological and dynamical invariants such as the Lyapunov's exponents, the Kaplan-Yorke dimension and Kolmogorov entropy and others are computed. It has been shown that an advanced computing has confirmed an existence of a low-D chaos in the cited system. For the first time new advanced approach is presented and applied to quite satisfactory short-terminal prediction of the atmospheric pollutant fluctuations dynamics.

Keywords: new mathematical models, new microsystem technologies, anthropogenic factor, atmospheric pollutants fluctuations, time series analysis and prediction

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НОВИЙ ПІДХІД І МІКРОСИСТЕМНА ТЕХНОЛОГІЯ ВДОСКОНАЛЕНОГО АНАЛІЗУ І ПРОГНОЗУ ЧАСОВОЇ ДИНАМІКИ КОНЦЕНТРАЦІЙ ЗАБРУДНЮЮЧИХ РЕЧОВИН В АТМОСФЕРІ ПРОМИСЛОВИХ МІСТ

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Реферат

Мета роботи полягає у розробці та презентації нового підходу та, відповідно, нової мікросистемної технології для поглибленого, вдосконаленого аналізу, моделювання та прогнозування часової динаміки концентрацій забруднювачів повітря та застосування її до вивчення часової динаміки концентрації забруднюючих атмосферу речовин для конкретних індустріальних міст. В роботі представлені результати вдосконаленого аналізу, моделювання і прогнозування часової динаміки концентрацій забруднюючих речовин (двоокису азоту) в атмосфері промислових міст (Одеса, Україна, Гданськ, Польща) з використанням комплексу нових моделей і нової мікросистемної технології.

Застосовані методика нелінійного аналізу, теорія хаосу і методи теорії динамічних систем. Для аналізу виміряних часових періодів концентрацій діоксиду азоту фазовий простір системи було реконструйовано методом затримок. З метою виконання удосконаленого аналізу використовуються метод взаємної інформації, алгоритм кореляційного інтеграла, алгоритм помилкових найближчих сусідів, аналіз на основі показників Ляпунова і метод сурогатних даних. Метод кореляційної розмірності дозволив виявити дивний атрактор із відповідною фрактальної розмірністю. Статистична значимість результатів була підтверджена тестуванням сурогатних даних.

В рамках вдосконаленого підходу чисельно досліджена хаотична поведінка часових рядів концентрації двоокису азоту на декількох сайтах в містах Одеса (Україна) і Гданськ (Польща). Розраховані різноманітні топологічні та динамічні інваріанти, зокрема, показники Ляпунова, розмірності Каплана-Йорка, ентропія Колмогорова та інші. Вдосконалений підхід природно підтвердив існування детерміністичного хаосу в досліджуваній системі. Запропоновано новий ефективний метод коротко-і середньо-термінового прогнозування часової динаміки флуктуацій концентрацій забруднюючих атмосферу речовин на прикладі двоокису азоту.

Ключові слова: нові математичні моделі, нові мікросистемні технології, антропогенний вплив, флуктуації атмосферних забруднювачів, аналіз та прогнозування часових рядів