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A chaos-geometric approach to analysis, modelling and forecasting atmospheric pollutants dynamics for industrial regions

We applied an advanced chaos-geometric approach to analysis, modeling, forecasting and processing the time series of the air pollutants (NO_2) concentrations in an atmosphere of the industrial cities (regions). The approach includes such advanced non-linear analysis and a chaos theory methods such as a multifractal approach, correlation integral algorithm, the Lyapunov's exponents and Kolmogorov entropy analysis, a power spectrum analysis, prediction models with neural networks blocks etc. The dynamical and topological invariants (including the Lyapunov's exponents spectrum, Kaplan-Yorke dimension, Kolmogorov entropy etc) for the air pollutants (NO_2) concentrations time series in an atmosphere of the industrial cities are computed. Our study has shown an existence of a deterministic chaos in the atmospheric pollutants fluctuations dynamics. It is presented an effective prediction model for description of the temporal evolutionary dynamics of the air pollutants concentration in atmosphere of the industrial city.

***Key words**: atmospheric pollutants dynamics, chaos-geometric approach.*

Introduction. In this paper we present an advanced version of the chaos-geometric approach to analysis, processing and prediction of the scalar environmental measurement data, in particular, the time series of the atmospheric pollutants (dioxide of nitrogen) concentrations in an atmosphere of the industrial cities. The studies concerning non-linear behaviour in the time series of nature dynamical systems are sparse, and their outcomes are ambiguous (c.g., [1-8]). In Refs. [8-15] it has been presented an advanced chaos-geometric approach to analysis, modeling, forecasting and processing the time series of the air pollutants concentrations in an atmosphere of the industrial cities (regions). The approach includes such advanced non-linear analysis and a chaos theory methods such as a multifractal approach, correlation integral algorithm, the Lyapunov's exponents (LE) and Kolmogorov entropy (KE) analysis, a power spectrum analysis, prediction models with neural networks blocks etc. Here the results of computing the dynamical and topological invariants (including the Lyapunov's exponents spectrum, Kaplan-Yorke dimension, KE etc) for the air pollutants (NO_2) concentrations time series in an atmosphere of the industrial cities are listed. It is presented an advanced prediction model for description of the temporal evolutionary dynamics of the air pollutants.

The input data. Chaos-geometric approach. In our study, we have used the nitrogen dioxide concentration data, namely, the multi year hourly concentrations, observed at several sites of the Odessa (one year total of 20x6570 data points) and

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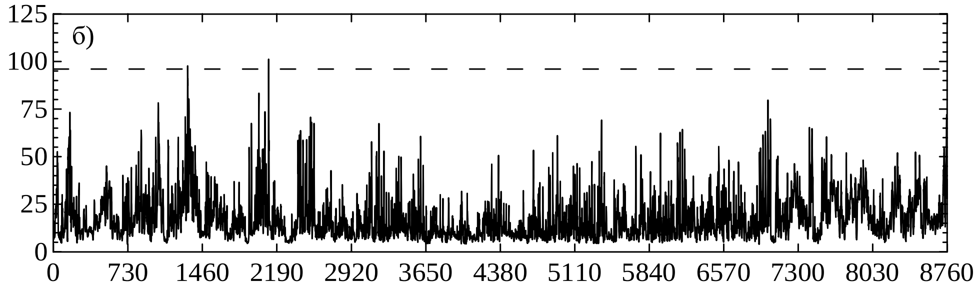

Fig. 1. The time series of concentrations (μg/m^3) of the of the NO_2

Gdansk (20x8760 data points) regions during 2001-2006 years. The typical time series of concentrations (in μg/m^3) of the NO_2 are listed in fig.1 [8].

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 (see [1,8] and Refs. therein). In Refs. [8-12] it has been developed the computational code for studying chaotic features of the complex non-linear systems and in details described a procedure of testing of the chaos elements in the corresponding time series. In Table 1 we present the block-scheme of a chaos-geometric approach in application to air pollutants dynamics.

The detailed description of all blocks can be found in Refs. [5-12]. Below we are

Table 1.

A chaos-geometric approach to nonlinear analysis, modeling and prediction of atmospheric pollutants concentrations temporal and spatial dynamics

I. Preliminary study and assessment of the presence of chaos: 1. Test by Gottwald-Melbourne: $K \rightarrow 1$ – chaos; 2. Fourier decompositions, irregular nature of change – chaos; 3. Spectral analysis, Energy spectra statistics, the Wigner distribution, the spectrum of power, "Spectral rigidity";
⇓
II. The geometry of the phase space. Fractal Geometry: 4. Computation time delay τ using autocorrelation function or mutual information; 5. Determining embedding dimension d_E by the method of correlation dimension or algorithm of false nearest neighbouring points; 6. Calculation multi-fractal spectra. Wavelet analysis;
⇓
III. Prediction: 7. Computing global Lyapynov dimensions LE: λ_α; Kaplan-York dimension d_L, KE, average predictability measure Pr_{max}; 8. Determining the number of nearest neighbour points NN for the best prediction results; 9. Nonlinear prediction. Neural network algorithm, algorithm optimized trajectories.

limited only by the key aspects. As usually, we study the concentration data $s(n)=s(t_0+ n\Delta t) = s(n)$,where t_0 is a start time, Δt is time step, and n is number of the measurements. The first fundamental step of modelling is in reconstruction of the corresponding phase space using as well as possible information contained in $s(n)$. Using collection of time lags τ to create a vector in d dimensions, $y(n)= [s(n), s(n+\tau), s(n + 2\tau),..,s(n +(d–1)\tau)]$, 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. From the mathematical viewpoint, this procedure results in set of d-dimensional vectors $y(n)$ replacing scalar measurements. There are a few approaches to the choice of proper time lag [5-9]. This point 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. The alternative approach is based on using method of an average mutual information. The correlation integral analysis is one of the widely used techniques to investigate the signatures of chaos in a time series. This method is based on using the correlation integral, $C(r)$. As usually, if the corresponding time series is characterized by an attractor, then the correlation integral $C(r)$ is related to the radius r as $d = \lim\limits_{\substack{r\to 0\\ N\to\infty}}[\log C(r) / \log r]$, where d is correlation exponent. The saturation value of this exponent is defined as the correlation dimension (d_2) of the attractor (c.g. [5-12]). Another method for determining d_E is given by the method of false nearest neighbours. As a rule, the simultaneous application of two methods provides more exact determination d_E. The further important step in studying the chaotic time series is determination of predictability, which can be estimated by the KE. The KE is proportional to a sum of the positive LE. The largest positive value of the LE determines some average prediction limit. Since the LE defined as asymptotic average rates, they are independent of the initial conditions. The estimate of the attractor dimension is provided by the conjecture d_L and the LE are taken in descending order. The further development of the chaos-geometric approach was provided by development of new prediction models with standard interpolation methods (e.g., spline or polynomial) and neural networks blocks (all details are in refs. [11,13-16]).

Some results and conclusion. In Table 2 we present our advanced data on the parameters τ, K, correlation dimension (d_2), embedding dimension (d_E), two LE (λ_1, λ_2), Kaplan-York dimension (d_L), and average limit of predictability (Pr_{max}, hours), KE K_{ent} for time series of the NO_2 at sites of the Odessa (2001) and Gdansk (2003) regions. If time lags determined by average mutual information are used, then algorithm of false nearest neighbours provides $d_E = 6$ for all air pollutants. 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. It is very important to pay the attention on the presence of the two (from six) positive LE λ_i . This fact suggests that the system broadens in the line of two axes and converges along four axes that in the six-dimensional space [8,9,13].

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 Odessa and Gdansk sites

τ	d_2	d_E	λ_1	λ_2	d_L	Pr_{max}	K_{ent}	K
Site 2 Odessa region (2001)								
8	5.29	6	0.0191	0.0050	3.92	42	0.024	0.70
site 6 of Gdansk region (2003)								
9	5.31	6	0.0184	0.0061	4.11	40	0.025	0.68

As example of using an approach to predict the time series, in Figure 2 we present the empirical (solid line 1) and forecasting (solid line 2 and dotted line 3) data for the NO_2 concentration for the last one hundred points (Gdansk region, 2003) [8].

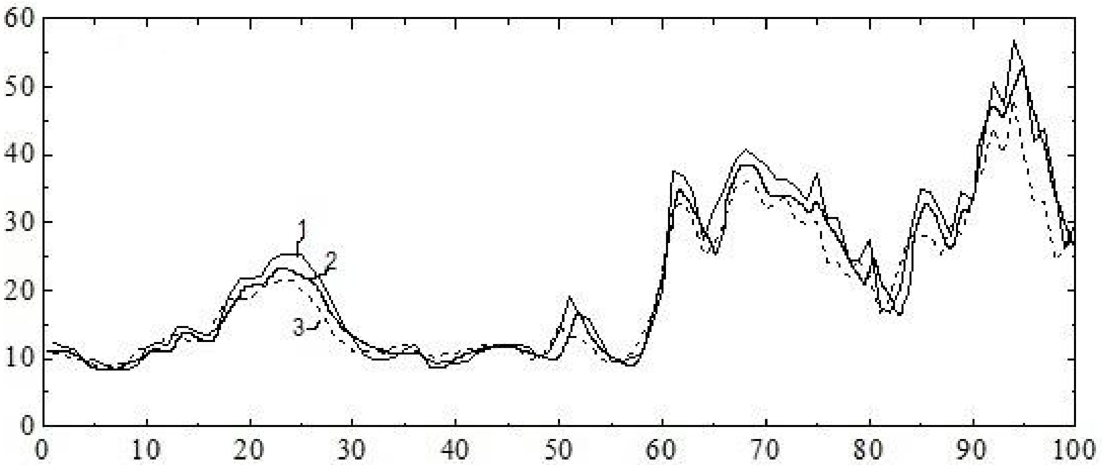

Fig. 2. The empirical (solid line 1) and forecasting (solid line 2 and dotted line 3) NO_2 concentration lines for the last one hundred points (see text).

The theoretical predicted data (solid line 2) are obtained with using the Schreiber-type prediction algorithm with neural networks block and the theoretical data (dotted line 3) are obtained with using the standard Schreiber-type algorithm. 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. In Table 3 we list the quantitative indictors of the forecast effectiveness. It can be seen that with decreasing predictability the quality of the forecast improves, that is, the results of the method are very similar to those that can be obtained by other methods. In order to check how well the model is built, it reflects the entire time series, a forecast was also made for 900 randomly selected terms. The success of the forecast turned out to be slightly improved (Table 3).

Table 3.

Correlation coefficient (r) between actual and predictive series and rms prediction error (σ) for different predictions timeliness (NO_2 ; two sites) for the last 100 raw points and 900 randomly chosen raw points

	6h	12h	18h	24h		6h	12h	18h	24h
Site 1; Last 100 points of a raw					Site 1; 900 random points				
R	0.98	0.98	0.97	0.96	*r*	0.99	0.99	0.98	0.98
Σ	3.825	4.019	5.233	6.025	σ	3.711	3.891	4.338	5.011
Site 2; Last 100 points of a raw					Site 2; 900 random points				
R	0.99	0.99	0.98	0.97	*r*	0.99	0.99	0.99	0.98
Σ	3.611	3.938	4.839	5.636	σ	3.567	3.899	4.287	4.978

To conclude, we have presented results of advances studying the temporal dynamics (time series) of the atmospheric pollutants (dioxide of nitrogen) concentration in atmosphere of the industrial ccities using earlier developed chaos-geometric approach and new prediction models. To reconstruct the corresponding attractor, the time delay and embedding dimension are determined. The LE spectrum, Kaplan-Yorke dimension, KE etc are calculated. It is presented a new effective prediction model for description of the temporal dynamics of the air pollutants concentration.

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Хаос-геометричний підхід до аналізу, моделювання і прогнозування динаміки забруднюючих речовин в атмосфері промислових регіонів

АНОТАЦІЯ

Узагальнений хаос-геометричний підхід застосований до аналізу, моделювання та прогнозування часової динаміки концентрацій забруднюючих речовин (NO2) в атмосфері промислових міст. Підхід включає в себе такі методи нелінійного аналізу та теорії хаосу, як мультифрактальний формалізм, метод кореляційного інтеграла, аналіз на основі показників Ляпунова, ентропії Колмогорова, спектральні і прогнозні моделі, в т.ч., вперше з нейронномуреживим блоком. 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 кореля-

ційної розмірності дозволив виявити дивний аттрактор з відносно невисокою фрактальною розмірністю. Розраховані динамічні і топологічні інваріанти, в тому числі, розмірності: вкладення, кореляційна, Каплана-Йорка, показники Ляпунова, ентропія Колмогорова та ін. Аналіз отриманих даних підтвердив наявність елементів детермінованого хаосу в флуктуаційної часовій динаміці концентрацій атмосферних забруднювачів. Розроблено нову ефективну модель прогнозування тимчасової еволюційної динаміки концентрації забруднювачів повітря в атмосфері промислового міста. Наведено чисельні дані для коефіцієнта кореляції між фактичним і прогностичним рядами.

***Ключові слова**: флуктуаційна динаміка атмосферних забруднювачів, хаос-геометричний підхід.*

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Хаос-геометрический подход к анализу, моделированию и прогнозированию динамики загрязняющих веществ в атмосфере промышленных регионов

АНОТАЦИЯ

Обобщённый хаос-геометрический подход применен к анализу, моделированию и прогнозированию временной динамики концентраций загрязняющих веществ (NO_2) в атмосфере промышленных городов. Подход включает в себя такие методы нелинейного анализа и теории хаоса, как мульти фрактальный подход, метод корреляционного интеграла, анализ на основе показателей Ляпунова, энтропии Колмогорова, спектральные и прогнозные модели, в т.ч., впервые с нейронносетевым блоком. 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 относительно невысокой фрактальной размерностью. Рассчитаны динамические и топологические инварианты, в том числе, размерности: вложения, корреляционная, Каплана-Йорка, показатели Ляпунова, энтропия Колмогорова и др. Анализ полученных данных показал наличие элементов детерминированного хаоса в флуктуационной временной динамике концентраций атмосферных загрязнителей. Разработана новая эффективная модель прогнозирования временной эволюционной динамики концентрации загрязнителей воздуха в атмосфере промышленного города. Приведены численные данные для коэффициента корреляции между фактическим и прогностическим рядами.

***Ключевые слова**: флуктуационная динамика атмосферных загрязнителей, хаос-геометрический подход.*