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ANALYSIS AND FORECAST OF THE ANTHROPOGENIC IMPACT ON INDUSTRIAL CITY'S ATMOSPHERE BASED ON METHODS OF CHAOS THEORY: NEW GENERAL SCHEME

The theoretical basis's of a new general formalism for an analysis and forecasting an impact of anthropogenic factors on the atmosphere of an industrial city are presented. It is developed a new compact general scheme for modeling temporal fluctuations of the air pollution concentration field temporal fluctuations ,based on the methods of a chaos theory.
***Keywords**: air basin of the industrial city, the ecological state of the, time series of concentrations, pollutants, analysis and prediction methods of the theory of chaos*

1. Introduction

Problem of studying the dynamics of chaotic dynamical systems arises in many areas of science and technology. We are talking about a class of problems of identifying and estimating the parameters of interaction between the sources of complex (chaotic) oscillations of the time series of experimentally observed values. Such problems arise in environmental sciences, geophysics, chemistry, biology, medicine, neuroscience, engineering, etc. Problem of an analysis and forecasting the impact of anthropogenic pressure on the state of atmosphere in an industrial city and development of the consistent, adequate schemes for modeling the properties of the concentration fields of air pollutions is one of the most important and fundamental problems of modern environmental sciences, in particular, applied ecology and urban ecology [1-18]. Most of the models currently used to assess a state (as well as, the forecast) of an air pollution are presently by the deterministic models or simplified ones, based on a simple statistical regressions. The success of these models, however, is limited by their inability to describe the nonlinear characteristics of the pollutant concentration behaviour and lack of understanding of the involved physical and chemical processes. Although the use of methods of a chaos theory establishes certain fundamental limitation on the long-term predictions, however, as has been shown in a series of our papers (see, for example, [1-11]), these methods can be successfully applied to a short-or medium-term forecasting. As example, let us remind about quantitatively correct description of the temporary changes in the concentration of nitrogen dioxide (NO2) and sulfur dioxide (SO2) in several industrial cities (Odessa, Triste, Allepo and cities of the Gdansk region) with discovery of the low-dimensional chaos. Some elements of this technique have been successfully applied to several tasks of prediction of the other nature system ecological state [6-11]. The main purpose of this paper is formally to present theoretical basis of a new general formalism for an analysis and forecasting an impact of anthropogenic factors on the atmosphere of an industrial city and develop a new compact general scheme for modeling temporal fluctuations of the air pollution concentration field temporal fluctuations ,based on the methods of a chaos theory.

2. New general formalism for analysis of and forecasting an impact of anthropogenic factors on the atmosphere of an industrial city

Preliminary we start from the first key task on testing a chaos in the time series of air pollutants [1-11]. As usually, let us consider scalar measurements $s(n)=s(t_0+ n\Delta t) = s(n)$, where t_0 is a start time, Δt is time step, and n is number of the measurements. In a general case, $s(n)$ is any time series (f.e. 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 $s(n)$. Such reconstruction results in set of d-dimensional vectors $\mathbf{y}(n)$ replacing scalar measurements. 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, $\mathbf{y}(n)=[s(n),s(n+\tau),s(n+2\tau),..,s(n+(d-1)\tau)]$, the required coordinates are provided. In a nonlinear system, $s(n+j\tau)$ are some unknown nonlinear combination of the actual physical variables. The dimension d is the embedding dimension, d_E.

The choice of proper time lag is important for the subsequent reconstruction of phase space. If τ is chosen too small, then the coordinates $s(n+j\tau)$, $s(n+(j+1)\tau)$ are so close to each other in numerical value that they cannot be distinguished from each other. If τ is too large, then $s(n+j\tau)$, $s(n+(j+1)\tau)$ are completely independent of each other in a statistical sense. If τ is too small or too large, then the correlation dimension of attractor can be under-or overestimated.

One needs to choose some intermediate position between above cases. 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. It's better to use approach with a nonlinear concept of independence, e.g. an average mutual information. The mutual information I of two measurements a_i and b_k is symmetric and non-negative, and equals to 0 if only the systems are independent. The average mutual information between any value a_i from system A and b_k from B is the average over all possible measurements of $I_{AB}(a_i, b_k)$. Usually it is necessary to choose that τ where the first minimum of $I(\tau)$ occurs.

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. $d_E > d_A$. In other words, we can choose a fortiori large dimension d_E, e.g. 10 or 15, since the previous analysis provides us prospects that the dynamics of our system is probably chaotic. The correlation integral analysis is one of the widely used techniques to investigate the signatures of chaos in a time series. The analysis uses the correlation integral, $C(r)$, to distinguish between chaotic and stochastic systems.

According to [4], it is computed 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

$$d = \lim_{\substack{r\to 0 \\ N\to\infty}} \frac{\log C(r)}{\log r}, \quad (1)$$

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. [3,4]).

Another method for determining d_E comes from asking the basic question addressed in the embedding theorem: when has one eliminated false crossing of the orbit with itself which arose by virtue of having projected the attractor into a too low dimensional space? In other words, when points in dimension d are neighbours of one other? By examining this question in dimension one, then dimension two, etc. until there are no incorrect or false neighbours remaining, one should be able to establish, from geometrical consideration alone, a value for the necessary embedding dimension. Such an approach was described by Kennel et al. [16,17]. In dimension d each vector $\mathbf{y}(k)$ has a nearest neighbour $\mathbf{y}^{NN}(k)$ with nearness in the sense of some distance function. The Euclidean distance in dimension d between $\mathbf{y}(k)$ and $\mathbf{y}^{NN}(k)$ we call $R_d(k)$:

$$R_d^2(k)=[s(k)-s^{NN}(k)]^2+[s(k+\tau)-s^{NN}(k+\tau)]^2+ \\ ...+[s(k+\tau(d-1))-s^{NN}(k+\tau(d-1))]^2. \quad (2)$$

$R_d(k)$ is presumably small when one has a lot a data, and for a dataset with N measurements, this distance is of order $1/N^{1/d}$. In dimension d + 1 this nearest-neighbour distance is changed due to the (d + 1)st coordinates $s(k + d\tau)$ and $s^{NN}(k + d\tau)$ to

$$R_{d+1}^2(k)=R_d^2(k)+[s(k+d\tau)-s^{NN}(k+d\tau)]^2. \quad (3)$$

We can define some threshold size R_T to decide when neighbours are false. Then if

$$\frac{|s(k+d\tau)-s^{NN}(k+d\tau)|}{R_d(k)}>R_T, \quad (4)$$

(the nearest neighbours at time point k are declared false). Kennel et al. [16] showed that for values in the range $10 \le R_T \le 50$ the number of false neighbours identified by this criterion is constant. In practice, the percentage of false nearest neighbours is determined for each dimension d. A value at which the percentage is almost equal to zero can be considered as the embedding dimension.

As usually, the predictability can be estimated by the Kolmogorov entropy, which is proportional to a sum of positive Lyapunov exponents. The spectrum of the Lyapunov 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 global Lyapunov exponents, which can be determined from measurements. The Lyapunov 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.

For chaotic systems, being both stable and unstable, Lyapunov exponents indicate the complexity of the dynamics. The largest positive value determines some average prediction limit. Since the Lyapunov 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 exponents. The estimate of the attractor dimension is provided by the conjecture d_L and the Lyapunov exponents are taken in descending order. The dimension d_L gives values close to the dimension estimates discussed earlier and is preferable when estimating high dimensions. To compute the Lyapunov exponents, we use a method with linear fitted map, although maps with higher order polynomials can be used too [18-23].

3. Conclusions

Summing up above said and results of Refs. [1-3], it is useful to summarize the key points of the investigating system for a chaos availability and wording the forecast model (evolution) of the system. The above methods are just part of a large set of approaches (see our versions in [1-11]), which is used in the identification and analysis of chaotic regimes in the time series. Generally speaking, the short technique of processing any time series of the air pollutants can be formulated as follows:

a) check for the presence of a chaotic regime (the Gottwald-Melbourne's test; the method of correlation dimension);

b) reducing the phase space (choice of the time delay, the definition of the embedding space by methods of correlation dimension algorithm and false nearest neighbor points);

c) determination of the dynamic invariants of a chaotic system (global Lyapunov exponents);

d) forecasting evolution of the dynamical system.

Algorithm for calculating the characteristics of the chaotic time series and use it to forecast the non-linear method is presented in Figure 1. The most important stage of this technique are the first two points, as the accuracy of the recovery will depend on the dimension of the attractor chaotic classification system and forecast its evolution. Therefore it is preferable not to use any one method, and several compare results. There is another very important aspect related to the invariants of the system. The fact is that if the aggregate and dynamic topological invariants (see details in [1-3]), the two systems are identical, then we can say that the evolution of these systems are also subject to the same laws. Further, if one of these systems is known differential equation (or system of equations) describing its dynamics, it can be assumed that an analogous equation (or system) and the other describes the evolution of the system.

I. Preliminary conclusion about the presence of chaos

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1. The Gottwald-Melbourne test: K → 1 - chaos

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2. The Fourier expansion irregular change - chaos

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II. The phase space

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3. Computation of the time delay τ using the autocorrelation function or the mutual information

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4. Determining embedding dimension d_E by the method of the correlation dimension or algorithm of the false nearest neighbor points

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III. Forecasting

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5. Computation of the global Lyapunov dimension λ_α; determination of the Kaplan-York dimension d_L and average limits of predictability Pr_{max}

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6. Determining the number of nearest neighboring points NN for the best forecast results

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7. Application of a nonlinear prediction method

Figure 1 – General compact algorithm for computation of the characteristics of the air pollutant chaotic time series and application of the non-linear prediction method to it

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Аналіз і прогноз антропогенного впливу на повітряний басейн промислового міста на основі методів теорії хаосу: Нова загальна схема. Глушков О.В.

З метою розвитку теоретичних основ загального апарату аналізу та прогнозу впливу антропогенного навантаження на стан атмосфери промислового міста і розробки нової схеми моделювання властивостей полів концентрацій забруднюючих повітряний басейн речовин на основі методів теорії хаосу, виконано аналіз тестів на наявність хаосу в системі (повітряний басейн промислового міста) і викладено удосконалену методику відновлення фазового простору.

Ключові слова: *повітряний басейн промислового міста, екологічний стан, часові ряди концентрацій, забруднюючі речовини, аналіз і прогноз, методи теорії хаосу*

Анализ и прогноз антропогенного воздействия на воздушный бассейн промышленного города на основе методов теории хаоса: Новая общая схема. Глушков А.В.

Изложены теоретические основы общего аппарата анализа и прогноза влияния антропогенной нагрузки на состояние атмосферы промышленного города, Представлена компактная общая схема моделирования временных флуктуаций полей концентраций загрязняющих воздушный бассейн веществ на основе методов теории хаоса.

Ключевые слова: *воздушный бассейн промышленного города, экологическое состояние, временные ряды концентраций, загрязняющие вещества, анализ и прогноз, методы теории хаоса*