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ANALYSIS AND FORECAST OF THE HYDROECOLOGICAL SYSTEM POLLUTION DYNAMICS BASED ON METHODS OF CHAOS THEORY: NEW GENERAL SCHEME

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We present firstly a new whole technique of analysis, processing and forecasting any time series of the chemical pollutants in the typical hydroecological systems , which is schematically looked as follows: a). A general qualitative analysis of dynamical problem of the typical hydroecological systems (including a qualitative analysis from the viewpoint of ordinary differential equations, the "Arnold-analysis"); b) checking for the presence of a chaotic (stochastic) features and regimes (the Gottwald-Melbourne's test; the method of correlation dimension); c) 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); d). Determination of the dynamic invariants of a chaotic system (Computation of the global Lyapunov dimension λ_α; determination of the Kaplan-York dimension d_L and average limits of predictability Pr_{max} on the basis of the advanced algorithms; e) A non-linear prediction (forecasting) of an dynamical evolution of the system. The last block indeed includes new (in a theory of hydroecological systems and environmental protection) methods and algorithms of nonlinear prediction such as methods of predicted trajectories, stochastic propagators and neural networks modelling, renorm-analysis with blocks of the polynomial approximations, wavelet-expansions etc.

Key words: hydroecological systems, the ecological state, 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 [1-10]. 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 has been in details considered, for example, in Ref.[3]. In modern theory of the hydroecological systems, water resources and environmental protection a problem of quantitative treating pollution dynamics is also one of the most important and fundamental problems, in particular, applied ecology and urban ecology [1-18]. Let us remind [1-3] that most of the models currently used to assess a state (as well as, the forecast) of an environment 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. Especially serious problem is arised during studying dynamics of the hydroecological systems. 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. In Ref.[1-4] we presented the successful examples of the 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. Moreover, some elements of this technique have been successfully applied to several prediction tasks for other nature system. Here we mean a prediction of the ecological state evolution (temporal or even spatial) [6-11]. As example, let us remind the results of the research into dynamics of variations hydroecological (nitrates and sulphates concentrations in the Small Carpathians river's watersheds in the Earthen Slovakia) systems in the definite region by using the non-linear prediction approaches and the recurrence plots method. We at first discovered a chaotic behaviour in the nitrates and sulphates concentration time series in the watersheds of the Small Carpathians. Naturally, except different physical and chemical features, from the formal mathematical point of view a difference between atmospheric and hydrological environmental systems is not essential, because in the both problems we are dealing with the time series of fundamental pollution characteristics and therefore construction of the technique for studying pollution dynamics of hydroecological systems will have only some differences in details. The main purpose of this paper is formally to represent theoretical basis of a new general formalism for an analysis and forecasting an impact of anthropogenic factors on the hydroecological systems (water resources) and develop a new compact general scheme for modeling temporal fluctuations of the pollution concentration field temporal fluctuations , based on the methods of a chaos theory. Earlier it had been successfully realized in a case of the atmosphere (air bassein) of large industrial cities (regions). So, below we will follow the corresponding atmospheric formalism [2-4] and dive the necessary comments in a case of the important features.

2. NEW GENERAL FORMALISM FOR ANALYSIS OF AND FORECASTING POLLUTANTS DYNAMICS OF THE HYDROECOLOGICAL SYSTEMS

As usually, we start from the first key task on testing a chaos in the time series of hydroecological pollutants. Following to [2-4], one should consider scalar measurements of the system dynamical parameter, say:

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

Here t_0 is a start time, Δt is the time step, and n is number of the measurements. In a general case, $s(n)$ is any time series (hydroecological 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,

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

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 (see details, for example, in Refs. [2-4]).

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.

Further it is an important task 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 [1-3]. 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 [2-4].

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 [2-4], one should calculate 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

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

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. [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? [2-4]. 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 $R_d(k)$ [3]

$$R_d^2(k) = [s(k) - s^{NN}(k)]^2 + [s(k+\tau) - s^{NN}(k+\tau)]^2 + \\ \ldots + [s(k+\tau(d-1)) - s^{NN}(k+\tau(d-1))]^2. \quad (4)$$

$R_d(k)$ 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

$$R_{d+1}^2(k) = R_d^2(k) + [s(k+d\tau) - s^{NN}(k+d\tau)]^2. \quad (5)$$

We can define some threshold size R_T to decide when neighbours are false. Then if [3]

$$\frac{|s(k+d\tau) - s^{NN}(k+d\tau)|}{R_d(k)} > R_T, \quad (6)$$

(the nearest neighbours at time point k are declared false). Kennel et al. [17] 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.

If one compute the whole spectrum of the Lyapunov exponents, other invariants of the system, i.e. the Kolmogorov entropy and the attractor's dimension can be found. The Kolmogorov entropy measures the average rate at which information about the state is lost with time. An estimate of this measure is the sum of the positive Lyapunov exponents. The estimate of the dimension of the attractor is provided by the Kaplan and Yorke conjecture (see details in Refs. [2-4,16,18]):

$$d_L = j + \frac{\sum_{\alpha=1}^{j} \lambda_\alpha}{|\lambda_{j+1}|}, \quad (7)$$

where j is such that $\sum_{\alpha=1}^{j} \lambda_\alpha > 0$ and $\sum_{\alpha=1}^{j+1} \lambda_\alpha < 0$, 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, one should use a method with linear fitted map, although maps with higher order polynomials can be used too [18-23]. Another new approach has been recently developed by Glushkov-Prepelitsa et al and in using the neural networks technique [25].

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) for the typical hydroecological systems (rivers, water resources etc.). Naturally, a difference between the atmospheric and hydrological systems is not essential and connected only with blocks of treating dynamics of these systems from the viewpoint of the evolutionary differential equations theory.

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 for the typical hydroecological systems. Shortly speaking, the whole technique of analysis, processing and forecasting any time series of the chemical pollutants in the typical hydroecological systems will be looked as follows (see figure below):

A). A general qualitative analysis of dynamical problem of the typical hydroecological systems (including a qualitative analysis from the viewpoint of ordinary differential equations, the “Arnold-analysis”);

B) checking for the presence of a chaotic (stochastic) features and regimes (the Gottwald-Melbourne’s test; the method of correlation dimension);

C) 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);

D). Determination of the dynamic invariants of a chaotic system (Computation of the global Lyapunov dimension λ_α; determination of the Kaplan-York dimension d_L and average limits of predictability Pr_{max} on the basis of the advanced algorithms;

E) A non-linear prediction (forecasting) of an dynamical evolution of the system.

The last block indeed includes new methods and algorithms of nonlinear prediction such as methods of predicted trajectories, stochastic propagators and neural networks modelling, renorm-analysis with blocks of the polynominal approximations, wavelet-expansions [10,11,25]). Indeed, one should use a few algorithms at any step of studying.

Naturally, if the aggregate and dynamic topological invariants (see [1-11]) are identical for two chosen systems, then evolutions of these systems are also subject to the same laws, including the same or analogous systems of differential equations. This fact is very useful especially with using such new methods and algorithms of nonlinear prediction as methods of predicted trajectories, stochastic propagators and neural networks modelling with blocks of the polynominal approximations, wavelet-expansions [1,10,11,25].

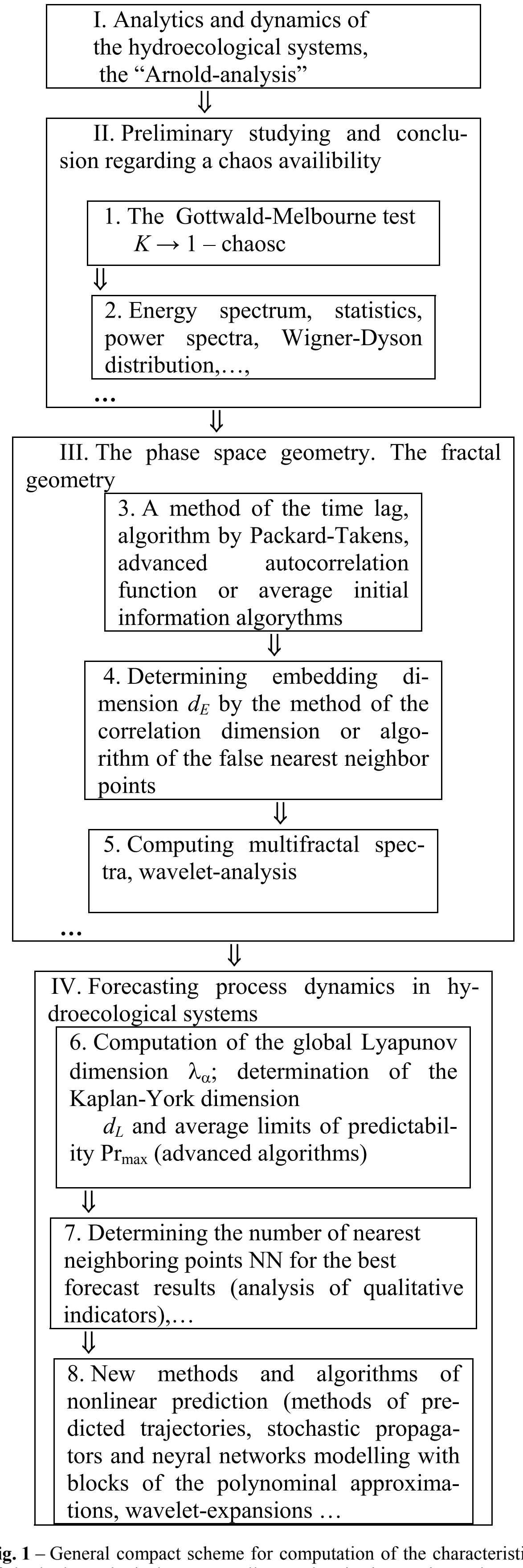

Fig. 1 – General compact scheme for computation of the characteristics of the hydroecological system pollutant chaotic time series and a nonlinear analysis, modelling and prediction

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АНАЛИЗ И ПРОГНОЗ ДИНАМИКИ ЗАГРЯЗНЕНИЯ ГИДРОЭКОЛОГИЧЕСКИХ СИСТЕМ, ОСНОВАННЫЕ НА МЕТОДАХ ТЕОРИИ КВАНТОВОЙ ГЕОМЕТРИИ И ХАОСА: НОВАЯ ОБШАЯ ТЕХНИКА

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Мы представляем новый общий аппарат анализа, обработки и прогнозирования характеристик временных рядов концентраций загрязняющих веществ для типичных гидроэкологических систем, который схематически включает следующие блоки и уровни исследований: а). Общий качественный анализ динамических особенностей задачи эволюции типичных гидроэкологических систем (в том числе, качественный анализ с точки зрения обыкновенных дифференциальных уравнений, "Арнольд-анализ»); б) проверка на наличие хаотических (стохастических) особенностей, элементов, режимов (тест Готвальда-Мельбурна, метод корреляционной размерности); в) Исследование фазового пространства (выбор времени задержки, определение пространства вложения методами и алгоритмами корреляционной размерности и ложных ближайших соседних точках); г). Определение динамических инвариантов хаотической системы (вычисление глобальной размерности, показателей Ляпунова λ_{α}; определение размерности Каплана-Йорка d_L и среднего предела предсказуемости Pr_{max} на основе усовершенствованных алгоритмов; е) нелинейный анализ и предсказание (прогнозирование) динамической эволюции систем. Последний блок действительно включает в себя новые (в теории гидроэкологических систем и охраны окружающей среды) методы и алгоритмы нелинейного прогнозирования, такие как методы прогнозируемых траекторий, формализм случайных пропагаторов, нейросетевые алгоритмы, ренорм-анализ с блоками полиномиальных аппроксимаций, вейвлет-разложений и т.д.

Ключевые слова: гидроэкологические системы, экологическое состояние, временные ряды концентраций, загрязняющие вещества, анализ и прогнозирование на основе методов теории хаоса.

АНАЛІЗ І ПРОГНОЗ ДИНАМІКИ ЗАБРУДНЕННЯ ГІДРОЕКОЛОГІЧНИХ СИСТЕМ, ЗАСНОВАНІ НА МЕТОДАХ КВАНТОВОЛЇ ГЕОМЕТРІЇ ТА ТЕОРІЇ ХАОСУ: НОВА ЗАГАЛЬНА ТЕХНІКА

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Ми представляємо новий загальний апарат аналізу, обробки та прогнозування характеристик часових рядів концентрацій забруднюючих речовин для типових гідроекологічних систем, що схематично включає наступні блоки і рівні досліджень: а). Загальний якісний аналіз динамічних особливостей завдання еволюції типових гідроекологічних систем (у тому числі, якісний аналіз з погляду звичайних диференціальних рівнянь ", Арнольд-аналіз»); б) перевірка на наявність хаотичних (стохастичних) особливостей, елементів, режимів (тест Готвальда-Мельбурна , метод кореляційної розмірності); в) Дослідження фазового простору (вибір часу затримки, визначення простору вкладення методами і алгоритмами кореляційної розмірності і помилкових найближчих сусідніх точках) ;. г) Визначення динамічних інваріантів хаотичної системи (обчислення глобальної розмірності, показників Ляпунова λ_{α}; визначення розмірності Каплана-Йорка d_L і середнього межі передбачуваності Pr_{max} на основі вдосконалених алгоритмів ;. е) нелінійний аналіз і прогноз (прогнозування) динамічної еволюції систем Останній блок дійсно включає в себе нові (в теорії гідроекологічних систем та охорони навколишнього середовища) методи та алгоритми нелінійного прогнозування , такі як методи прогнозованих траєкторій, формалізм випадкових пропагатор, нейромережеві алгоритми, Ренорм-аналіз з блоками поліноміальних апроксимацій, вейвлет-розкладів і т.д.

Ключові слова: гідроекологічні системи, екологічний стан, часові ряди концентрацій, забруднюючі речовини, аналіз та прогнозування на основі методів теорії хаосу.

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