UDC 504.06

STUDYING AND FORECASTING THE SULPHATES POLLUTION DYNAMICS BY USING A CHAOS THEORY METHODS: APPLICATION TO THE SMALL CARPATHIANS RIVER'S WATERSHEDS

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Purpose. of this article is advanced quantitative studying results of a pollution dynamics for variations hydroecological systems, namely, the sulphates concentrations dynamics for a number of the Small Carpathians river's watersheds in the Eastern Slovakia. **Methodology**. We have used methods and algorithms of the chaos theory (chaos-geometric approach) and dynamical systems theory in the advanced versions. **Results**. New more exact data on chaotic behaviour of the sulphates concentration time series in the watersheds of the Small Carpathians are presented. The required time delay and embedding dimension have been computed by the methods of autocorrelation function and average mutual information. Besides, the advanced versions of the correlation dimension method and algorithm of false nearest neighbours were used. The Fourier spectrum of the concentration of sulphates in the water catchment area Vydrica (C.Most) for the period 1991 - 1993 is listed. Here we present new advanced data on the correlation dimension (d_2), embedding dimension (d_E), Kaplan-Yorke dimension (d_L), average limit of predictability (Pr_{max}) and parameter K for the sulphates concentrations in in the watersheds of the Small Carpathians. **Originality**. For the first time the chaos theory was used to forecast sulphates and other contaminators concentration time series by the methods of autocorrelation function and average mutual information, correlation dimension method and algorithm of false nearest neighbours. **Practical value**. The results themselves present a high ecological value for contaminaotrs concentration forecast. Moreover, developed approach on studying dynamics of variations of the sulphates concentrations in the river's water reservoirs using the non-linear prediction approaches and a chaos theory methods can be used to similar calculations for different water bodies.

Key words: hydroecological systems dynamics, studying and forecasting, sulphates concentrations, the Small Carpathians river's watersheds, chaos theory methods

МОДЕЛЮВАННЯ ТА ПРОГНОЗУВАННЯ ДИНАМІКИ ЗАБРУДНЕННЯ ГІДРОЕКОЛОГІЧНИХ СИСТЕМ ЗА ДОПОМОГОЮ МЕТОДІВ ТЕОРІЇ ХАОСУ: УТОЧНЕНІ ДАНІ ЩОДО ЗАБРУДНЕННЯ ВОДОДІЛІВ РІЧОК МАЛИХ КАРПАТ

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Дана робота продовжує кількісні дослідження динаміки забруднення різних гідроекологічних систем, зокрема, часовій динаміці зміни концентрацій сульфатів у ряді вододілів річок Малих Карпат у Східній Словаччині. Різні методи і алгоритми теорії хаосу (хаос-геометричного підходу) і теорії динамічних систем використані у найбільш досконалих версіях. Представлені нові більш точні дані, що характеризують хаотичну поведінку часових рядів концентрацій сульфатів для ряду вододілів річок Малих Карпат. У попередніх роботах (див. [1]) для відновлення відповідного аттрактора, попередньо обчислювалися час затримки (часовий лаг) і розмірності вкладення. Шукані параметри були визначені з використанням методів автокореляційної функції та середньої взаємної інформації. Крім того, були застосовані більш досконалі версії методу кореляційної розмірності і алгоритму помилкових найближчих сусідів. Тут наведені нові більш точні результати по кореляційній розмірності (d_2), розмірності вкладення (d_E), розмірності Каплан-Йорка (d_L), середній межі передбачуваності (Pr_{max}) і параметру хаосу К для концентрацій сульфатів для ряду вододілів.

Ключові слова: гідроекологічні динамічні системи, вивчення та прогнозування, нітрати і сульфати концентрації, вододіли Малих Карпат, методи теорії хаосу

PROBLEM STATEMENT. Our paper concerns results of the research into dynamics of variations hydroecological (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. Earlier the same program has been in details performed for the sulphates in the same system. Many studies in various fields of science have appeared, where chaos theory was applied to a great number of dynamical systems [1-14]. The studies concerning non-linear behaviour in the time series of atmospheric constituent concentrations are sparse, and their outcomes are ambiguous In ref. [5] there is an analysis of the NO_2, CO,

O_3 concentrations time series and is not received an evidence of chaos. 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 refs. [2, 10,12] there is an analysis of the NO_2, CO, O_3 concentrations time series in the Gdansk and Trieste region and it has been definitely received an evidence of chaos. More over it has been given a short-range forecast of atmospheric pollutants using 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. It opens very attractive perspectives using the same methods in studying dynamics of pollution of other ecological and hydrological systems. In this work we study the pollutions dynamics of the hydrological systems, in particular, variations of the sulphates concentrations in the river's water reservoirs in the Earthen Slovakia by using the non-linear prediction approaches and chaos theory method (in versions) [2,9-14]. A chaotic behaviour in the sulphates concentration time series in the watersheds of the Small Carpathians is investigated».

EXPERIMENTAL PART AND RESULTS OBTAINED. As the initial data we use the results of empirical observations made on six watersheds (fig.1.)in the region of the Small Carpathians, carried out by coworkers of the Institute of Hydrology of the Slovak Academy of Sciences [2]. Fig.2 shows the temporal changes in the concentrations of sulphates in the catchment areas. In fig. 3 we list the Fourier spectrum of the concentration of sulphates in the water catchment area Vydrica (C.Most)for the period 1991 - 1993. The X-axis - frequency, the axis Y – energy. The Fourier spectrum looks the same as in the case of a random process, so there exists the possibility of using methods of chaos theory and subsequent short-term prediction method for nonlinear pollutant concentrations.

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.

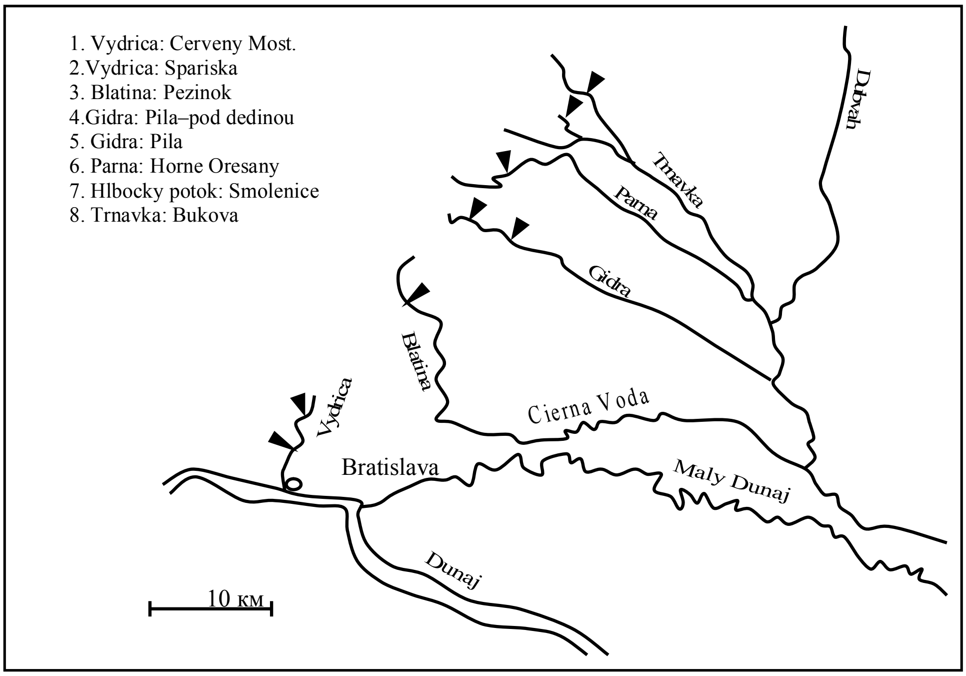

Figure 1 – Scheme of the f observation points in the Small Carpathians (Slovakia) [2].

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 $I_{AB}(a_i, b_k)$. In ref. [4] it is suggested, as a prescription, that it is necessary to choose that τ where the first minimum of $I(\tau)$ occurs

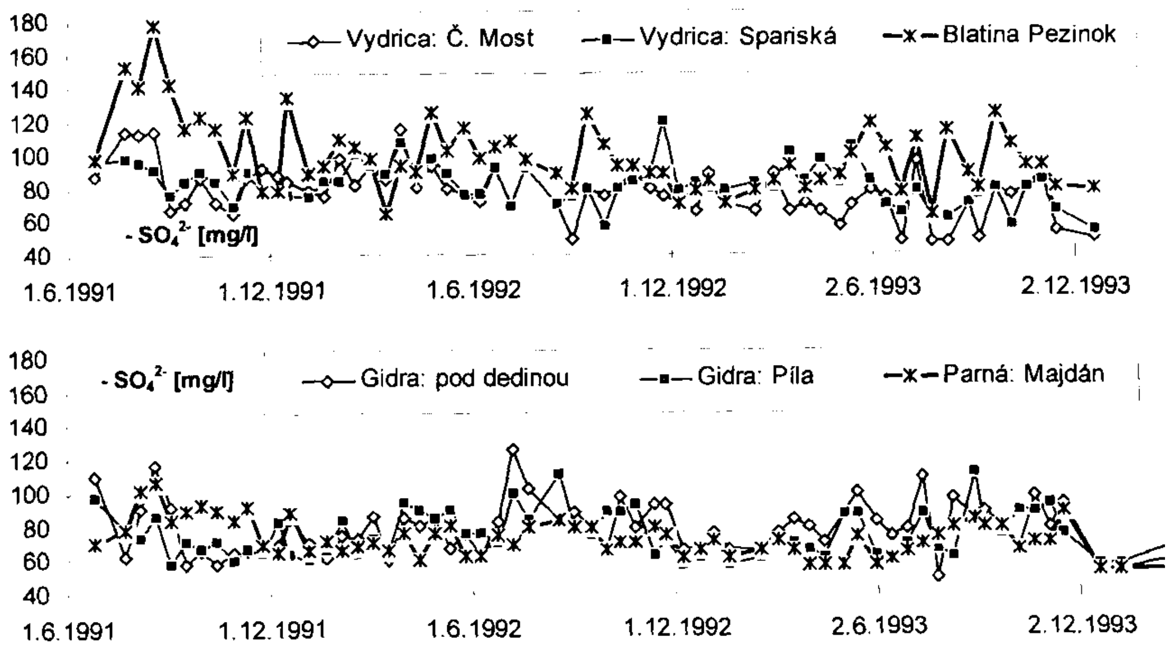

Figure 2 – The temporal changes in the concentrations of sulphates in some catchment of the Small Carpathians (Slovakia) [2].

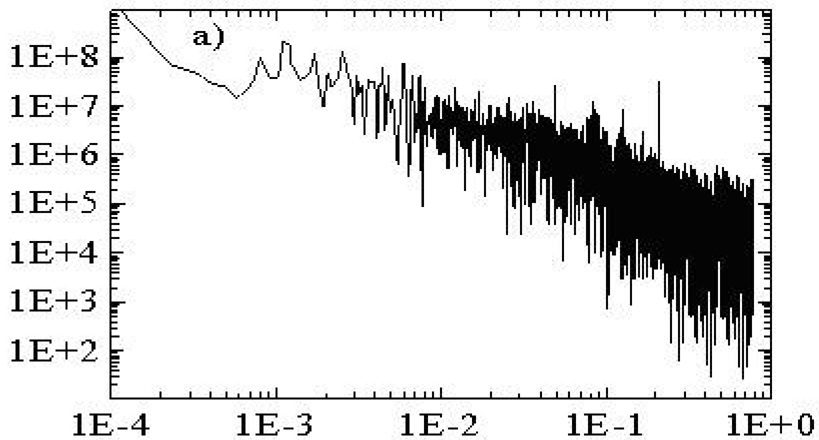

Figure 3 – The Fourier spectrum of the concentration of sulphates in the water catchment area Vydrica (C.Most) for the period 1991 - 1993

Table 1 – Time lag (τ), correlation dimension (d_2), embedding dimension (d_E), Kaplan-Yorke dimension (d_L), average limit of predictability (Pr_{max}) and parameter K for the sulphates concentrations in the watersheds of the Small Carpathians

River (Site)	τ	d_2	d_E	d_L	Pr_{max}	K
Vydrica (C.Most)	15	5,63	6	5,73	11	0,69
Vydrica (Spariska)	14	4,89	5	4,41	10	0,82
Blatina (Pezinok)	20	4,73	5	4,52	11	0,74
Gidra (Main)	17	5,47	6	5,68	11	0,81
Gidra (Pila)	14	5,69	6	5,79	12	0,69
Pama (Majdan)	16	4,68	5	4,13	10	0,72
Hlbocsky (Smolenice)	18	4,06	5	4,53	9	0,81

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. 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 [8], 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

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

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. [2,8]).

The correlation dimension of attractor (d_A) is defined as the value of the correlation dimension at which it is not affected by increasing the embedding dimension Before we discuss the results of a reconstruction of the attractor dimension by the method of the correlation dimension, we also check a similar result by the algorithm (version [2] of the false nearest neighboring points). The dimension of the attractor in this case was defined as the embedding dimension, in which the number of false nearest neighboring points was less than 3%

First of all, it's important to define how predictable is a chaotic system? The predictability can be estimated by the Kolmogorov entropy, which is proportional to a sum of the positive Lyapunov's exponents. The spectrum of 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 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. For chaotic systems, being both stable and unstable, 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. The dimension d_L gives values close to the dimension estimates discussed earlier and is preferable when estimating high dimensions. To compute Lyapunov's exponents, we use a method with linear fitted map [1,2], although the maps with higher order polynomials can be used too. The sum of positive Lyapunov's exponents determines the Kolmogorov entropy, which is inversely proportional to the limit of predictability (Pr_{max}).

The Tables 1 summarizes the results of the numerical reconstruction of the attractors, as well as average limit of predictability (Pr_{max}) and the Gottwald-Melbourne chaos availability parameter K [8] for the sulphates concentrations in the watersheds of the Small Carpathians region. We also note that the length and discrete time series in Table 1 is one night; τ and Pr_{max} have the corresponding dimensions.As it is indicated, the sum of the positive Lyapunov's exponents λ_i determines the Kolmogorov entropy, which is inversely proportional to the limit of predictability (Pr_{max}). Let us remind since the conversion rate of the sphere into an ellipsoid along different axes is determined by the λ_i, it is clear that the smaller the amount of positive dimensions, the more stable is a dynamic system. Consequently, it increases the predictability of it. 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. Our data show that the greatest degree of predictability is observed for the time series of sulphates in the watershed Gidra (Main) (fourteen slots, i.e. seven months), and in other cases the limit of predictability is slightly less. Such predictability is quite sufficient for the prediction of pollution.

CONCLUSIONS. In this paper we present the results of studying dynamics of variations of the sulphates concentrations in the river's water reservoirs in the Earthen Slovakia using the non-linear prediction approaches and a chaos theory methods. A chaotic behaviour in the sulphates concentration time series in the watersheds of the Small Carpathians is investigated. To reconstruct the corresponding attractor, the time delay and embedding dimension are needed. The former is determined by the methods of autocorrelation function and average mutual information, and the latter is calculated by means of correlation dimension method and algorithm of false nearest neighbours. It is shown that low-dimensional chaos exists in the time series under investigation and quite sufficient predictability is obtained in the forecasting the sulphates pollution concentrations dynamics in the watersheds of the Small Carpathians (as example of the hydroecological system).

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МОДЕЛИРОВАНИЕ И ПРОГНОЗИРОВАНИЕ ДИНАМИКИ ЗАГРЯЗНЕНИЯ ГИДРОЭКОЛОГИЧЕСКИХ СИСТЕМ С ИСПОЛЬЗОВАНИЕМ МЕТОДОВ ТЕОРИИ ХАОСА: УТОЧНЕННЫЕ ДАННЫЕ ПО ДИНАМИКЕ ЗАГРЯЗНЕНИЯ ВОДОРАЗДЕЛОВ РЕК МАЛЫХ КАРПАТ

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Данная работа продолжает количественные исследования динамики загрязнения различных гидроэкологических систем, в частности, временной динамики изменения концентраций сульфатов в ряде водоразделов рек Малых Карпат в Восточной Словакии. Различные методы и алгоритмы теории хаоса (хаос-геометрического подхода) и теории динамических систем использованы в наиболее совершенных версиях. Представлены новые более точные данные, характеризующие хаотическое поведение временных рядов концентраций сульфатов для ряда водоразделов рек Малых Карпат. В предыдущих работах (см. [1]) для восстановления соответствующего аттрактора, предварительно вычислялись время задержки (временной лаг) и размерности вложения. Искомые параметры определялись с использованием методов автокорреляционной функции и средней взаимной информации. Кроме того, были применены более совершенные версии метода корреляционной размерности и алгоритма ложных ближайших соседей. Здесь приводятся новые более точные результаты по корреляционной размерности (d_2), размерности вложения (d_E), размерности Каплан-Йорка (d_L), среднему пределу предсказуемости (Pr_{max}) и параметру хаоса К для концентраций сульфатов для ряда водоразделов.

Ключевые слова: гидроэкологические динамические системы, изучения и прогнозирования, нитраты и сульфаты концентрации, водоразделы рек Малых Карпат, методы теории хаоса