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MODELLING AND FORECASTING THE HYDROECOLOGICAL SYSTEMS POLLUTION DYNAMICS BY USING A CHAOS THEORY METHODS: I. ADVANCED DATA ON POLLUTION OF THE SMALL CARPATHIANS RIVER'S WATERSHEDS

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This paper presents the advanced quantitative studying results of a pollution dynamics for variations hydroecological systems, namely, the nitrates and sulphates concentrations dynamics for a number of the Small Carpathians river's watersheds in the Eastern Slovakia. The different methods and algorithms of the chaos theory (chaos-geometric approach) and dynamical systems theory have been used in the advanced versions. New more exact data on chaotic behaviour of the nitrates and sulphates concentration time series in the watersheds of the Small Carpathians are presented. To reconstruct the corresponding attractor, the time delay and embedding dimension are needed. The parameters are determined by the methods of autocorrelation function and average mutual information. Besides, there are used the advanced versions of the correlation dimension method and algorithm of false nearest neighbours. The Fourier spectrum of the concentration of nitrates in the water catchment area Ondava: Stropkov for the period 1969 – 1996 is listed.

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

1. INTRODUCTION

This work goes on our studying regular and chaotic features of different nature systems, namely, atmospheric, hydrological, hydroecological systems (water resources, environment protection) [1-12]. As usually let us remind that 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 nitrates and sulphates concentrations in the river's water reservoirs in the Earthen Slovakia [11,12] by using the non-linear prediction approaches and chaos theory method (in versions) [1-5,13-20] . A chaotic behaviour in the nitrates and sulphates concentration time series in the watersheds of the Small Carpathians is investigated too. However, in the cited studying the authors have used the most simplified algorithms of a chaos theory.

2. TESTING FOR CHAOS IN TIME SERIES

2.1 Data

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 co-workers of the Institute of Hydrology of the Slovak Academy of Sciences [21,22]. Fig.2 shows the temporal changes in the concentrations of nitrates in the catchment areas. Table 1 presents some of the important statistics (coordinates of sites 6 and 9 are 54°24'54"N, 18°34'47"E and 54°29'40"N, 18°33'15"E) [2]. In fig. 3 we list the Fourier spectrum of the concentration of nitrates in the water catchment area Ondava: Stropkov for the period 1969 - 1996. 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.

2.2 Testing for chaos in time series

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

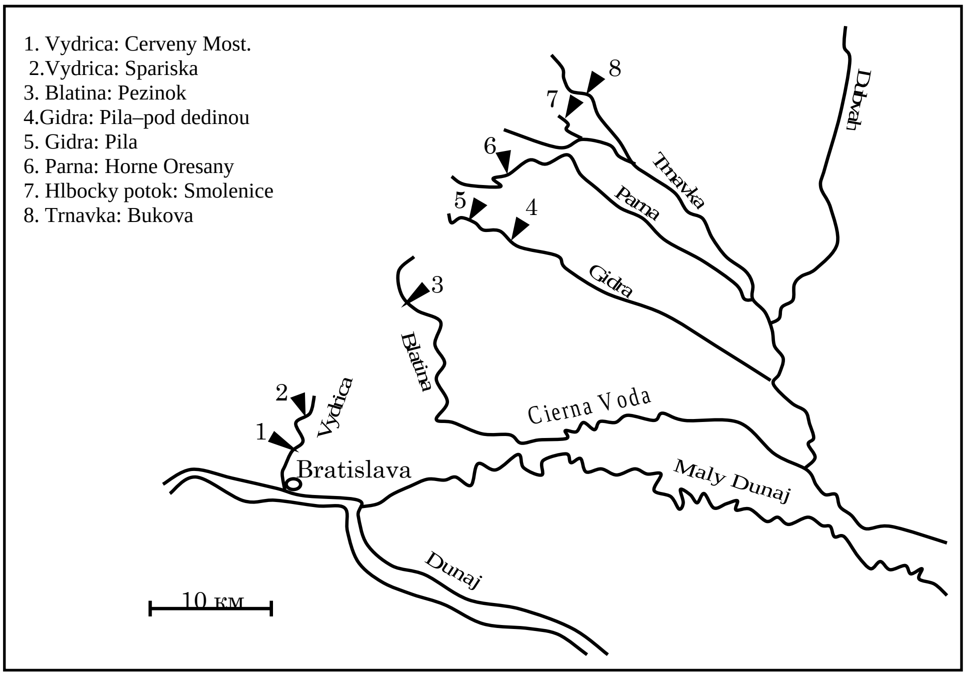

Fig. 1 - Scheme of the observation points in the Small Carpathians (Slovakia) (see text).

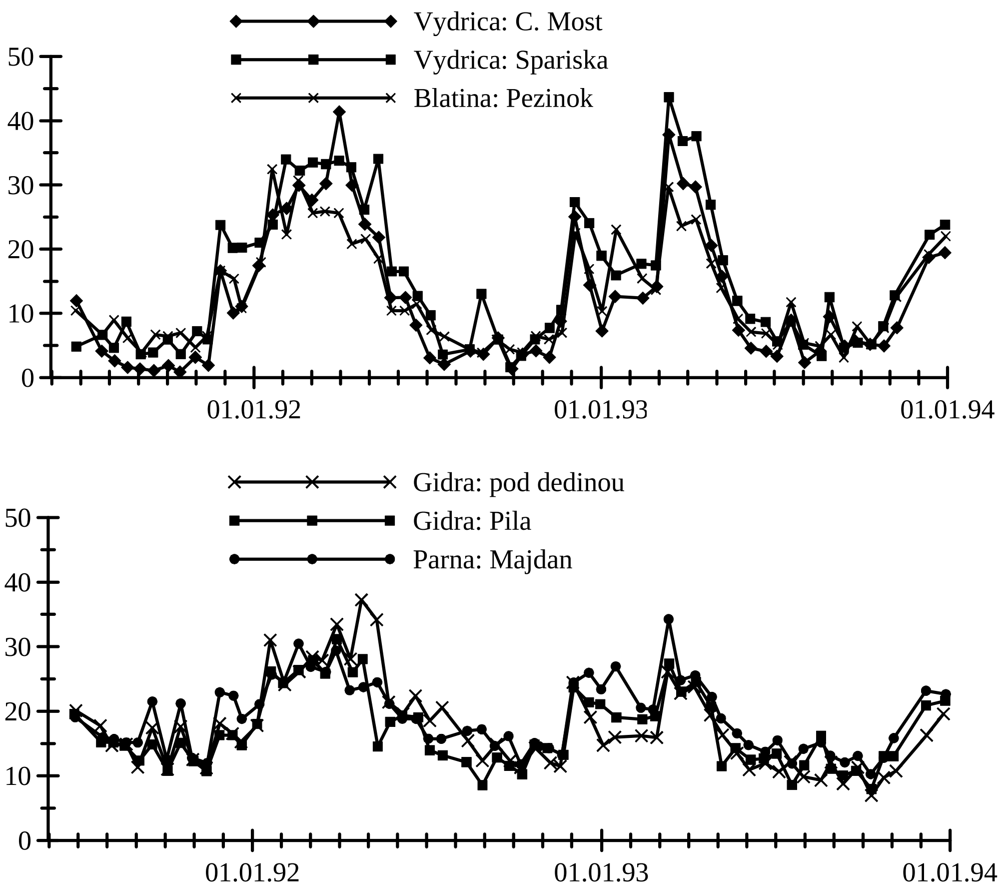

Fig. 2 - The temporal changes in the concentrations of nitrates in some catchment of the Small Carpathians (Slovakia) [2].

Table 1 - Some statistics of or measured values for the nitrate concentrations (in mg·l[-1]) in water flows Small Carpathian region during the period 1991-1995 (see text)

River Site	Vydrica C.Most	Vydrica Spariska	Blatina Pezinok	Gidra pod dedin.	Gidra Pila	Pama Majdan
Mean	10,96	14,48	11,65	16,71	16,59	18,53
min	0,73	0,75	1,74	7,70	8,55	10,10
max	40,20	42,10	31,40	36,60	31,50	34,20
Sq.deviation	10,41	11,09	8,05	6,66	5,61	5,22
c_s	1,03	0,70	0,79	1,08	0,75	0,62
c_v	0,95	0,77	0,69	0,40	0,34	0,28
c_{95}	29,77	33,47	25,20	29,29	26,70	26,89
c_{90}	28,00	32,56	22,97	26,72	25,93	25,61
c_{10}	1,52	3,31	3,55	10,09	10.50	12,58

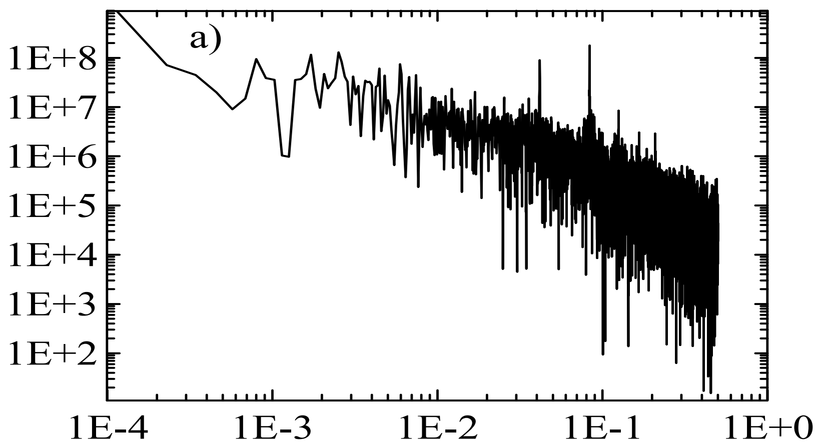

Fig. 3 - The Fourier spectrum of the concentration of nitrates in the water catchment area Ondava: Stropkov for the period 1969 - 1996

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.

2.3 Time lag

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.

Fig. 4 shows the results of these calculations for the time series of concentrations of nitrates in the water catchment area Ondava: Stropkov for the period 1969 to 1996.

In Tables 2 and 3 we list the values of the time delay (τ), depending on the different values of the autocorrelation function (C_L) and the first minimum of mutual in-formation (I_{min1}) for the concentration of nitrates (fig.2) and sulphates (fig.3) in the watershed of the Small Carpathians.

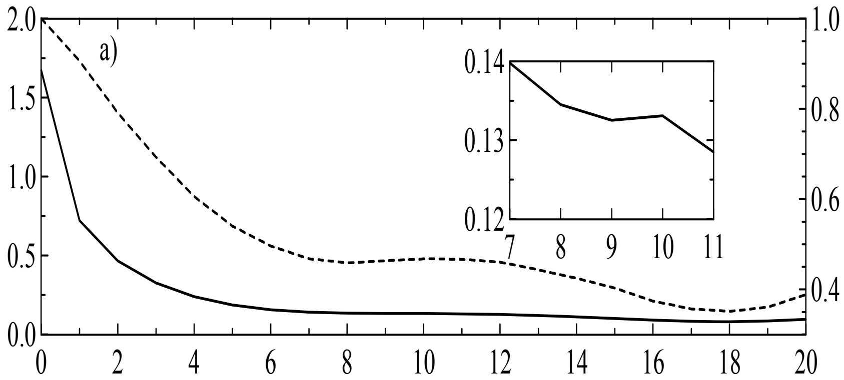

Fig. 4 - The mutual information (Y-axis on the left, solid line)and the autocorrelation function (Y-axis on the right, dashed line) as a functionfrom the time delay (axis X) for a concentration of nitratesin the watershed Ondava: Stropkov for the period 1969 - 1996

Table 2 - The values of the time delay (τ), depending on the different values of the autocorrelation function (C_L) and the first minimum of mutual information (I_{min1}) for the concentration of nitrates in the watershed of the Small Carpathians

River (Site)	C_L = 0	C_L = 0,1	C_L = 0,5	I_{min1}
Vydrica (C.Most)	–	282	52	19
Vydrica (Spariska)	–	280	51	18
Blatina (Pezinok)		305	60	18
Gidra (Main)	–	266	48	16
Gidra (Pila)	–	258	47	20
Pama (Majdan)	–	304	57	18
Ondava: (Stropkov)	–	246	43	10
Ladomirka (Svidnik)	–	143	26	10
Ondava (Svidnik)	–	132	26	10
Babie (Olsavka)	–	142	25	8
Manelo (Gribov)	322	175	27	7

Table 3 - The values of the time delay (τ), depending on the different values of the autocorrelation function (C_L) and the first minimum of mutual information (I_{min1}) for the concentration of sulphates in the watersheds of the Small Carpathians

River (Site)	C_L = 0	C_L = 0,1	C_L = 0,5	I_{min1}
Vydrica (C.Most)	–	282	48	15
Vydrica (Spariska)	–	280	48	14
Blatina (Pezinok)		305	47	20
Gidra (Main)	–	266	50	17
Gidra (Pila)	–	258	51	14
Pama (Majdan)	–	304	52	16

2.4 Embedding dimension

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

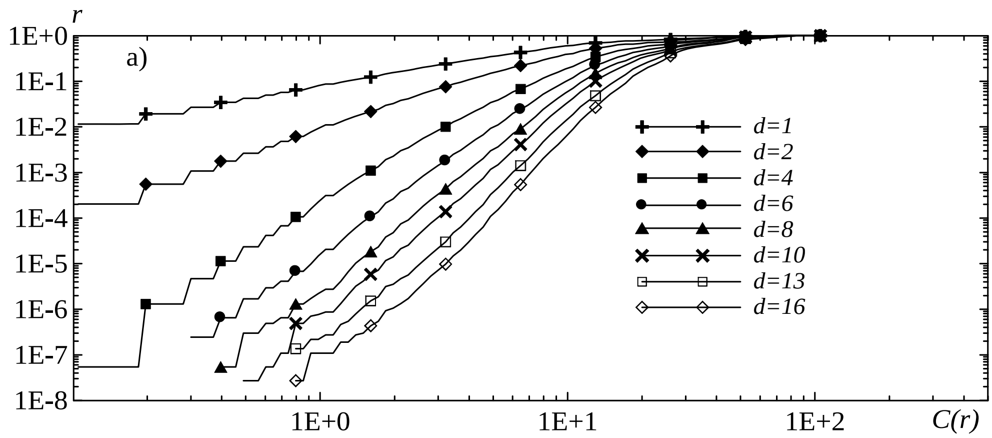

Fig. 5 - Dependence of the correlation integral *C (r)* of radius *r* for different embedding dimensions *d* for concentrations of nitrates in the watershed Ondava: Stropkov (1969 – 1996).

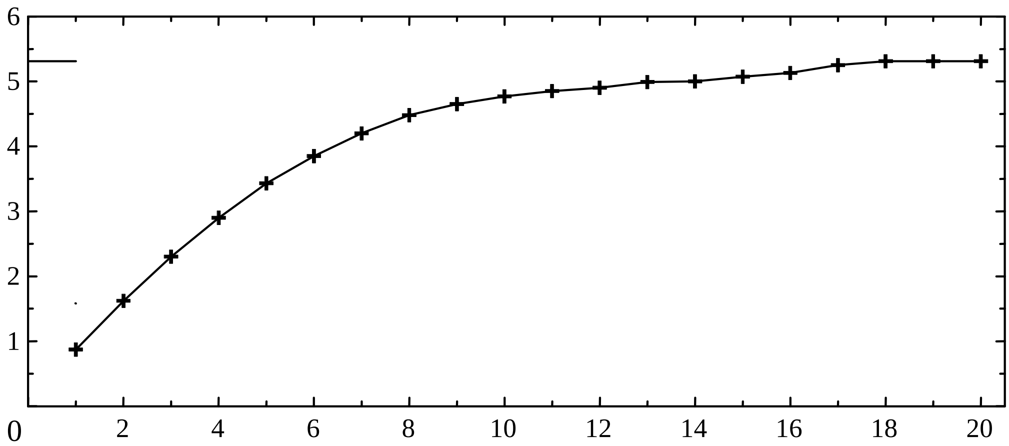

Fig. 6 - The dependence of the correlation dimension (axis Y) on the embedding dimension (axis X) for a concentration of nitrates in the watershed Ondava: (Stropkov) for period 1969-1996.

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]).

In figure 5 we present calculated dependence of the correlation integral *C (r)* of the radius *r* investments in different dimensions d for concentrations of nitratesin the watershed Ondava: (Stropkov) for the period 1969 – 1996. In figure 6 there is listed the dependence of the correlation dimension (axis Y) on the embedding dimension (axis X) for concentration of the nitrates in the watershed Ondava: (Stropkov) for period 1969-1996.

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. In fig. 5 we list the dependence of the correlation dimension (axis Y) on the embedding dimension (axis X) for a concentration of nitrates in the watershed Ondava: (Stropkov) for the period 1969 – 1996.

There is the corresponding curve, analysis of which shows that the saturation value for d_2 concentrations nitrates in the watershed Ondava: (Stropkov) for the period 1969 - 1996 amounts to 5.31 and was achieved by embedding dimension *ds*, at 18.

Before we discuss the results of a reconstruction of the attractor dimension by the method of the correlation dimension, we also give 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%.

3. CONCLUSSIONS

In first part of the paper we present renewed quantitative studying results for the nitrates and sulphates concentrations dynamics for a number of the Small Carpathians river's watersheds in the Earthen Slovakia. The different methods and algorithms of the chaos theory (chaos-geometric approach) and dynamical systems theory have been used in the advanced versions. New more exact data on chaotic behaviour of the nitrates and sulphates concentration time series in the watersheds of the Small Carpathians are presented. To reconstruct the corresponding attractor, the time delay and embedding dimension are needed. The parameters are determined by the methods of autocorrelation function and average mutual information. Besides, there are used the advanced versions of the correlation dimension method and algorithm of false nearest neighbours. We list the Fourier spectrum of the concentration of nitrates in the water catchment area Ondava: Stropkov for the period 1969 – 1996 too listed.

In the next parts of the work we will present the combined and final data on the time lags (τ), correlation dimensions (d_2), embedding dimensions (d_E), Kaplan-Yorke dimensions (d_L), average limits of predictability (Pr_{max}) and the known chaos parameter K for the nitrates and sulphates concentrations time series in the watersheds of the Small Carpathians. On the basis of the advanved data we will demonstrate the low-dimensional chaos in investigated time series , consider the advanced prediction model and list the results of forecasting the pollution concentrations dynamics in the watersheds of the Small Carpathians (as example of the hydroecological system).

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

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У статті представлені о уточнені кількісні дані по динаміці забруднення різних гідроекологічних систем, зокрема, часовій динаміці зміни концентрацій нітратів і 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 нітратів і сульфатів для ряду вододілів річок Малих Карпат. Для відновлення відповідного атрактору, попередньо обчислюються час затримки (часовий лаг) і розмірності вкладення. Шукані параметри визначаються з використанням методів автокореляційної функції та середньої взаємної інформації. Крім того, застосовані більш досконалі версії методу кореляційної розмірності і алгоритму помилкових найближчих сусідів. Представлений також розрахований спектр Фур'є концентрації нітратів для водозбору Ондава-Стропков за період 1969-1996гг.

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

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

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В статье представлены уточненные количественные данные по динамике загрязнения различных гидроэкологических систем, в частности, временной динамике изменения концентраций нитратов и 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 нитратов и сульфатов для ряда водоразделов рек Малых Карпат. Для восстановления соответствующего аттрактора, предварительно вычисляются время задержки (временной лаг) и размерности вложения. Искомые параметры определяются с использованием методов автокорреляционной функции и средней взаимной информации. Кроме того, применены более совершенные версии метода корреляционной размерности и алгоритма ложных ближайших соседей. Представлен также рассчитанный спектр Фурье концентрации нитратов для водосбора Ондава-Стропков за период 1969-1996гг.

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

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