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An advanced analysis and modelling the air pollutant concentration temporal dynamics in atmosphere of the industrial cities: Odessa city

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Abstract. Results of analysis and modelling the air pollutant (dioxide of nitrogen) concentration temporal dynamics in atmosphere of the industrial city Odessa are presented for the first time and based on computing by nonlinear methods of the chaos and dynamical systems theories. A chaotic behaviour is discovered and investigated. To reconstruct the corresponding strange chaotic attractor, the time delay and embedding dimension are computed. 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 nitrogen dioxide concentration time series under investigation. Further, the Lyapunov's exponents spectrum, Kaplan-Yorke dimension and Kolmogorov entropy are computed.

1. Introduction

The problem of quantitative treating air pollution temporal and spatial dynamics in atmosphere of the industrial cities is remained by one of the most actual and important problem of the modern applied ecology, the environmental protection [1-6]. As a rule, the deterministic models or simplified ones, based on a simple statistical regressions, are usually used to estimate air pollution [1-3]. The problem of any prediction of air pollutants temporal or spatial dynamics is remained practically unsolved hitherto. In the last years a new approach to air pollution problem is provided by using methods of advanced non-linear analysis, chaos, dynamical systems theories (see [5-21] and Refs. therein). 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. Also, it was shown that O_3 concentrations in Cincinnati (Ohio) and Istanbul are evidently chaotic, and non-linear approach provides satisfactory results [4]. In Ref. [6] it has been fulfilled the detailed analysis of the NO_2, CO, CO_2 concentration time series in the Gdansk region (Polland) and it has been definitely obtained the evidence of a chaos. Moreover it has been given a short-range forecast of atmospheric pollutants time evolution using non-linear prediction method. These studies show that a chaos and dynamical system theories methodology can be applied and the short-range forecast by the non-linear prediction method can be satisfactory.

In this paper for the first time we present the results of analysis and numerical modelling the air pollution (dioxide of nitrogen) concentration temporal dynamics in atmosphere of the industrial city Odessa. A chaotic behaviour has been discovered and in details investigated by using nonlinear methods of the chaos and dynamical systems theories [7-22]. To reconstruct the corresponding strange chaotic attractor, the time delay and embedding dimension are computed. 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. All calculations are performed with using "Geomath" and "Quantum Chaos" computational codes [21-35].

2. Data and method of analysis and modelling

In our study, we use the nitrogen dioxide (NO_2) concentration data observed in the atmosphere of the Odessa city from 1976 till 2000 years [2]. The multi-year hourly concentrations (one year total of 20x8760 data points, 1990) are analyzed. The typical temporal series of concentration (in mg/m^3) of the NO_2 (cite 1) is presented in figure 1.

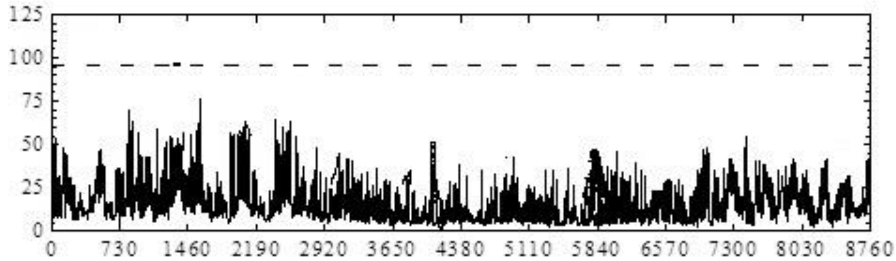

Figure 1. The temporal series of concentrations (in mg/m3) of the of the NO_2 (see text).

In Refs. [7-20] it has been developed 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. Here we are limited only by the key aspects. As usually, we 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, but here $s(n)$ corresponds to an atmospheric pollutant concentration. The first fundamental step of modelling is in reconstruction of the corresponding phase space using as well as possible information contained in $s(n)$. From the mathematical viewpoint, this procedure results in set of d-dimensional vectors $\mathbf{y}(n)$ replacing scalar measurements. One should further to operate with 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 set of the 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. The dimension d is defined as an embedding dimension, d_E.

In Refs. [6-8,14,15] a few approaches to the choice of proper time lag are presented. This point is important for the subsequent reconstruction of phase space. The 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 [9]. Let us remind that 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. The fundamental goal of the d_E calculation is in the further reconstruction of the 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 the corresponding chaotic attractor, d_A, i.e. $d_E > d_A$. 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, $C(r)$. According to Ref. [10], the correlation integral is defined as:

$$C(r) = \lim_{N\to\infty} \frac{2}{N(n-1)} \sum_{\substack{i,j \\ (1\le i<j\le N)}} H\left(r - \| \mathbf{y}_i - \mathbf{y}_j \|\right)$$

where H is the Heaviside step function with $H(u) = 1$ for $u > 0$ and $H(u) = 0$ for $u \le 0$, r is the radius of sphere centered on $\mathbf{y}_i$ or $\mathbf{y}_j$, and N is the number of data measurements. As usually, if the corresponding time series is characterized by an attractor, then the correlation dimension d is defined by a limit of relation of the log $C(r)$ to log of the corresponding radius (look details in Ref. [10]. In a case of the chaotic system the correlation exponent attains saturation with an increase in the embedding dimension. The saturation value of this exponent is defined as the correlation dimension (d_2) of the attractor. The technique of application the correlation integral method (say, the Grassberger-Procaccia algorithm [10]) is presented in Refs. [14,15].

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? This method is called as the method of false nearest neighbours. As a rule, the simultaneous application of two methods provides more exact determination d_E. It is noteworthy that the nearest integer above the saturation value provides the minimum or optimum embedding dimension for reconstructing the phase-space or the number of variables necessary to model the dynamics of the system. This concept can be applied, since the embedding dimension determined by both the correlation dimension method and the algorithm of false nearest neighbours are identical. The further important step in studying the chaotic time series of the dynamical system is determination of predictability, which can be estimated by the Kolmogorov entropy. The Kolmogorov entropy is proportional to a sum of the positive Lyapunov's exponents. Let us remind that the Lyapunov's exponents spectrum is one of the fundamental dynamical invariants for non-linear system with chaotic behaviour. According to definition, the Lyapunov's exponents are related to the eigenvalues of the linearized dynamics across the attractor. These parameters indicate the complexity of dynamics of the studied system. As usually, the positive values the Lyapunov's exponents show local unstable behaviour of the system, and respectively, their negative values show stable behaviour. The largest positive value of the Lyapunov's exponents 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 (version [14], although the maps with higher order polynomials can be used too.

3. The results and conclusions

Table 1 summarizes the results for the time lag, which is computed for first ~10^3 values of time series. The autocorrelation function crosses 0 only for the NO_2 time series, whereas this statistic for other time series remains positive. The values, where the autocorrelation function first crosses 0.1, can be chosen as τ, but earlier it had been showed that an attractor cannot be adequately reconstructed for very large values of τ. So, before making up final decision we calculate the dimension of attractor for all values in Table 1. If time lags determined by average mutual information are used, then algorithm of false nearest neighbours provides $d_E = 6$ for all air pollutants. Table 2 shows the results of computing a set of the dynamical and topological invariants, namely: correlation dimension (d_2), embedding dimension (d_E), two Lyapunov exponents λ_1,λ_2), Kaplan-York dimension (d_L) and average

Table 1. Time lags (hours) subject to different values of C_L and first minima of average mutual information (I_{min1}) for the time series of NO_2, SO_2 concentrations for two sites of the Odessa city (see text)

	NO_2 (cite 1)	NO_2 (cite 2)
$C_L = 0$	-	-
$C_L = 0.1$	142	156
$C_L = 0.5$	7	9
I_{min1}	10	13

limit of predictability (Pr_{max}, hours) for two the NO_2 concentration time series for the Odessa during the period: Jan.-Dec., 1990. From the data 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 Lyapunov's exponents λ_i (i=1,2). One could conclude that the system broadens in the line of two axes and converges along four axes that in the six-dimensional space. Other values of the Lyapunov's exponents λ_i are negative.

Table 2. The correlation dimension (d_2), embedding dimension (d_E), first two Lyapunov exponents, (λ_1,λ_2), Kaplan-Yorke dimension (d_L), and the Kolmogorov entropy, average limit of predictability (Pr_{max}, hours) for the time series of the NO_2 and SO_2 concentrations (Odessa city, 1990)

	Site 1 (Odessa) NO_2	Site 2 (Odessa) NO_2
λ_1	0.0187	0.0191
λ_2	0.0059	0.0049
d_2	5.28	5.26
d_E	6	6
d_L	4.09	3.92
K_{entr}	0.025	0.024
Pr_{max}	41	42

To conclude, for the first time we have presented the results of analysis and modelling the air pollutant (NO_2) concentration temporal dynamics in the Odessa's atmosphere. We have applied a number of nonlinear methods of a modern chaos and dynamical systems, such as an autocorrelation function method and the mutual information approach, a correlation integral analysis and the false nearest neighbours algorithm, the Lyapunov exponent's analysis and surrogate data method etc. To reconstruct the corresponding strange chaotic attractor, the time delay and embedding dimension are computed. 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. Further, the Lyapunov's exponents spectrum, Kaplan-Yorke dimension and Kolmogorov entropy are computed. A chaotic behaviour in the time series of NO_2 concentrations for two sites of the Odessa city was discovered and investigated. It has been shown that the low-dimensional chaos exists in the nitrogen dioxide concentration time series under investigation. The Lyapunov exponent's analysis has supported this conclusion.

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