Investigation of nonlinear dynamical properties by the observed complex behaviour as a basis for construction of dynamical models of atmospheric photochemical systems

Alexander M. Feigin, Yaroslav I. Molkov, Dmitrii N. Mukhin and Eugenii M. Loskutov

Institute of Applied Physics, Russian Academy of Sciences, 46 Ulyanov Street, Nizhny Novgorod 603950, Russia

Received 2nd April 2001
First published as an Advance Article on the web 12th November 2001

The importance of the investigation of nonlinear dynamical properties (NDPs) of the atmospheric photochemical systems (PCSs) was demonstrated in ref. 1 and 2 (A. M. Feigin and I. B. Konovalov, *J. Geophys. Res.*, 1996, **101** (D20), 26038; 1. B. Konovalov, A. M. Feigin and A. Y. Mukhina, *J. Geophys. Res.*, 1999, **104** (D3), 3669). The only known way to study NDPs of any natural dynamical system (including atmospheric PCSs) is to construct a mathematical model of the system. The key point here is adequacy of the NDPs of the constructed model to the system observed. We propose a new approach to construction of such an adequate model for systems manifesting nonstationary chaotic behaviour and describe an algorithm based exclusively on nonlinear dynamical analysis of the observed time series (TS) without invoking any *a priori* knowledge about the properties of the system observed. Potentialities of the algorithm are demonstrated with the aid of a computer model of the mesospheric PCS. The duration of the "observed" TS is limited so that the system demonstrates only one—chaotic—type of behaviour, without any bifurcations throughout the observed TS. The proposed algorithm enabled us to make a correct prognosis of bifurcation sequences and calculate probabilities to reveal, at the time instant of interest, predicted regimes of the system's behaviour for times much greater than the length of the initial TS.

1. Introduction

1.1.

Atmospheric photochemical systems (PCSs) are ensembles of interrelated chemical processes, including photolysis processes, that occur in the Earth's atmosphere and affect dynamics of minor gaseous constituents of the atmosphere (*i.e.*, all chemical compounds present in the atmosphere, excluding molecular nitrogen and oxygen). The processes and their characteristics differ appreciably in different regions of the atmosphere. The following PCSs are typically distinguished: PCS of the boundary layer, of the free troposphere, of the polar lower stratosphere, of the mesosphere, and others. Photochemical processes are among the principal elements in the chain of global atmospheric processes defining the thermal structure of the Earth's atmosphere, its radiation balance and global circulation. Analysis of PCS evolution is of key importance for investigation of changes in the state of the ozone layer, climatic consequences of civilization (in particular, the

greenhouse effect), control of the chemical composition of the air in densely populated regions and in regions of intensive plant cultivation, *etc.*

1.2.

One of the principal goals in investigating the problems mentioned above and many others is prognosis of the expected changes in the characteristics of the processes and phenomena observed in the atmosphere today. Nonlinearity is the inherent property of atmospheric photochemistry. Therefore, knowledge of NDPs of atmospheric PCSs, namely, types of possible regimes of behaviour for different combinations of parameter values, is of principal importance for construction of an adequate prognosis of phenomena in which photochemistry plays a significant role. Firstly, it allows for prognosis of possible (due to parameter trends) switchings of the system between regimes of behaviour co-existing in its phase space under current parameter values. Secondly, knowledge of NDPs enables one to foresee bifurcations (disappearance of the existing regimes and birth of the new ones) and evaluate their consequences.

A general approach to the study of NDPs is well known and consists in investigation of the structure of the phase space of the system and analysis of changes occurring in this structure when the values of control parameters vary, in other words investigation of the structure of the space of the parameters of the system. Apparently, this approach implies that there is a definite mathematical model of the system under consideration.

A traditional method of modelling—construction of a model on the basis of "first principles"—demands general understanding of the origin of the processes playing the main role in the studied phenomenon, as well as specific knowledge about the composition of the "ensemble" of processes of "required" origin. The generally adopted method of verification of the "first principles" models is comparison of results of modelling with the observed ones (and earlier observed results) by *quantitative* characteristics of the phenomenon under consideration. Clearly, in terms of *prognosis* of the evolution of a *nonlinear* dynamic system (DS), such verification is sound only under the condition of revealing the bifurcations that occurred in the course of observations and were reproduced by the model. However, for "natural" DSs another situation is typical, when, in spite of the "intrinsic" nonlinearity of such systems and *nonstationarity* of the processes running in them, no bifurcations occur during the observation time. In this case, the traditional method of verification can only testify to adequate reproduction by the model of the current type of behaviour of the system, giving no guarantees as regards prognosis of possible future bifurcations. Indeed, satisfactory quantitative adequacy of the model of the observed evolution can be attained by either taking into account or neglecting processes that introduce into the model *qualitatively different* NDPs. A "qualitative" error in creating the "first principles" model of such complex and insufficiently studied DSs as various natural systems is highly probable.

1.3.

The above is absolutely true for atmospheric PCSs. A classical mathematical model of an atmospheric PCS is a set of equations of chemical kinetics, complicated to a greater or lesser extent by contributions from processes of a non-chemical nature. In the simplest case, such a model is a box in which "correctly" selected chemical reactions proceed. This model can be written in the form of a system of first-order ordinary differential equations for concentrations of minor gaseous constituents of the atmosphere:

$$\frac{\mathrm{d}X_i}{\mathrm{d}t} = f_i(\vec{X}, \vec{A}),\ \vec{X} = \{X_i\}_{i=1}^{N},\ \vec{A} = \{A_j\}_{j=1}^{M}. \tag{1}$$

Here, X_i is the concentration of the chemical constituents which are part of the PCS, A_j are the parameters determining the character of the evolution of the system, and t stands for time. The functions $f_i(\vec{X}, \vec{A})$ on the right-hand side of eqn. (1) describe the sources and sinks of the corresponding chemical components; and f_i are the nonlinear functions of the arguments $\vec{X}$. The local character of the function $f_i(\vec{X})$ means that model (1) includes only chemical (and photochemical) reactions proceeding in the atmosphere. Such box models are usually part of complex models describing more or less adequately the interrelated atmospheric processes (chemical processes,

heat and mass transfer, radiation transfer) characterised by definite temporal and spatial scales as a whole.

One of the main features of atmospheric PCSs is their nonstationarity. Conditions, that are external relative to photochemical processes, vary in the course of time for different reasons, both of natural and anthropogenic nature. Correspondingly, mathematical models of atmospheric PCSs of the form (1) are nonautonomous; the control parameters entering these models are functions of time.

1.4.

The essential influence exerted by processes of a non-chemical nature upon variations of concentrations of chemical components significantly impedes clarification of the role of NDPs of "chemical" origin in the observed phenomena. Nevertheless, today we are in a position to speak about possible manifestations of a multistable box model of a *boundary layer* PCS and multistability induced bifurcations of the birth/disappearance of a pair of "additional" equilibrium states in the change of the so-called regimes with high and low concentration of NO_x (a family of odd nitrogen) in the boundary layer of the troposphere.[3,4]† Another phenomenon that may be caused by NDSs of a *mesospheric* PCS is multiple amplification of the so-called quasi-2-day oscillations of different characteristics (zonal and meridional wind amplitudes, temperature, *etc.*) that occur in the upper mesosphere and thermosphere in the summer season.‡ The corresponding bifurcation of period doubling of a limit cycle, that corresponds to "conventional" oscillations of concentrations of chemical components with a period of one day, occurs with variation of control parameters, such as water vapour concentration, coefficient of vertical eddy diffusion and temperature.[6–9]

Of special interest is manifestation of NDPs of a *polar lower stratospheric* PCS in formation of an Antarctic ozone hole. This phenomenon first revealed in 1985[10] could not be explained within the scope of the known models and, consequently, had not been predicted by them (*cf. e.g.*, ref. 11). It did not take much time to understand that the cause of the error was neglect of heterogeneous chemical reactions with participation of particles of polar stratospheric clouds.[12,13] One of the properties of these reactions, that is most important in terms of construction of an adequate prognosis, is a special type of nonlinearity which they introduce into equations of chemical kinetics. It was shown recently[1,2] that the influence of heterogeneous reactions on the phase space structure of a polar lower stratospheric PCS increased as one of the control parameters (concentration of inorganic chlorine) increased and resulted in a sequence of unpredicted bifurcations in the behaviour of Antarctic PCS in the 1980s. Note that, in the course of formation of an ozone hole, the evolution of a given PCS depends weakly on processes of non-chemical origin, so that the box model of the form (1) reproduces the key quantitative characteristics of the phenomenon to a satisfactory accuracy. Therefore, we have strong arguments to believe that NDSs of the polar lower stratospheric PCS played a decisive role in the appearance of the Antarctic ozone hole and can cardinally affect its future evolution.

1.5.

The above allows us, firstly, to speak about the need to investigate NDPs of atmospheric PCSs in constructing a prognosis of evolution of different atmospheric phenomena. Secondly, the use for this purpose of "first principle" models is fraught with prognostic error that is possible even in modelling future behaviour of "long-lived" systems in nature that demonstrate stable evolution.

We propose a basically new method of constructing mathematical models of different systems existing in nature, intended for investigation of their NDPs and long-range prognosis of their

† The rate of emission into the atmosphere of free radicals is the control parameter whose seasonal variations may lead to these bifurcations. Study of this phenomenon is of practical importance: the two mentioned regimes correspond to essentially different (by two orders of magnitude and more) boundary ozone concentrations, increased values of which are the cause of exacerbation of many diseases in humans, lead to decreased productivity of crop and forest reproductivity, and so on.

‡ A fairly detailed analysis of experimental data was given in ref. 5 for more than 20 years of observations.

qualitative behaviour. The method is based on analysis of the observed time series and is most effective for systems demonstrating nonstationary chaotic dynamics. This behaviour is typical, in particular, for various systems determining the occurrence of paramount processes in the Earth's atmosphere and hydrosphere (evolution of the ozone layer,[14] behaviour of the concentrations of chemical components within the boundary layer,[15] large-scale variations of surface temperature of the tropical Pacific Ocean (the El Niño phenomenon)[16,17]). Note that even today the scope of real systems demonstrating chaotic dynamics ranges from the above enumerated atmospheric and atmospheric–oceanic processes to diverse systems in living organisms[18,19] and tectonic activity[20] and has a tendency to expand as modern methods of nonlinear dynamical analysis are applied to new data bases of different nature.

We will address the case when a chaotic time series (TS) *only* is available, and there is no additional information about the dynamic system that generated it. As was said above, our goal is to construct a model that would be adequate in its NDPs to the observed system. In other words, it must not only reproduce the observed evolution of the system but also allow us to predict qualitative changes in the system's behaviour (bifurcations). We will refer to such models as *prognostic* ones. We will also suppose that no bifurcations occur in the course of the observed time series and the system demonstrates only one—chaotic—type of behaviour.

Because the change in the type of behaviour of the system is a consequence of the variation of control parameters, the time series generated by such a system is nonstationary. Obviously, nonstationarity of the observed TS can be revealed only if the corresponding process is characterised by at least two, strongly differing timescales.§ This lays the basis for two hypotheses that are natural in terms of physics.

Hypothesis 1. The observed nonstationary time series is generated by a *weakly nonautonomous* "*fast*" dynamical subsystem, the parameters of which vary slowly on characteristic timescales of the evolution of its dynamical variables.

Hypothesis 2. Evolution of a "slow" subsystem, interaction with which is the cause of nonautonomy of the "fast" subsystem, remains unchanged in the not too remote future of the "slow" subsystem. By the "not too remote future" of the slow subsystem we mean a time interval of the order of several lengths of the observed TS during which changes of the parameters of the fast subsystem are relatively small.

Interpretation of nonstationarity of TS as nonautonomy of the observed DS (hypothesis 1) is meaningful when the time dependence of parameters of the system is known. The second hypothesis allows one to reconstruct the trends of parameters of a fast subsystem over a sufficiently extended time interval.

Productivity of this approach was first demonstrated in ref. 24 and 25, where an algorithm based on the hypotheses formulated above was proposed for construction of prognostic models of systems demonstrating low-dimensional chaotic dynamics. The potential of this algorithm was illustrated by means of computer models. A computer modelled nonstationary chaotic series was used to construct a prognostic model that was employed for constructing prognosis of bifurcations of the "observed" system. The algorithm allowed us to predict correctly a sequence of bifurcations and determine other characteristics of prognosis for times much greater than the length of the initial series.

In Section 2 of this paper we propose a much more universal algorithm that enables one to create prognostic models for both low- and high-dimensional dynamical systems. In Section 3 the new algorithm is used for construction of the prognostic model of a mesospheric PCS employing a nonstationary chaotic time series generated by a computer model of the system. We also consider criteria for choosing technical parameters of a prognostic model. In the concluding section, results of the present research are formulated and possible further development of the proposed approach and its application to analysis of real time series is discussed.

§ Several methods for revealing nonstationarity of TS were proposed (see, *e.g.*, ref. 21–23). Still another is part of the algorithm that will be described in this paper.

2. Algorithm of constructing a prognostic model by observed time series

2.1.

The proposed algorithm can be represented as the following step-by-step procedure:

(1) The phase space of the observed system is reconstructed.

(2) A prognostic model is elaborated in the form of a discrete time map written in an analytic form.

(3) A covariance matrix of parameters of the prognostic model is found, and parameter trends and their covariance matrix are extrapolated to the "future" (outside the scope of the initial TS).

(4) A bifurcation prognosis is constructed: a bifurcation sequence is predicted and the time dependence of the probability to reveal the predicted regimes of the system's behaviour is determined.

Methods of phase space reconstruction have been discussed in many papers (see, for instance, ref. 26 and the literature cited therein). Therefore, in Section 2.2 we will restrict ourselves to a brief consideration of the first step of the procedure and to some comments on its features within the framework of the proposed algorithm. The next step will be quite novel, which distinguishes the proposed algorithm from that proposed earlier[24,25] for elaboration of prognostic models of low-dimensional DSs. This step will be addressed in more detail in Section 2.3. Steps 3 and 4 do not differ "ideologically" from the corresponding steps of the "low-dimensional" algorithm. Nevertheless, bearing in mind the key importance of these steps in construction of bifurcation prognosis and aiming at giving the reader a complete picture of the proposed approach we will address in more detail the most significant aspects of the corresponding operations in Sections 2.4 and 2.5.

2.2.

In this work, as in ref. 24 and 25, the model of the observed DS is constructed in the form of a discrete time map. In conformity with the choice of a discrete model, the vector of state in the reconstructed phase space at the time instant t_k is specified by co-ordinates with delays:[27]

$$\vec{Y}(t_k) = \{y(t_k), y(t_k + \Delta t), \ldots, y(t_k + (d_E - 1)\Delta t)\}, \quad (2)$$

where $y(t)$ is the initial time series, d_E is the dimension of phase space (minimal embedding dimension), and Δt is the delay time determined, for example, from the condition of the first minimum of the mutual information function.[28] The value of d_E was calculated by the "false neighbours" method.[26,29]

Further, in the reconstructed phase space we chose the Poincare section for which we used the zero of the second co-ordinate $y_k^{(2)} = y(t_k + \Delta t) = 0$. As a result, a new data series $\{\vec{X}_j = \vec{Y}(t_j)\}_{j=1}^{J}$ (where t_j are the instants at which the reconstructed phase trajectory intersects the Poincare section in a definite direction) was obtained from the initial TS. It is worthy of note that $\{\vec{X}_j\}$ can be determined to a finite accuracy that depends on the discretization scale of the initial TS.

2.3.

The model was constructed in the form of a certain function $f(.)$ approximating the discrete time map:

$$x_j = f(x_{j-1}, \ldots, x_{j-N}; t_{j-1}; \vec{\mu}) + \xi_j, \quad (3)$$

$$f(x_{j-1}, \ldots, x_{j-N}; t_{j-1}; \vec{\mu}) = f_0(x_{j-1}, \ldots, x_{j-N}; \vec{\mu}_0) + \vec{\beta} \cdot t_{j-1} \cdot \vec{f}_1(x_{j-1}, \ldots, x_{j-N}; \vec{\mu}). \quad (4)$$

Here, N is the order of mapping, ξ_j is the error of approximation, and $\vec{\mu} = \{\vec{\mu}_0, \vec{\mu}_1, \vec{\beta}\} \in \mathscr{R}^{\{M_0 + M_1 + B\}}$ is a set of parameters of the model. The evolution operator was written in the form (4) employing the hypotheses 1 and 2 formulated in Section 1.5. Namely, the slow dependence on time t of parameters of the observed DS and small relative variation of their values over the time interval of about several lengths of the initial TS allowed us to describe nonautonomy as a time-dependent correction $[\vec{\beta} \cdot t \cdot \vec{f}_1(.)]$ to the autonomous part of the model $f_0(.)$. In other words, slowness of the dependence of evolution operator on time means the possibility of its Taylor series expansion in time with a restricted number of terms. In this work we took into account only the linear terms of the expansion. Apparently, this approximation is equivalent to reconstruction of

nonautonomy of the observed DS in the form of a linear time dependence only of those parameters that enter the model linearly, which is clearly seen in eqn. (4).¶

A nontrivial issue is a choice of the form of functions $f_0(.)$ and $\vec{f}_1(.)$. For the algorithm to allow for construction of prognostic models of various *high-dimensional* DSs, these functions must enable one to approximate nearly any single-valued function of an arbitrary number of variables with an arbitrary preset accuracy. Such universality is inherent in artificial neural networks[30] that allow one to increase approximation accuracy by a simple increase in the number of neurons, while the form of the function remains unchanged. Still another property of a neural network (NN) is its dissipativity outside the "learning region" (the region of variation of the arguments of the function within the scope of the initial TS), thus providing global stability of the obtained models.‖

In this research we chose as $f_0(.)$ and $\vec{f}_1(.)$ functions a perceptron, *i.e.*, the simplest three-layer NN,[30] in which the linearly entering parameters were sought in the form of linear functions of time:

$$f(x_{j-1}, \ldots, x_{j-N}; t_{j-1}; \vec{\mu}) = \sum_{i=1}^{m} (\alpha_i + t_{j-1}\beta_i)\tanh\left(\sum_{k=1}^{N} w_{ki}\, x_{j-k} + \gamma_i\right). \tag{5}$$

Here, m is the number of neurons in the hidden layer of the network and $\mu = \{\alpha, \beta, w, \gamma) \in \mathscr{R}^{(N+3)m}$ is the complete set of model parameters. In eqn. (5) the number of NN inputs is chosen to be equal to the order of the mapping.

As soon as the specific form of the discrete time map has been chosen, construction of a model reduces to finding optimal values of its parameters. The slowness of the time dependence of the evolution operator, that was used in writing a prognostic model in the forms (3) and (4), enables us to employ the corresponding perturbation theory and optimise parameter values in two stages. At the first stage, we seek the values of the parameters $\tilde{v},\tilde{w},\tilde{\gamma}$ that would provide the minimum of "autonomous" r.m.s error.**

$$\chi_a^2 = \left\langle \left[x_j - \sum_{i=1}^{m} v_i \tanh\left(\sum_{k=1}^{N} w_{ki}\, x_{j-k} + \gamma_i\right)\right]^2 \right\rangle_j, \tag{6}$$

where $\langle . \rangle_j$ has the meaning of an average for the corresponding subscript. At the second stage, the values of parameters $w = \tilde{w},\gamma = \tilde{\gamma}$ are fixed and the values of parameters $\bar{\alpha},\bar{\beta}$ corresponding to the minimum of "nonautonomous" r.m.s. error are found:

$$\chi_n^2 = \left\langle \left[x_j - \sum_{i=1}^{m} (\alpha_i + t_j \beta_i)\tanh\left(\sum_{k=1}^{N} \tilde{w}_{ki}\, x_{j-k} + \tilde{\gamma}_i\right)\right]^2 \right\rangle_j. \tag{7}$$

The resulting model may be interpreted as an autonomous DS

$$x_j = \sum_{i=1}^{m} \bar{v}_i(t)\tanh\left(\sum_{k=1}^{N} \tilde{w}_{ki}\, x_{j-k} + \tilde{\gamma}_i\right) + \xi_j, \quad \bar{v}_i(t) = \bar{\alpha}_i + \bar{\beta}_i t, \tag{8}$$

the qualitative behaviour of which is determined by a *single* control parameter, namely, time t.

2.4.

The model constructed in Section 2.3 reproduces not only the topological structure of the observed attractor, but slow variations of this structure also. This makes it possible to investigate *future* NDSs of the observed system by constructing bifurcation prognosis, *i.e.* analyse the depen-

¶ Linear approximation is insufficient when quantitative characteristics of the observed attractor, that vary due to the system's nonautonomy, reach their extreme values *within* the initial TS. Such a situation occurs, for example, in construction of a prognostic model of a mesospheric PCS by a TS corresponding to the so-called "external" chaotic attractor of the given system (see ref. 24 and 25, as well as Section 3.1).

‖ Problems encountered when using NNs will be considered in Sections 3.1 and 3.4.

** Note that the search of the "best" approximation of the data series $\{x_j = y(t_j)\}_{j=1}^{J}$ by minimising the errors (6) and (7) corresponds to the use of the method of least squares, which imposes restrictions on the application of the algorithm to analysis of noisy TS. This issue will be addressed in Section 4.3.

dence of qualitative behaviour of model (8) with time. It is quite obvious that results of such analysis depend significantly on errors inevitable in constructing a prognostic model that are characterised by a random quantity ξ_j entering into eqn. (8). The cause of such errors is, firstly, non-zero accuracy of reconstruction of the phase trajectory and the corresponding point map with respect to *finite* and *discrete* TS. Secondly, error may be due to incomplete correspondence of the operator, describing evolution of the prognostic model, to the analogous operator of the DS that generated the initial TS. The most dangerous consequence of the above-mentioned errors in constructing the prognosis of qualitative behaviour of the DS by the prognostic model (8) is the error in seeking values of the parameters α and β controlling changes in the behaviour of the model in the course of time. Available information about the observed DS (*i.e.*, the initial time series) does not allow one to determine the magnitude of this error accurately. Nevertheless, reasonable physical assumptions can give an upper estimate of this error.

Assume that there exists a set of parameters $\{\alpha^*, \beta^*\}$ for which a prognostic model describes the observed DS *exactly*, and the differences between the model and the modelled system, characterised in eqn. (8) by a random quantity ξ_j, are generated exclusively by error in determining these parameters. Assume also that ξ_j is normally distributed white noise with zero mean. Then, parameters $\{\alpha, \beta\}$ are normally distributed random quantities with average values $(\bar{\alpha}, \bar{\beta})$ minimising the "nonautonomous" error (7), with $\{\bar{\alpha}, \bar{\beta}\} = \{\alpha^*, \beta^*\}$, and with the covariance matrices $C_{\alpha\alpha}$, $C_{\alpha\beta}$, $C_{\beta\alpha}$, $C_{\beta\beta}$ determined from expansion of this error near the minimum:

$$\chi_n^2(\alpha, \beta) \approx \chi_n^2(\bar{\alpha}, \bar{\beta})(1 + J^{-1}((\alpha - \bar{\alpha})^{\mathrm{T}}(C_{\alpha\alpha}^{-1})(\alpha - \bar{\alpha}) + (\alpha - \bar{\alpha})^{\mathrm{T}}(C_{\alpha\beta}^{-1})(\beta - \bar{\beta}) + (\beta - \bar{\beta})^{\mathrm{T}}(C_{\beta\alpha}^{-1})(\alpha - \bar{\alpha}) + (\beta - \bar{\beta})^{\mathrm{T}}(C_{\beta\beta}^{-1})(\beta - \bar{\beta}))). \quad (9)$$

2.5.

The last step is investigation of future NDPs of the observed DS, *i.e.*, construction of the prognosis of bifurcations of its qualitative behaviour. Within the framework of the proposed algorithm it is sufficient to study the dependence of qualitative behaviour of the prognostic model (8) on the single control parameter t. This dependence is specified by a random, normally distributed set of parameters $v(t)$ with an average

$$\bar{v}(t) = \bar{\alpha} + \bar{\beta}t, \quad (10)$$

and a covariance matrix

$$C_{vv}(t) = C_{\alpha\alpha} + t(C_{\alpha\beta} + C_{\beta\alpha}) + t^2 C_{\beta\beta}. \quad (11)$$

The random spread of parameter trend $v(t)$ means that the predicted bifurcations must be considered as random events, and the instants of the bifurcation transitions as random values. Consequently, prognosis of bifurcations is expected to give answers to the following questions: What is the probability with which the predicted bifurcations will occur up to a definite instant of time? What is the mathematical expectation of the instant of a specific bifurcation transition? What is the accuracy of prediction of an average instant of a specific bifurcation? What is the probability to reveal the type of the system's behaviour of interest to us at a given instant of time?

We use the Monte Carlo method to find answers to the formulated questions. Consider a set of "II" supplementary to the $\bar{v}(t)$ trends constructed in the parameter space of the model so that the sets of parameters specified by them at an arbitrary time instant t should be described by a normal probability distribution characterised by the found dependences $\bar{v}(t)$ and $C_{vv}(t)$. On having constructed a bifurcation diagram (BD) corresponding to each supplementary trend we obtain an ensemble of bifurcation instants for each predicted bifurcation transition. To answer the questions posed above, it is sufficient to find the time dependence of the probability density of the instants of all the predicted bifurcations. For this we divide the entire timescale into sufficiently small intervals δt_i and record how often elements of each of the obtained ensembles fall within these intervals; this quantity is denoted by v_b^i. The time dependence of the probability density of the b-bifurcation, $\varphi_b(t)$, is defined as

$$\varphi_b = \frac{v_b^i}{\delta t_i \Pi}, \qquad b = 1, \ldots, B. \quad (12)$$

Here, B is the total number of predicted bifurcations.

Knowledge of $\varphi_b(t)$ gives answers to the first three of the four questions formulated above if we determine in a standard manner the dependence on slow time of the integral probability Φ_b of the corresponding bifurcation:

$$\Phi_b(t^*) = \int_T^{t^*} \varphi_b(t)\mathrm{d}t, \qquad t^* > T \tag{13}$$

and calculate the mathematical expectation of the bifurcation instant and the corresponding dispersion.

In addition, analysis of the whole set of functions $\varphi_b(t_s)$ allows us to determine the probability P_k with which the "k"-th type of behaviour of the system can be revealed at a given instant of time t^*:

$$P_k(t^*) = P_k^+(t^*)(1 - P_k^-(t^*)). \tag{14}$$

Here,

$$P_k^{+,-}(t^*) = \int_T^{t^*} \varphi_k^{+,-}(t)\mathrm{d}t, \qquad t^* > T \tag{15}$$

and the functions $\varphi_k^+(t)$ and φ_k^- are the sums of probability densities of all possible bifurcations of the transition to and from the regime (type of behaviour), respectively. In eqn. (13) and (15) T denotes the boundary of the observed TS.

3. Construction of prognostic model of a mesospheric PCS

3.1.

In this section we demonstrate the proposed algorithm taking as a data source a system describing the behaviour of minor chemical constituents of the Earth's atmosphere in the mesopause region (heights of 70 to 90 km).[6,7] For the convenience of the reader, we present below a brief description of this system and its NDPs described earlier in ref. 7 and 31.

The system includes five first-order nonlinear differential equations under periodic external forcing:

$$\begin{aligned}
\frac{\mathrm{d}x_1}{\mathrm{d}t} &= -(a_9 + 2a_{11}x_1 + a_{10}x_3 + a_4x_4 + a_5x_5)x_1 + a_1x_2x_5 + a_{15}x_4^2 + a_{16}s(t)x_3 + 2a_8s(t)\\
\frac{\mathrm{d}x_2}{\mathrm{d}t} &= -(a_6 + a_{12}x_3 + (a_1 + a_2 + a_{14})x_5)x_2 + a_4x_1x_4 + a_7s(t)r\\
\frac{\mathrm{d}x_3}{\mathrm{d}t} &= -(a_{10}x_1 + a_{12}x_2 + a_{13}x_4 + a_{16}s(t))x_3 + a_9x_1\\
\frac{\mathrm{d}x_4}{\mathrm{d}t} &= -(a_4x_1 + 2a_{15}x_4 + a_3x_5 + a_{13}x_3)x_4 + a_5x_1x_5 + a_{12}x_2x_3 + 2a_{14}x_2x_5 + a_7s(t)r\\
\frac{\mathrm{d}x_5}{\mathrm{d}t} &= -(a_5x_1 + a_3x_4 + (a_1 + a_2 + a_{14})x_2)x_5 + a_6x_2 + a_{13}x_3x_4.
\end{aligned} \tag{16}$$

These are equations of chemical kinetics for 16 chemical reactions (including photolysis reactions) running in the mesosphere. The system contains five chemical species (O, H, O_3, HO, HO_2) whose concentrations are dynamical variables denoted, respectively, by $x_1, \ldots, x_5$. The dynamics of these species is determined by the magnitudes of the coefficients $a_1 \cdots a_{16}$ (constants of the reactions) and has a characteristic timescale of one day or less under mesospheric conditions. The concentrations of the other reagents participating in the reaction are much higher than those of the above five species and are supposed to be constant. Periodic external forcing is due to daily variations of exposure to light as a result of sunrise and sunset and is manifested by periodic modulation of photodissociation rates of the molecules of ozone, one of the dynamical variables of system (16),

oxygen, the concentration of which is assumed to be constant, and water vapour, whose relative concentration "r"†† is one of the control parameters of the system. This modulation enters into system (16) in the form of the periodic function $s(t)$ that reaches its maximum $s_{max} = 1$ at midday and minimum $s_{min} = 0$ at midnight.‡‡ By virtue of such nonautonomy, the phase space of system (16) has dimension six.

The variable x_1 (the concentration of atomic oxygen [O]) is the dynamical variable whose time series "was observed", although this choice is not of fundamental importance. Fig. 1(a) displays a BD where the concentration of atomic oxygen at the instant of sunrise is on the vertical axis, and the magnitude of relative concentration of water vapour "r", that is the control parameter of the system, is on the horizontal axis. Clearly, the system possesses a wide set of dynamic regimes that are realised depending on the value of the control parameter. If several values of [O] correspond to some value of r, then a regime with a period of the same number of days is realised. The "dark" regions in the BD are for those intervals of parameter values in which the system behaves chaotically.

One can see that the system has three regions of chaotic behaviour in the considered range of variation of the control parameter. Of particular interest are two of them that are realised at relatively small values of $r \in [1.5; 2.1]$. The corresponding fragment is magnified to scale on the abscissa in Fig. 1(b). It is clearly seen that the two regions of chaotic behaviour partially overlap. This feature is a consequence of the bistable behaviour of the system accompanied by hysteresis with the variation of the control parameter. As the control parameter changes from the left to the right within the limits of Fig. 1(b), a sequence of bifurcations takes place. First, the motion with a

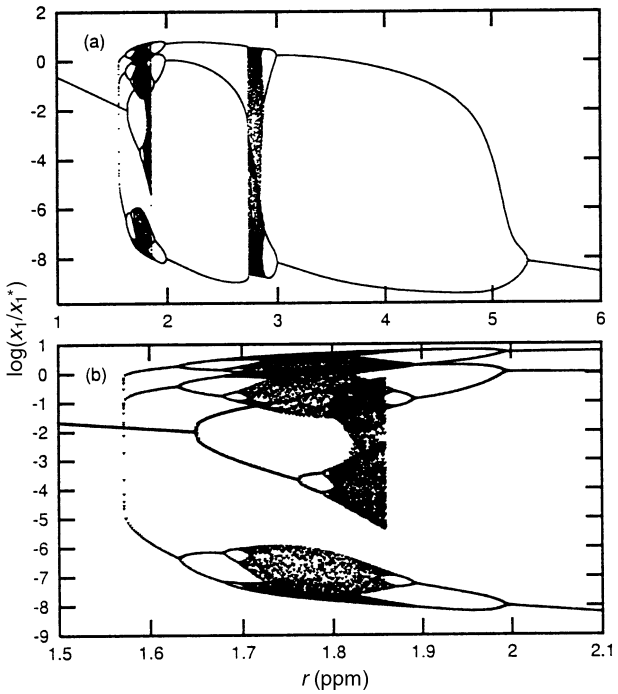

Fig. 1 (a) Bifurcation diagram of system (16); (b) fragment of bifurcation diagram with the scale extended along the abscissa axis. Logarithm of atomic oxygen concentration at sunrise, normalised to $x_1^* = 1.13 \times 10^9$ cm^{-3} along the vertical axis; value of relative concentration of water vapour r along the horizontal axis.

†† Given below in ppm units (particles per million) defined as the number of molecules of water vapour per million molecules of air.

‡‡ Detailed consideration of system (16) (values of coefficients a_1–a_{16}, ranges of variation of control parameter "r", form of function $s(t)$), and its nonlinear-dynamical properties can be found in ref. 31 and 32.

period of one day loses stability (at $r \approx 1.65$) and period doubling occurs (a stable regime with a period of two days is born). Then follows a cascade of such doublings, and the dynamics becomes chaotic at $r \approx 1.8$. We will call the resulting chaotic set an "internal attractor". Finally, for $r \approx 1.87$, this motion disappears and the system jumps into an absolutely different regime of behaviour.

With a reverse change of parameter, we start at $r = 2.1$ from stable motion with a period of three days which doubles at $r \approx 2$, quadruples at $r \approx 1.9$, and then a transition to a chaotic regime through a cascade of doublings occurs. The obtained chaotic set will be referred to as an "external attractor". As is clear from Fig. 6(b), this attractor consists of three regions and, with a period of external forcing of one day, the map jumps successively from one region into another. With a further decrease of the control parameter, an inverse cascade of doublings is initiated at $r \approx 1.7$, a regime with a three-day period is, again, realised at $r \approx 1.63$ and vanishes at $r \approx 1.58$, and the system passes to a stable one-day regime. Thus, catastrophic bifurcations occur in the system both with an increase and a decrease of parameter r.

3.2.

In this paper we use chaotic evolution of a mesospheric photochemical system (MPCS) "observed" within the basin of internal attractor for construction of prognostic models for the given dynamical system.§§

So, we generate a TS of variable x_1 having duration $T = 1500$ days within the limits of which parameter r decreases (linearly in time) from 1.855 to 1.82 (Fig. 2(a)), and make use of the algorithm described in Section 2.

First, we reconstruct the attractor in phase space and establish that (i) the minimal embedding dimension of system (16) is equal to 3; and (ii) the correlation dimension of the attractor is 1.9.¶¶

We take as the Poincare section the surface $\dot{x}_1 = 0$ and record the intersections of this section by the phase trajectory from the side of $\dot{x}_1 < 0$ (local minima of variable x_1). Such a section in the expanded phase space corresponds to the instant of sunrise. A first-order discrete time map corresponding to the chosen Poincare section is given in Fig. 2(b). This discrete time map is multivalued (Fig. 2(b)) due to the presence of an "additional" branch in the left-hand side of the map. Since in ref. 24 and 25 we used the low-dimensional algorithm, the constructed prognostic model neglected the multivalued nature of the map. The high-dimensional algorithm described in Section 2 permits one to construct a model in the form of a higher-order discrete time map, thus avoiding rough approximation of the observed data.

The prognostic model was constructed in the form of the NN (8) (number of inputs being $N = 2$) approximating the second-order discrete time map extracted from the initial TS. The total number of model parameters was $\mu = \{\alpha, \beta, w, \gamma\} = (N + 3)\ m = 5m$, of which $2m$ parameters $\{\alpha_i, \beta_i\}_{i=1}^{m}$ determine the behaviour of the model outside the scope of the initial TS. The number of neurons m is a technical parameter of the model; its influence on the characteristics of prognosis of qualitative behaviour of the system will be discussed in Section 3.3.

In line with the general algorithm, the NN was learnt in two stages. At the first stage, the values of the parameters $\{\tilde{v},\tilde{w},\tilde{\gamma}\}$ minimising the autonomous error (6) were sought; at the second stage $\{\tilde{w},\tilde{\gamma}\}$ were fixed, and the values of the parameters $\{\tilde{\alpha},\tilde{\beta}\}$ minimising the nonautonomous error (7) were found. The minimum of the first error was sought by *Variable Metric Methods in Multidimensions* (also called *quasi-Newton methods*),[33] and the minimum of the second one by the *Singular Value Decomposition* (*SVD*) *Method*.[33] At the first stage we had to take into account that a complicated nonlinear dependence of the NN (8) on parameters $\{w, \gamma\}$ may result in the existence of many local minima of the error (6). For construction of a model that would be maximally sensitive to a change of dynamical variables within the range of values corresponding to the initial TS, the "observed" series $\{x_j\}$ was normalised to provide $\langle x_j \rangle_j = 0$, $\langle x_j^2 \rangle_j = 1$, after which the right-hand side of (6) was supplemented by the factor $(1 + \lambda(4m)^{-1} \sum_{i=1}^{m} (v_i^2 + w_{1i}^2 + w_{2i}^2 + \gamma_i^2))$,

§§ No specific problems arise when a prognostic model is constructed by the time series generated by two other chaotic attractors given in Fig. 1(a) and (b).

¶¶ The cause of such low values of the dimensions of system (16) was discussed in detail in ref. 31 and 32.

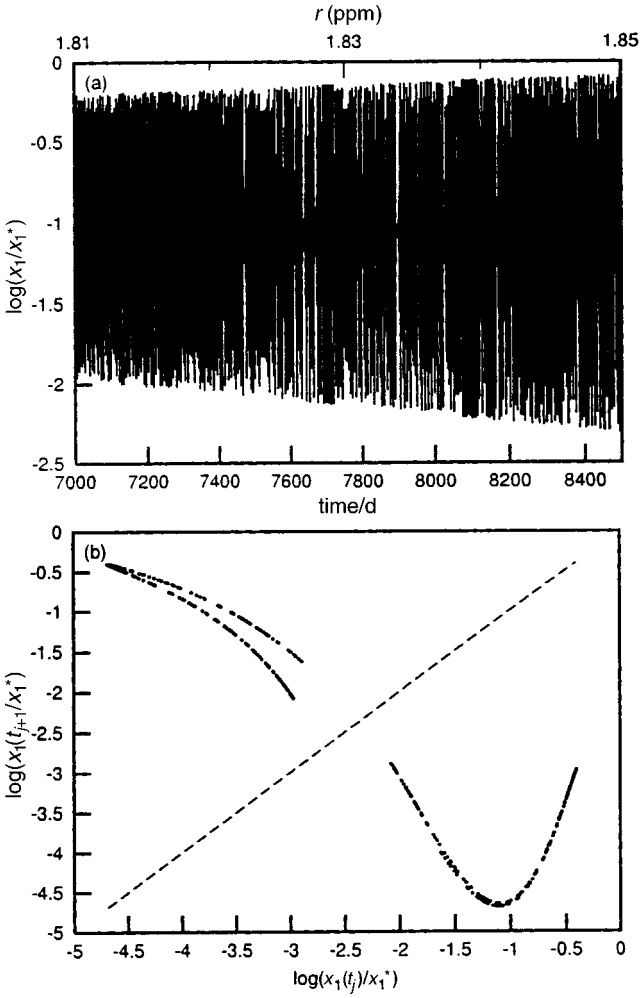

Fig. 2 (a) "Observed" TS employed for construction of prognostic model. Logarithm of atomic oxygen concentration, normalised to $x_1^* = 1.13 \times 10^9$ cm^{-3} along the vertical axis; time along the lower horizontal axis and current value of r along the upper horizontal axis; (b) first-order discrete time map reconstructed by the given TS.

where λ is the technical parameter of order unity, and the minimum of the autonomous error corrected in this manner was sought.‖‖

Further, steps 3 and 4 of the general algorithm were accomplished. Namely, the error (7) was expanded into series (9) and the covariance matrix $\begin{pmatrix} C_{\alpha\alpha} & C_{\alpha\beta} \\ C_{\beta\alpha} & C_{\beta\beta} \end{pmatrix}$ of parameters $\{\alpha, \beta\}$ characterising nonautonomy of the prognostic model was calculated.

Still further, the time dependence of qualitative behaviour of the prognostic model was investigated. For this, 1000 trends of parameters $v(t) = \alpha + \beta\ t$ were specified so that, at each time instant, distribution of these parameters should be normal, with the average (10) and the covariance matrix (11). Analysis of changes in the behaviour of the model in the "future"*** determined by each trend, allows one to set up a statistical ensemble of bifurcation instants for each of the

‖‖ Note that for $\lambda \ll 1$ this procedure means minimisation of (6) with minimal norm of the values of parameters $\{v_i, w_{1i}, w_{2i}, \gamma_i\}_{i=1}^m$.

*** Apparently, the "future" is conventional here because the proposed alogirithm allows for analysis of the changes in the model's behaviour in both directions of the time axis.

bifurcation transitions found and calculate the probability characteristics (12)–(14) of the predicted bifurcations and regimes of behaviour.

3.3.

Before we pass to discussion of the results of the considered research, consider an important issue of choosing a technical parameter of model (8), namely, the number of neurons m. Since the order of the discrete time map N (the number of inputs of the NN) is defined by the dimension of the reconstructed phase space of the observed system (the minimal embedding dimension), m determines completely the total number of prognostic model parameters $\mu = \{\alpha, \beta, w, \gamma\} = (N + 3)\, m$. Therefore, we will actually speak about the optimal number of parameters of the model.

On the one hand, for the model to guarantee sufficiently accurate reproduction of the observed evolution of the system, the number of parameters must not be too small: the reproduction error is obviously a monotonically decreasing function of the number of parameters. This statement is illustrated in Fig. 3(a) and (b), where the monotonically decreasing autonomous (6) and nonautonomous (7) errors, normalised to dispersion of the observed signal, are plotted *vs.* the number of neurons m.

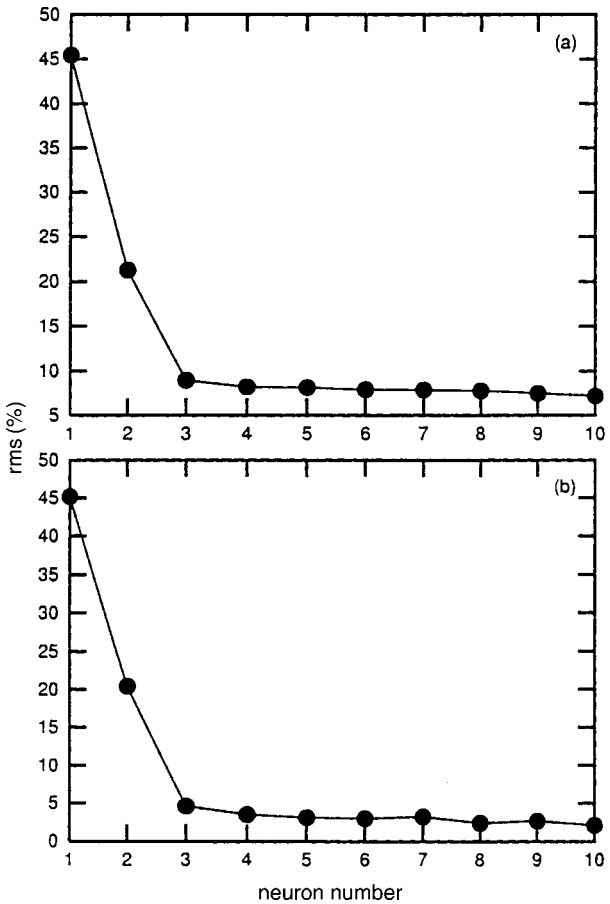

Fig. 3 Least r.m.s. error plotted *vs.* the number of neurons in the hidden layer of NN (8): (a) for autonomous error (6); (b) for nonautonomous error (7).

Our task, however, is not pinpoint accuracy of reproducing the observed evolution, but *prognosis of changes in the qualitative behaviour* of the observed system. The informativity of such a prognosis within the scope of the algorithm under consideration is determined by the probability characteristics (12)–(14). Clearly, the prognosis is the more informative the more accurately the bifurcation instants are predicted and the greater the probability of revealing the most probable regime of behaviour at the time instant of interest. Both these characteristics depend significantly on "arrangement" of m-dimensional space of nonautonomous parameters of the model $\{v_i\}_{i=1}^m = \{\alpha_i + t\beta_i\}_{i=1}^m$. An increase in m means an increase in the dimension of this space and, generally speaking, the complication of its structure. The resulting number of qualitatively different regimes of behaviour co-existing in time for different trends $v(t)$, forming a statistical ensemble of bifurcation instants, can increase too. Therefore, it should be expected that a too large number of parameters will result in deterioration of the characteristics of prognosis.

So, we can conjecture that there exists an optimal range of the number of model parameters that provides the most informative prognosis of qualitative behaviour of observed DS with the aid

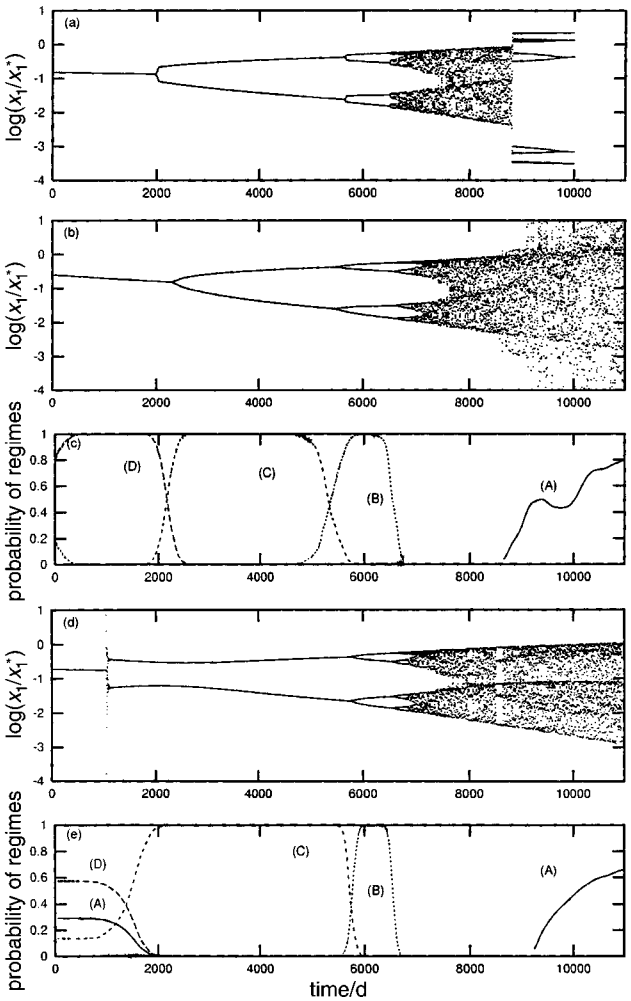

Fig. 4 (a) Fragment of bifurcation diagram of system (16) from Fig. 1. Prognosis of qualitative behaviour of mesospheric PCS constructed using model (8): (b), (d) bifurcation diagrams corresponding to average trend (10) with the number of neurons $m = 3$ and $m = 4$, respectively; (c), (e) time dependence of the probability to reveal different regimes: "regime" of catastrophe (A); oscillatory regimes with a period of four (B), two (C) and one (D) days for $m = 3$ and $m = 4$, respectively.

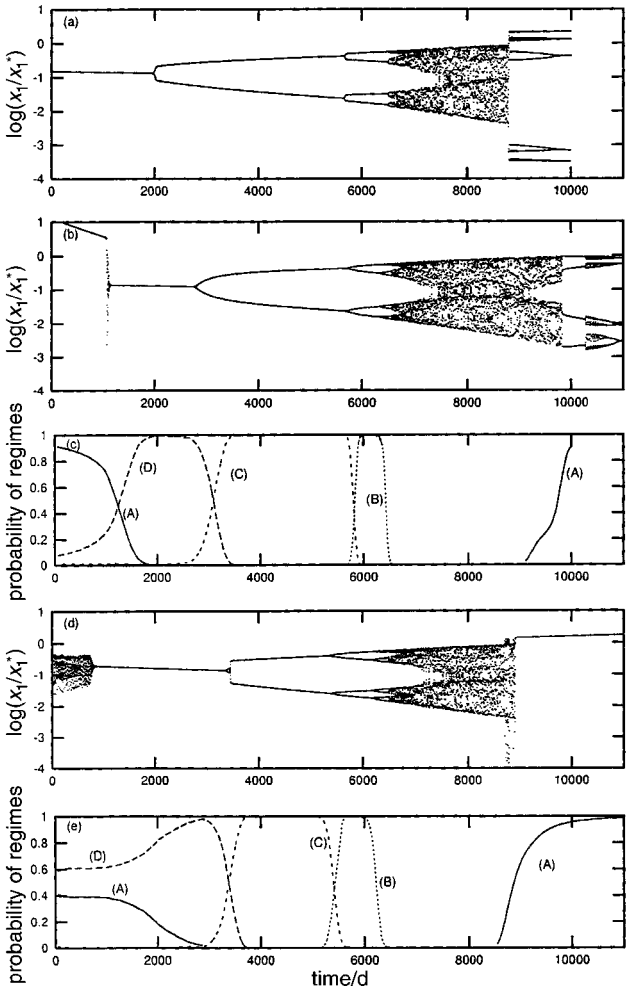

Fig. 5 The same as in Fig. 4 but for $m = 5$ (b) and (c) and $m = 6$ (d) and (e).

of a prognostic model of the given form. The lower limit of this range (*i.e.*, the minimal needed number of parameters) can be found in a standard manner by analysing the dependence of the quality of reproduction of the *observed* behaviour of a DS on the number of parameters of the model. For example, for the situation under consideration, analysis of Fig. 3(a) and (b) leads straightforwardly to the conclusion that the number of neurons in the NN (8) must be not less than three: $m \geqslant 3$. As to the upper limit of the range, we do not find it possible to make any conclusions *before* we construct the prognosis; moreover, it is necessary to compare the characteristics of the prognoses constructed using a different number of parameters (different number of neurons in the hidden layer of the NN in the model (8) of interest to us). It is also worthy of note that the informativity of the prognosis using a "good" prognostic model must depend sufficiently weakly on the number of parameters, if this number falls within the optimal range.

To conclude this section we would like to note the following circumstance. Representation of the evolution operator in the form of the expansion (4) in time explicitly entering this expression means that the proposed algorithm can be employed as long as the nonautonomous part of the operator is of the order of its autonomous part or less. Our calculations verify that, for models with $m \in [3; 10]$, the applicability limit of the algorithm is a time interval having duration of

about four lengths of the initial TS $T \in [7000; 8500]$ calculated from its centre (moment $t = 7750$). Thus, we can expect to obtain a correct prognosis over the time interval $1750 \approx < t < \approx 13\,750$.†††

3.4.

We investigated prognoses of bifurcations constructed using model (8) with the number of neurons $m \in [1; 10]$. As was to be expected, for $m = 1, 2$ the model does not reproduce even the observed evolution of the system. The most informative was prognosis for $m = 5, 6$. For a greater number of neurons, prognosis informativity decreases.

In Fig. 4(b) and (d), 5(b) and (d) and 6(b) we present the bifurcation diagrams corresponding to the average trend (10) for $m = 3$–7, respectively. Time dependences of the probability to reveal different predicted regimes of behaviour, determined by the expression (14), are shown on the panel below each diagram (Fig. 4(c) and (e), 5(c) and (e) and 6(c)). This characteristic allows one to judge the accuracy of prediction of bifurcation transition instants as well as the maximal probability of the regime most probable at the current time instant. We remind the reader that all the results given here were obtained *exclusively* on the basis of analysis of the TS that represented variations of one dynamical variable (concentration of atomic oxygen) over the time interval $T \in [7000; 8500]$ days (see Fig. 2(a)) *without* any other information about the system (16) that generated it. For estimation of the quality of prognosis, correct bifurcation diagrams obtained by direct computation of the system (16) and describing variations of qualitative behaviour of this system over the entire time interval are shown on the upper panel of each figure (Fig. 4(a), 5(a) and 6(a)). Finally, the bifurcation diagram corresponding to the average trend and time dependences of the probability of predicted regimes plotted for the same initial TS (see Fig. 2(a)) but using a low-dimensional algorithm[24,25] are given for comparison in Fig. 6(d) and (e).

Prognoses for different values of parameter m will be compared by analysing the time dependence of the probabilities of the predicted regimes, $P_k(t)$. Being the most typical "representatives" of the corresponding statistical ensembles, the bifurcation diagrams for the average trend (10) may, however, reproduce local features of the structure of the space of parameters of prognostic model, that are not typical of the statistical ensemble as a whole. For example, in Fig. 4(d) one can see that no bifurcations are predicted in the "future" $t > 8500$ prognosticated within the limits of this panel for a model with $m = 4$, whereas statistical analysis shows (see Fig. 4(e)) that a catastrophic bifurcation will occur by the time instant $t = 11\,000$ with probability $P_\infty \simeq 0.62$, as a result of which the chaotic attractor that generated the initial TS will disappear.

As noted above, comparison of the time dependences of the regime probabilities depicted in Fig. 4(c) and (e), 5(c) and (e) and 6(c) shows that the most informative are prognoses made employing models with $m = 5$ and $m = 6$. Indeed, one can see in Fig. 5(c) and (e) that the maximal probabilities of all predicted regimes are equal to unity in this case. An exception is a catastrophic "regime", the most remote into the "past" ($t < 7500$), to which the model passes when a single-periodic regime breaks up. Comparison with the correct bifurcation diagram (Fig. 5(a)) reveals that this regime, unlike all the others, was predicted erroneously; the observed system has no such regime. However, it should be taken into consideration that the probability of this "false" regime is rather small at the boundary of the prognosis interval (for $t \approx 1750$): $P_\infty \approx 0.2$ for $m = 5$ and $P_\infty \approx 0.3$ for $m = 6$.

Models with a larger or smaller number of neurons predict much worse the catastrophic regime that actually occurs in the future for $t > 8800$. Note that the corresponding catastrophic bifurcation is a natural restriction of the interval of prognosis into the "future". Moreover, in good agreement with what was said in Section 3.3, models with a large number of neurons provide a better accuracy of prediction of the instants of nearest bifurcations in the "past", and a model with $m = 3$ gives the most accurate prognosis of the bifurcation of the birth of a single-periodic regime, that is the most remote into the past, which is not prognosticated at all by models with

††† It is the upper estimate of the prognosis interval. The interval of prognosis may be, for example, shortened as a result of a catastrophic bifurcation, when the system passes to the earlier unattainable region of phase space.

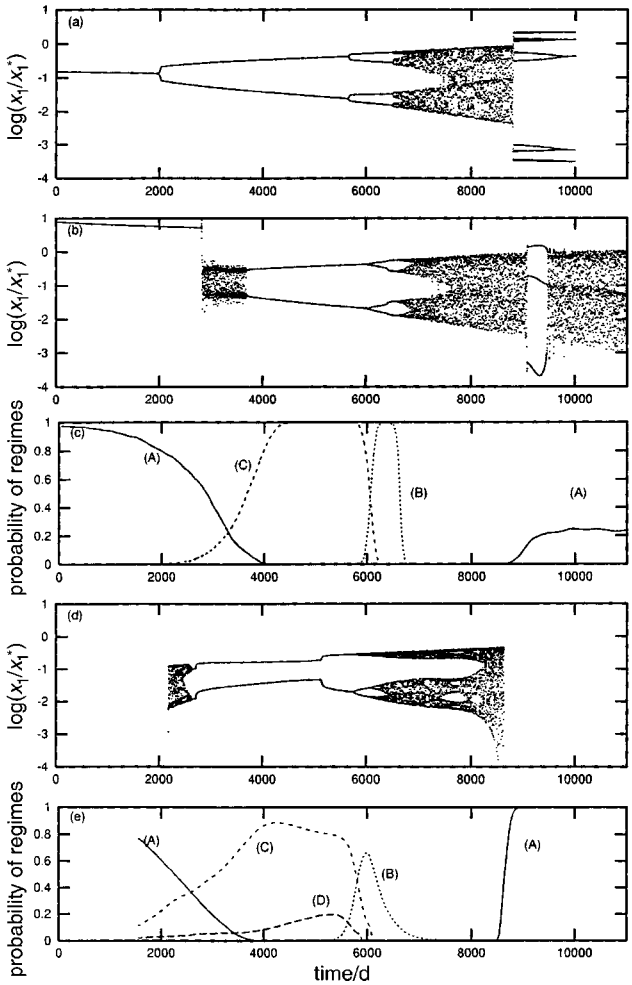

Fig. 6 The same as in Fig. 4 but for $m = 7$ (b) and (c) and calculated using low-dimensional algorithm[24,25] (d) and (e).

$m \geqslant 7$. Nevertheless, we can conclude that the informativity of the prognosis constructed with the aid of model (8) depends weakly on the number of parameters for $m \in [3; 7]$.

Let us make some conclusions from the results presented in Fig. 4–6:

(1) The prognostic model (8) with the optimal number of neurons $m = 5$ and $m = 6$ predicted correctly all the bifurcation transitions within the prognosis interval, with the maximal probabilities of all regimes of behaviour predicted over this interval being equal to unity.

(2) The "future" catastrophe—the nearest bifurcation to the boundaries of the initial TS—is predicted worse than other bifurcations that are more remote in time. This result has two causes. Firstly, dissipativity of a NN that provides global stability of the prognostic model decreases sensitivity of the model *outside* the "learning region" (the region of variation of the arguments of a discrete time map *within* the initial TS). Secondly, it is exactly the situation that occurs for the internal attractor of a mesospheric PCS: the characteristic size of the attractor grows with approaching catastrophe. Consequently, model (8) prognosticates the future worse than the past, recession into which results in a decreased range of variation of dynamical variables.

(3) The prognosis constructed employing a low-dimensional algorithm[24,25] shown in Fig. 6(d) and (e) predicts bifurcations and regimes of behaviour in the past much worse than the NN (8),

but it is better in predicting the future catastrophe. The cause of a poor prognosis of the "past" is insufficiently accurate reproduction of the observed behaviour of the DS, which is due primarily to the use of evolution operator in the form of a first-order discrete time map. However, the form of this function—the fifth degree polynomial—provides a more informative prognosis of the "future" bifurcation that is very near in time. Clearly, the use of polynomial functions of many variables in a "pure" form for construction of prognostic models of high-dimensional DSs is hardly promising because of the inevitable global instability of such models. However, hybrid models that combine, for instance, a NN as an autonomous component of the prognostic model (3),(4) and a system of multidimensional polynomials orthogonalised on the observed attractor as a nonautonomous component may be an optimal solution for modelling some high-dimensional DSs.

4. Conclusion

4.1.

We proposed an algorithm for constructing prognostic models of systems demonstrating complex (high-dimensional) dynamic behaviour. The basis for this algorithm is an investigation of a NDPs of the system exclusively by analysing the TS that represents variations of one dynamical variable, *without* any additional information about the system that generated this TS. Prognostic models are intended for prediction of qualitative behaviour of observed DS and its bifurcations. The algorithm essentially broadens the scope of the general approach to analysis of nonstationary TS recently proposed by the authors.[24,25]

The algorithm was used for analysis of the TS generated by a computer model of a mesospheric photochemical system. We employed the TS calculated for slow change in the control parameter of the system, namely, relative concentration of water vapour. The duration of the "observed" series was restricted so that the system demonstrated *only one*—chaotic—type of behaviour, *without* any bifurcations.

The constructed prognostic model enabled us to make a correct prognosis of bifurcation sequences and calculate probabilities to reveal at the time instant of interest predicted regimes of the system's behaviour for times much greater than the length of the initial TS.

4.2.

Of basic importance for application of the developed approach is *prediction of bifurcations of the more complex behaviour to the simpler one*: the dimension of attractors arising in the phase space of a DS as a result of bifurcations must not exceed the dimension of the attractor corresponding to the initial TS. It is quite obvious, for example, that the described general procedure does not allow for prediction of a cascade of period doubling bifurcations for the case when the initial TS contains information about the type of behaviour that is simplest for such a cascade. We emphasise that the proposed algorithm enables one to overcome windows of regular behaviour between chaotic attractors, but use of the most complex type of behaviour is decisive for construction of a prognostic model.

4.3.

The assumption that the noise is additive and dynamical, to which corresponds additive allowance for the random component in eqn. (3), imposes significant restrictions in terms of the applicability of the algorithm proposed in this research to analysis of real data bases. The assumption of additivity imposes purely quantitative restrictions on the degree of noise of the analysed TS. Whereas the dynamical noise enabled us to use the simplest way for optimising parameters of the model—the method of least squares. This permitted us to write cost functions (errors) in the form (6), (7), to find covariance matrices of the parameters characterising nonautonomy of the system from eqn. (9), and to use for these parameters a normal distribution function. It is clear, however, that a stochastic component of the actual TS nearly always contains the so-called measurement noise. Under these conditions, the method of least squares gives a systematic error in seeking optimal values of parameters.[34] Then, the procedure of finding a distribution function of the parameters of a prognostic model based on this method also becomes incorrect. One of the ways

to solve this problem is to employ the method of total least squares.[35] The corresponding modification of the algorithm is being undertaken at present, and we expect that it will enable us to use the elaborated approach for construction of prognostic models of real atmospheric processes on the basis of observed TS.

4.4.

Consider, in conclusion, possible practical applications of the prognostic models. We take as an example the construction of a prognostic model of a system determining ozone layer evolution in middle and low latitudes. The analysis of satellite measurements of ozone abundance in an atmosphere in ref. 14 showed that the corresponding time series is generated by a chaotic (strange) attractor, which makes this dynamic system an appropriate candidate for construction of a prognostic model.

The prognostic model is expected to provide the following opportunities:

First, reconstruction of nonautonomy of the considered system and, consequently, finding nonstationary characteristics of the ozone layer.

Second, prediction of bifurcations, *i.e.*, of qualitative changes in ozone evolution caused by nonstationarity.

Third, verification of the available "first principles" models by which the future state of the ozone layer is estimated at present. We mean comparison of NDPs of the prognostic model and of the "first principles" model. Note that the system under consideration is typical for the Earth's atmosphere in the sense that direct analysis of the NDPs of the "first principles" model is nearly impossible because of a high order of this system. Therefore, for verification we will first have to construct the so-called essential (or basic) dynamical model possessing the minimal possible number of degrees of freedom and, at the same time, retaining the NDPs of the complete "first principles" model. The general algorithm of constructing dynamical models was first described in ref. 31 and was used successfully for construction of essential dynamical models of the polar lower stratospheric[1] and mesospheric[31] PCSs.‡‡‡ Discrepancy between the NDPs of the essential and prognostic models will indicate that the essential and, hence, the complete "first principles" model must be corrected.

Finally, comparison of the verified "first principles" model with the prognostic model will allow one to set a correspondence between dynamical variables and nonautonomous parameters of the prognostic model and real physical and chemical characteristics of the ozone layer. This will enable one (i) to identify the "principal" dynamical variables that determine ozone layer evolution; (ii) to ascertain the trends of which parameters may lead the system to the revealed bifurcations and (iii) estimate the bifurcation instants and their quantitative consequences.

Acknowledgements

The research was done under support of the RFBR (project 99-02-16162).

References

1 A. M. Feigin and I. B. Konovalov, *J. Geophys. Res.*, 1996, **101**(D20), 26023.
2 I. B. Konovalov, A. M. Feigin and A. Y. Mukhina, *J. Geophys. Res.*, 1999, **104**(D3), 3669.
3 L. I. Kleinman, *J. Geophys. Res.*, 1991, **96**, 721.
4 L. I. Kleinman, *J. Geophys. Res.*, 1994, **99**, 16831.
5 T. Thayaparan, W. K. Hocking and J. MacDougall, *J. Geophys. Res.*, 1997, **102**, 9461.
6 B. Fichtelmann and G. Sonnemann, *Ann. Geophys.*, 1992, **10**, 719.
7 G. Sonnemann and B. Fichtelmann, *J. Geophys. Res.*, 1997, **102**, 1193.
8 G. Sonnemann and A. M. Feigin, *Phys. Rev. E*, 1999, **59**(2-A), 1719.
9 G. R. Sonnemann, A. M. Feigin and Y. I. Molkov, *J. Geophys. Res.*, 1999, **104**(D23), 30591.
10 J. C. Farman, B. G. Gardiner and J. D. Shanklin, *Nature*, 1985, **315**, 207.
11 *National Research Council. Causes and Effects of Changes in Stratospheric Ozone: Update 1983*, National Academy Press, Washington, DC, 1984.

‡‡‡ A particular version of this algorithm was quite recently published in ref. 36.

12 S. Solomon, *Rev. Geophys.*, 1988, **26**(1), 131.
13 S. Solomon, *Nature*, 1990, **347**, 347.
14 P. Yang, G. P. Brasseur and J. C. Gille *et al.*, *Physica D*, 1994, **76**, 331.
15 I.-F. Li, P. Biswas and S. Islam, *Atmos. Environ.*, 1994, **28**, 1707.
16 J. D. Neelin and M. Latif, *Phys. Today*, 1998, **N12**, 32.
17 B. Wang, A. Barcilon and Z. Fang, *J. Atmos. Sci.*, 1999, **56**, 5.
18 H. D. I. Abarbanel, R. Huerta and M. I. Rabinovich *et al.*, *Neural Comput.*, 1996, **8**(8), 1567.
19 G. W. Frank, T. Lookman and M. A. H. Nerenberg *et al.*, *Physica D*, 1990, **46**, 427.
20 H. N. Srivastava, S. N. Bhattacharya and K. C. Sinha Ray, *Geophys. Res. Lett.*, 1996, **23**(24), 3519.
21 R. Manuka and R. Savit, *Physica D*, 1996, **99**, 134.
22 T. Schreiber, *Phys. Rev. Lett.*, 1997, **78**, 843.
23 A. Witt, J. Kurths and A. Pikovsky, *Phys. Rev. E*, 1998, **58**, 1800.
24 A. M. Feigin, Y. I. Molkov, D. N. Mukhin and E. M. Loskutov, *Preprint No. 508*, *Institute of Applied Physics*, *RAS*, 1999, pp. 1–53.
25 A. M. Feigin, Y. I. Molkov, D. N. Mukhin and E. M. Loskutov, *Radiophys. Quantum Electron.*, 2001, **44**, 348.
26 H. D. I. Abarbanel, *Analysis of Observed Chaotic Data*, Springer-Verlag, New York, 1997.
27 F. Takens, in: *Dynamical Systems and Turbulence*, ed. D. A. Rand and L.-S. Young, 1981, Springer, Berlin, vol. 898, p. 366.
28 A. M. Fraser and H. L. Swinney, *Phys. Rev. A*, 1986, **33**, 1134.
29 M. B. Kennel, R. Brown and H. D. I. Abarbanel, *Phys. Rev. A*, 1992, **45**, 3403.
30 *The Handbook of Brain Theory and Neural Networks*, ed. M. A. Arbib, The MIT Press, 1995.
31 A. M. Feigin, I. B. Konovalov and Y. I. Molkov, *J. Geophys. Res.*, 1998, **103**(D19), 25447.
32 I. B. Konovalov and A. M. Feigin, *Nonlinear Proc. Geophys.*, 2000, **7**, 87.
33 H. W. Press, B. P. Flannery and S. A. Teukolskyl, *Numerical Recipes*, Cambridge University Press, Cambridge, 1990.
34 P. E. McSharry and L. A. Smith, *Phys. Rev. Lett.*, 1999, **83**, 4285.
35 S. Van Huffel and J. Vandewalle, *The Total Least Squares Problem*, SIAM, Philadelphia, 1991.
36 L. V. Kalachev and R. J. Field, *J. Atmos. Chem.*, 2001, **39**, 65.