Prediction of the atmosphere quality changes from monitoring data with estimation of indeterminacy

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We present a development of the technique for solving problems connected with dynamics of the atmosphere and ocean, as well as with the control for environment. New elements are numerical algorithms for optimum estimations of the predicted characteristics with allowance for indeterminacy. The latter can be interpreted as errors of models, parameters, and input data. The indeterminacy functions are introduced into the simulation system explicitly. The idea of the proposed approach is based on a special organization of the variational principle for non-linear models of the studied processes, which are considered in the generalized variational formulation. For this purpose, the objective functional is supplemented with functionals, expressing the total measure of all indeterminacies and, given the observational data, the measure of differences between the measured values and their images calculated by the models. The structure of the computational technology, which uses the universal algorithm of direct-inverse simulation for realization of this technique, is described. The proposed algorithms are intended to improve the organization of adaptive (or directed) strategies of monitoring and optimal forecasting of changes in the atmosphere quality.

Introduction

The problem of estimating indeterminacy in mathematical models exists from the very moment of appearance of models themselves and the statement of the forecasting problem on their base. The sources of indeterminacies, which are always present in the models, are imperfect knowledge about the physical processes, errors in numerical schemes and algorithms of their realization, and errors in definition of input data. Observational data are the main source of information for solving the forecast problem and estimating the indeterminacies. In its turn, monitoring data on the behavior of the studied processes introduce other indeterminacies, connected with measurement errors and inaccuracy of the mathematical model, used for calculation of images of the observed values.

In recent years, different approaches to estimation of indeterminacies are actively developed and ways to attenuation of their influence on the forecasting quality are proposed. A significant part in these approaches is played by the methods of adjoint equations developed by G.I. Marchuk.[1] As applied to models of the weather forecasting, the most progress was reached in the working out methods for improvement of the initial state of the predicted fields and formation of prognostic ensembles. Works on methods of the theory of sensitivity and assimilation of data for analysis of forecasting errors and formation of adaptive strategies of monitoring are activated. The descriptions of main approaches and the corresponding literature on the problem can be found in Refs. 2–7.

In this paper, we present a new stage in our simulation technique.[8–15] The idea of the proposed approach is based on a special organization of the variational principles for solving interconnected problems of ecology and climate on the base of non-linear models of dynamics of the atmosphere, ocean, and environmental control. The models of the processes are considered in a generalized variational formulation, which explicitly and additively includes the functions of indeterminacies. The objective functional is supplemented with functionals, expressing the total measure of all indeterminacies and, provided the observation data are in hand, the estimate of differences between the measured values and their images calculated in terms of functions of state. Further, the extended functional is formed and the universal algorithm of the direct-inverse simulation is constructed on the variational principle, which includes algorithms for calculation of functions of sensitivity and indeterminacy of the corresponding objects.

The optimal algorithms for forecasting and planning of the directed adaptive monitoring of evolution of natural processes are constructed by means of joint use of the basic and adjoint functions, as well as functions of indeterminacy and sensitivity. The indeterminacy functions introduce a regularization effect into the algorithms. When solving forecasting problems, assimilation of the observation data leads to the decrease of the degree of indeterminacy influence. If the domain of the model is insufficiently covered by observations from a stationary monitoring system, or if the observations are absent at all, then the indeterminacy functions can be used to identify the districts, where the stations of the adaptive (mobile) monitoring system should be located.

High efficiency of mixed strategies for monitoring the composition of the atmosphere with the use of stationary observational programs and mobile monitoring

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tools is proved by practice.[16–20] The mobile tools are more adapted to the organization of the directed monitoring by given objective criteria. The presented algorithms are intended to perfect the organization of such mixed strategies.

Problem statement

Write the mathematical model of the spatial-temporal evolution of the studied processes in the operator form

$$L(\varphi, \mathbf{Y}) \equiv \frac{\partial \varphi}{\partial t} + G(\varphi, \mathbf{Y}) - \mathbf{f} - \mathbf{r} = 0; \quad (1)$$

$$\varphi^0 = \varphi_a^0 + \xi \text{ for } t = 0; \ \mathbf{Y} = \mathbf{Y}_a + \zeta, \quad (2)$$

where $\varphi \in Q(D_t)$ is the vector-function of the state; $\mathbf{Y} \in R(D_t)$ is the vector of parameters; $G(\varphi, \mathbf{Y})$ is the spatial operator of the model; $D_t = D \times \left[0, \bar{t}\right]$ is the domain of variation of the spatial coordinates $\mathbf{x}$ and time t. The index a denotes the *a priori* estimates. Denote the set of the data measured in the set $D_t^m \subset D_t$ by φ_m and Ψ_m and define the set of observation models to form images of the measured values in terms of functions of state

$$\Psi_m = [H(\varphi)]_m + \eta. \quad (3)$$

Here $[\,]_m$ denotes the operator of information transfer from the net $D_t^h \subset D_t$ to the set D_t^m. Functions $\mathbf{r}$, ξ, ζ, and η describe indeterminacies and errors of the corresponding objects. When constructing algorithms, it is convenient to include into the vector of parameters both the internal characteristics of the model and sources, initial conditions, and indeterminacies of boundary conditions.

Introduce a collection of objective and controlling functionals, necessary for solving problems on estimation of the quality of models, monitoring, ecological forecasting, and design. Use the functionals of the general form

$$\Phi_k(\varphi, \mathbf{Y}) = \int_{D_t} F_k(\varphi, \mathbf{Y}) \chi_k(\mathbf{x}, t)\, \mathrm{d}D\mathrm{d}t = (F_k, \chi_k),$$
$$k = \overline{1, K}, \ K \geq 1, \quad (4)$$

where $F_k(\varphi, \mathbf{Y})$ are estimated functions and $\chi_k \geq 0$ are weight functions. The choice of all objects in Eq. (4) is determined by aims of the study. The functions $F_k(\varphi, \mathbf{Y}) \in Q(D_t)$ are chosen to be bounded, Lipschitz-continuous, and Gateaux differentiable with respect to their functional arguments $(\varphi, \mathbf{Y}) \in \{Q(D_t) \times R(D_t)\}$. The structure of the weight functions is defined by the following reasons.

1. In Eq. (4), we choose $\chi_k(\mathbf{x}, t) \in Q^*(D_t)$, where $Q^*(D_t)$ is the function space dual to $Q(D_t)$. These functions define Radon or Dirac measures $\chi_k(\mathbf{x}, t)\,\mathrm{d}D\mathrm{d}t$ in D_t. The properties of the measures are discussed in detail in Ref. 21. For definiteness, we introduce the normalization conditions

$$\int_{D_t} \chi_k(\mathbf{x}, t) \mathrm{d}D\mathrm{d}t = 1, \ \chi_k \geq 0. \quad (5)$$

2. The estimation domain D_t^v of the function $F_k(\varphi, \mathbf{Y})$ is defined in D_t by supports of non-zero values $\chi_k \geq 0$. In particular, in problems of data assimilation the support of the function χ_k describes the scheme of observations, which are taken into account in the functionals, on $D_t^v \subset D_t^m \subset D_t$.

3. The range of χ_k values is given in such a way that the domain D_t^v is ranked by the contribution of the function F_k into the total value of the functional Φ_k.

Indeterminacies in the models and data as a base for their unification

To solve the problems, we use the variational principle. Define an extended functional

$$\tilde{\Phi}_k^h(\varphi) = \left[I^h(\varphi, \mathbf{Y}, \varphi_k^*)\right]_{D_t^h} +$$
$$+\left\{\alpha_0 \Phi_k^h(\varphi, \mathbf{Y}) + 0.5\alpha_1 (\eta^T W_1 \eta)_{D_t^m}\right\}^h +$$
$$+0.5\left\{\alpha_2 (\mathbf{r}^T W_2 \mathbf{r})_{D_t^h} + \alpha_3 (\xi^T W_3 \xi)_{D^h} + \alpha_4 (\zeta^T W_4 \zeta)_{R^h(D_t^h)}\right\}^h \geq 0. \quad (6)$$

Here Φ_k is the objective functional of the form (4), and the functional

$$I(\varphi, \mathbf{Y}, \varphi_k^*) \equiv \left(L(\varphi, \mathbf{Y}), \varphi_k^*\right) = 0 \quad (7)$$

presents the integral identity for description of the model in the variational formulation; $\alpha_i \geq 0$, $i = \overline{0, 4}$ are weight coefficients. The upper index h denotes the discrete analogs of the corresponding objects here and below. Let us define the last four functionals in Eq. (6) by scalar products of the energy type. Formula (4) describes the structure of all functionals in Eq. (6). Their individuality is expressed through specific assignment of the estimated and weight functions. The functional of the integral identity (7) is chosen so that the balance equation for full energy of the system (1) is obtained from Eq. (7) at $\varphi^* = \varphi$. The observation part of the functional, containing the function η from Eq. (3), takes into account all available observational data for φ_m and ψ_m.

The weight matrices W_i in functionals (6) are defined as follows:

$$W_i = \tilde{W}_i \chi_{W_i}, \ i = \overline{1, 4}, \quad (8)$$

where $\tilde{W}_i$ are diagonal matrices defining the energy metric from the physical content of the corresponding functions; χ_{W_i} are diagonal matrices, whose elements represent the Radon and Dirac measures. They are of the same sense as the measures in the definition of the functionals (4). If the weight functions and measures are defined in such a way, all functionals for discrete and distributed characteristics are constructed by a common rule. This is important in construction and realization of adaptive algorithms, which are to operate in the regime of control for the spatial-temporal dynamics of the supports of different information fields.

The universal algorithm of the direct-inverse simulation

Following to Refs. 11 and 12, we construct a scheme of the universal algorithm of direct-inverse simulation with a quantitative estimation of indeterminacy functions. Without going into details of the calculation technique, present only its main elements, which realize the stability conditions of the extended functional (6) with respect to variations of its functional arguments $\partial\tilde{\Phi}^h/\partial s = 0$ $(s = \varphi, \varphi^*, r, \xi, \zeta)$. After making some transformations we obtain

1) the system of fundamental equations:

$$\left\{\frac{\partial\varphi}{\partial t} + G(\varphi, \mathbf{Y}) - \mathbf{f} - \mathbf{r}\right\}^h = 0; \qquad (9)$$

2) the system of adjoint equations:

$$\left\{-\frac{\partial\varphi^*}{\partial t} + A^*(\varphi, \mathbf{Y})\varphi^* + \alpha_0\frac{\partial\Phi_k}{\partial\varphi} + \alpha_1\left(\frac{\partial H}{\partial\varphi}\right)^* W_1(\Psi - H(\varphi))\right\}^h = 0; \qquad (10)$$

$$\varphi^*(\mathbf{x}, \bar{t}) = 0; \qquad (11)$$

3) the system of equations for estimation of indeterminacies:

$$\alpha_2 W_2\mathbf{r} - \varphi^*(\mathbf{x}, t) = 0, \qquad (12)$$

$$\alpha_3 W_3\xi - \varphi^*(\mathbf{x}, 0) = 0, \qquad (13)$$

$$\alpha_4 W_4\zeta + \alpha_0\frac{\partial\Phi_k^h}{\partial\mathbf{Y}} + \frac{\partial I^h}{\partial\mathbf{Y}} = 0. \qquad (14)$$

In Eq. (10), A^* is the adjoint operator to the Gateaux linearized operator of the model (1) in the discrete representation (9). The upper index "*" marks the adjoint (transposed) operators and functions from the dual space. In Eq. (14) we take into account only components of the sensitivity functions, which correspond to parameters with explicit allowance for indeterminacies in the functionals $\tilde{\Phi}_k^h$ and I^h. After having solved the problems (9)–(14), we obtain the sensitivity relation

$$\delta\Phi_k^h(\varphi, \mathbf{Y}) = \frac{\partial}{\partial a}\left\{\Phi_k^h(\varphi, \mathbf{Y} + a\delta\mathbf{Y}) + I^h(\varphi, \mathbf{Y} + a\delta\mathbf{Y}, \varphi_k^*)\right\}_{a=0} \equiv$$

$$\equiv \left(\frac{\partial\Phi_k^h}{\partial\mathbf{Y}}, \delta\mathbf{Y}\right), \qquad (15)$$

where a is the real parameter; φ_k^* is the solution of the problem (10) with the functional Φ_k. In contrast to Eq. (14), the sensitivity relation (15) takes into account all summands with variations of all characteristics related to the category of the model parameters.

The feedback equations

In practice, it is convenient to choose the objective functionals (4) as a sum of pairs of summands:

$$\Phi_k(\varphi, \mathbf{Y}) = \Phi_{ks}(\varphi) + \Phi_{kp}(\mathbf{Y}). \qquad (16)$$

In particular, the parametric part of the functional can be taken in the form

$$\Phi_{kp}(\mathbf{Y}) = 0.5\int_{D_t}\left\{\sum_{i=1}^{N}\left(\gamma_1\Gamma_{ip}^{(1)}\left|\operatorname{grad}\left(Y_i - \tilde{Y}_i\right)\right|^2 + \gamma_2\Gamma_{ip}^{(2)}\left(Y_i - \tilde{Y}_i\right)^2\right)\right\}\mathrm{d}D\mathrm{d}t. \qquad (17)$$

Here $\tilde{Y}_i$ are values of the parameters calculated by the schemes of physical parameterization of the models (for instance, coefficients of turbulence by the Smagorinskii scheme); $\gamma_1, \gamma_2 \geq 0$ are weight factors; $\Gamma_{ip}^{(\alpha)}$ are positive diagonal matrices of the scaling coefficients and weights, constructed by analogy with matrices (8); N is the total number of parameters.

Starting from the conditions of minimization for the objective functional and sensitivity relations,[10] we construct a system of feedback equations to refine the parameters:

$$\frac{\partial Y_i}{\partial t} = -\kappa\Gamma_i^{-1}\frac{\partial\Phi_k(\varphi, \mathbf{Y})}{\partial Y_i}, \quad i = \overline{1, N};$$
$$\kappa \cong \Phi_k(\varphi, \mathbf{Y})\Big/\left(\frac{\partial\Phi_k}{\partial\mathbf{Y}}, \frac{\partial\Phi_k}{\partial\mathbf{Y}}\right), \qquad (18)$$

where κ is the iteration parameter; Γ_i is the matrix of formation of a metric in the space of parameters. If the objective functionals are chosen in the form (16), (17), the feedback equations have the following structure:

$$\frac{\partial Y_i}{\partial t} = -\kappa\Gamma_i^{-1}\left\{\frac{\partial I^h(\varphi, \mathbf{Y}, \varphi^*)}{\partial Y_i} - \gamma_1\operatorname{div}\Gamma_{ip}^{(1)}\operatorname{grad}\left(Y_i - \tilde{Y}_i\right) + \gamma_2\Gamma_{ip}^{(2)}\left(Y_i - \tilde{Y}_i\right)\right\}. \qquad (19)$$

All numerical schemes for formation of problems (9)–(19) are generated by the variational principle for estimation of functional (6). The way, by which they are constructed, guarantees mutual agreement of all elements of the algorithm. In the general case, a set of problems (9)–(19) is solved by iteration methods. Functionals, included into Eq. (6), are approximated by the decomposition and split methods. Equations (19) are also solved via split schemes, coordinated with the general structure of the algorithm. It should be noted that if the "windows" of data assimilation are taken equal to intervals of model discretization in time, direct algorithms for on-line solution of problems (9)–(19) can be obtained. Some modifications of such algorithms are described in Ref. 13.

Algorithms for diagnostics of model quality and localization of mobile monitoring stations

1. Adaptive monitoring strategy for reducing the indeterminacy in a forecast

First, we consider the case when the interval $[0,\bar{t}\,]$ does not contain the data of a fixed system of observations $\{\psi_m\}$. Let us define a prognostic functional of type (4) in the estimation domain D_t^v. In fact, we put $\alpha_0 = 1$, $\alpha_1 = 0$ in Eq. (6); take F_k in the form

$$F_k(\varphi,\mathbf{Y}) = 0.5\big((\varphi-\varphi_{\mathrm{a}})W_k(\varphi-\varphi_{\mathrm{a}})\big) \qquad (20)$$

and $\chi_k(\mathbf{x},t) > 0$ for $(\mathbf{x},t)\in D_t^v$, where $\varphi_{\mathrm{a}}(\mathbf{x},t)$ is a given *a priori* estimate of the unknown function of state in D_t^v; W_k is a weight diagonal matrix. Its elements define the scale factors in formula (20), which describes the energy of perturbations of the function of state in D_t^v.

Perform one cycle of calculations by scheme (9)–(15) with *a priori* given values of the input data:

$$\left\{\varphi_{\mathrm{a}},\varphi_{\mathrm{a}}^0(\mathbf{x});\ \mathbf{Y}_{\mathrm{a}},\mathbf{f}_{\mathrm{a}},\mathbf{r}_{\mathrm{a}}=0,\zeta_{\mathrm{a}}=0,\xi_{\mathrm{a}}=0\right\}.$$

As output information, we obtain a set of values of the functions

$$\left\{\varphi(\mathbf{x},t),\ \varphi^*(\mathbf{x},t),\ \mathbf{r}(\mathbf{x},t),\ \xi(\mathbf{x},t),\ \zeta(\mathbf{x},t)\right\}$$

and a complete set of the sensitivity functions $\{\partial\Phi_k^h/\partial\mathbf{Y}\}_i$, $i=\overline{1,N}$, incoming into the sensitivity relation (15).

All functions are defined based on requirements of optimality of estimation of the prognostic functional (4), (20). The optimality is meant as independence of the estimated functional variation magnitude of variations $\delta\varphi(\mathbf{x},t)$ of φ in the domain D_t^v. A numerical scheme for finding $\varphi(\mathbf{x},t)$ is constructed so that the values of variations $\delta\tilde{\Phi}_k^h$ and $\delta I^h(\varphi,\mathbf{Y},\varphi^*)$ of the functionals (6) and (7) do not depend on $\delta\varphi^*$ variations of $\varphi^*(\mathbf{x},t)$ and variations of the functions of indeterminacy. As follows from equations (9) and (12), the indeterminacy functions of the model $\mathbf{r}$ are defined through the solution of adjoint problems generated by the variational principle for the extended functional up to weight matrices and coefficients. Here it is not important whether the observation data are available or not. In the general case, it is sufficient to have only the predicted functional Φ_k. The solution of the adjoint problem $\varphi_k^*(\mathbf{x},t)$ takes part also in calculations of sensitivity functions Φ_k to variations of $\delta\mathbf{Y}$ of the parameters $\mathbf{Y}$ in algorithms (15), (17), and (18). Recall that in the process of construction of the algorithms, the sources $\mathbf{f}(\mathbf{x},t)$, initial conditions, and heterogeneities of the boundary conditions were included in the set of parameters.

The indeterminacy and sensitivity functions are calculated through the same functions φ_k^* constructed for different Φ_k, $k=\overline{1,K}$. At the same time, their purposeful applications can have their own peculiarities. In particular, sensitivity functions are applied mostly to study trends in the behavior of functionals in the space of parameters. This is necessary in identification of parameters, sources, initial and boundary conditions, etc. Indeterminacy functions express errors under conditions of optimality of predicted characteristics and are used for analysis of the system as a whole and for organization of adaptive monitoring strategies. For instance, if the problem is to organize an adaptive scheme of localization of mobile monitoring tools to reduce indeterminacy of forecast, domains with larger values of indeterminacy and sensitivity functions can be most appropriate for these purposes. This is caused by the fact that all the functions are obtained from the conditions of optimality for estimates of the generalized forecasting characteristics.

2. Arrangement of mobile monitoring tools in addition to a stationary program of observations

Let us consider a situation when the data enter the interval $[0,\bar{t}\,]$ from a set of stationary monitoring stations situated in D_t^m, and it is required to solve the problem about adaptive arrangement of additional mobile tools of observation.

It is convenient to solve problems of such type in two steps. At the first step the extended functional (6) is formed, in the third summand of which all available observation data with weight $\alpha_1 = 1$ are taken into account; the objective functional Φ_k is excluded ($\alpha_0 = 0$). Under these initial prerequisites, the prediction-assimilation problem is solved via scheme (9)–(20). All sensitivity and indeterminacy functions are calculated as in Subsection 1. By configuration and ranges of the function values, domains in D_t with a preset level of observability from the monitoring stations are identified. Denote the domains as $D_t^H \in D_t$. Using the procedure of data assimilation in these domains, it is possible to reconstruct the necessary for prediction spatial-temporal structure of variables of state and parameters, which provide for the minimal value of the "observational" functional of quality, whence it follows that it is expedient to arrange the additional observations in the domain

$D_t^A = D_t^h / D_t^H$, i.e., beyond the observability domain D_t^H.

At the second step, the problem of prediction-assimilation of data is solved with the quality functionals (6) at $\alpha_0 = 1$ and $\alpha_1 = 1$ by scheme (9)–(19), as in Subsection 1. As a result, phase spaces of the state functions, sensitivity functions, and indeterminacy functions in the domain D_t^h are defined. The observability domain D_t^H, which was identified at the first step, has a guaranteed degree of covering by observational data from stationary stations. Therefore, the criterion of the choice of measurement localization in subdomains of higher values of the indeterminacy and sensitivity functions in $D_t^A \subset D_t^h$ should be used for adaptive arrangement of mobile observations. The idea of the algorithm of adaptive organization of observations, based on the minimization condition for indeterminacy functions in the domains that cannot be observed by stationary monitoring systems, belongs to A.V. Penenko (personal communication).

3. Sensitivity and indeterminacy functions in the system of simulation

These functions play a key part in organization of direct connections and feedbacks between parameters of the system and objective functionals. This is seen from the system of equations (9)–(19) as applied to problems of forecast and assimilation of observational data.

The scheme, first proposed in Ref. 9, is realized in different modifications of variational methods of the data assimilation, which are considered as traditional. The objective quality functional in it is minimized with respect to the function describing the initial state $\varphi^0(\mathbf{x})$. The feedback is realized only through solution of a conjugate problem at $t = 0$: $\varphi^*(\mathbf{x}, 0)$. Explicit introduction of indeterminacy functions into the structure of models and parameters changes the situation radically. The indeterminacy function $\mathbf{r}$ directly includes the whole 4-dimensional phase space of values of $\varphi^*(\mathbf{x}, t)$ in the feedback mode, and the indeterminacy function ζ includes all functions of the objective functional sensitivity to variations of the parameters.

Introduction of the indeterminacy functions brings a new quality into the simulation system on the whole. The case in point is the regularization of calculation algorithms. To demonstrate the idea of the proof of this fact, let us consider the case when the operators of the process and observation models are linear with respect to the state functions: $G(\varphi, \mathbf{Y}) = A(\mathbf{Y})\varphi$, $H(\varphi) = H\varphi$. This situation takes place, for instance, when the model of transfer and transformation of multi-component admixtures contains a linear (linearized) transformation operator. Under these assumptions, the system of equations (9)–(15) takes the form

$$\Lambda\varphi - \mathbf{f} - \mathbf{r} = 0; \quad \Lambda\varphi \equiv \left[\frac{\partial \varphi}{\partial t} + A(\mathbf{Y})\varphi\right]^h, \tag{21}$$

$$\Lambda^*\varphi^* + \alpha_0 W_0(\varphi - \varphi_a) + \alpha_1 H^T W_1(\Psi - H\varphi) = 0, \tag{22}$$

$$\mathbf{r} = \alpha_2^{-1} W_2^{-1} \varphi^*. \tag{23}$$

Excluding formally the functions φ^* and $\mathbf{r}$ from these equations, after some transformations we obtain the system of equations

$$\Lambda^* W_2 \Lambda\varphi + \alpha_2^{-1}\left[\alpha_0 W_0 + \alpha_1 H^T W_2 H\right]\varphi =$$
$$= \Lambda^* W_2 \mathbf{f} + \alpha_2^{-1}\left[\alpha_0 W_0 \varphi_a + \alpha_1 H^T W_2 \Psi\right]. \tag{24}$$

Since $\alpha_i \geq 0$ and W_i are diagonal weight matrices with positive elements, the systems (21)–(23) and (24) are well-posed. As is seen from Eq. (24), for $\alpha_0, \alpha_1 > 0$, incorporation of the quantitative tools of indeterminacy estimates introduces a regularization effect and, as a corollary, improves the convergence properties of iteration algorithms in solutions of inverse and optimization problems. Underline that the system (21)–(23) is solved by the scheme of the algorithm and the system (24) is written only for analysis of the algorithm behavior on the whole.

Conclusion

We have developed a new technique for forecasting of dynamics and quality of the atmosphere. In this technique, together with the sought state functions, the indeterminacy functions are calculated. The latter can be interpreted as errors of models, parameters, and input data. These functions are introduced into the simulation system explicitly as additional summands in the representation of the corresponding objects. The proposed algorithms are intended for better organization of adaptive monitoring strategies, for optimal forecasting of changes in the atmosphere quality.

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