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OPTIMAL FORECASTING OF NATURAL PROCESSES WITH UNCERTAINTY ASSESSMENT

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The problem of optimal forecasting of environmental changes induced by various factors is discussed. The proposed technique is based on variational principles and methods of the sensitivity theory with allowance for uncertainties in mathematical models and input data. Optimal forecasting is understood as forecasting where the estimates of cost functionals are independent of variations of the sought state functions. In addition to state functions, the forecasted characteristics include risk and vulnerability functions for receptor areas and quantification of uncertainties.

Key words: *optimal forecasting, mathematical modeling, quality of environment, sensitivity analysis, uncertainty assessment, convection, diffusion, and reaction equations.*

Introduction. The quality of forecasting of environmental changes by means of mathematical modeling depends to a large extent on the degree of uncertainty admitted in formulations of mathematical models and initial data for calculations. Sources of uncertainties, which are inevitable in mathematical models, are the lack of knowledge on physical processes, errors of numerical schemes and algorithms of their implementation, and errors in input information. This information, in turn, is taken from observations obtained with the use of monitoring systems, which involves other uncertainties due to measurement errors and inaccuracies in their presentation in mathematical models used to calculate the images of the registered quantities in terms of state functions of the models of various processes.

Various approaches to estimating uncertainties have been recently developed, and methods for attenuating the influence of uncertainties on the forecasting quality have been proposed. A significant role in these approaches belongs to methods of adjoint equations developed by Marchuk [1]. As applied to weather prediction, the greatest progress has been reached in diminishing uncertainties in the initial state of desired fields and forecast formation on the basis of results of ensemble rather than conventional single scenario calculations. New methods of the sensitivity theory and data assimilation for analyzing forecasting errors and organizing adaptive strategies of monitoring have been proposed recently. A description of the basic approaches and a review of publications on this topic can be found in [2–7].

One problem also dealing with forecasting of natural processes is considered in the present paper. The study involves not only forecasting of changes in the environment quality, but also estimating territorial risks and vulnerability and searching for optimal strategies of environment quality control, depending on varying parameters of the model and external effects. Various approaches developed for solving these problems are described, for instance, in [8]. Most of them are "forward" approaches. The essence of these approaches is obtaining results with the use of various sets of initial data by means of forward integration in time. Final conclusions can be obtained by comparing and analyzing particular situations. Obviously, a rather large number of variants have to be considered for reliable forecasting. Therefore, such a forecasting technology is not rational even if high-performance computers are used. Another drawback of forward modeling methods is noticeable difficulties inherent in determining the contributions of various sources of errors to forecasting results.

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An approach to overcoming these drawbacks is proposed in the present paper. A combination of forward and inverse modeling methods and methods of the model sensitivity theory [9–17] is based on specially constructed variational principles for solving interrelated problems of climatic and environmental processes on the basis of nonlinear models of dynamics of atmosphere and water objects, as well as transport and transformation of pollutants. Models of processes are included into the structure of variational principles in a generalized formulation, with uncertainty functions (UFs) being explicitly involved. The objective functional of the forecast is supplemented with functionals that express the total measure of all uncertainties and (if observation data are available) the assessment of deviations of the measured quantities from their images calculated in terms of state functions. The role of various factors in the formation of processes under study is elucidated with the use of sensitivity functions (SFs) on the basis of variational methods of the sensitivity theory, which provides qualitative and quantitative estimates of the influence of uncertainties in the description of these factors on the forecasting quality.

Formulation of the Problem. The mathematical model of space–time evolution of the examined processes includes models of atmosphere dynamics, which are designed for the formation of carrier medium hydrodynamics, and also models that describe the processes of transport and transformation of various substances, which are intended for reconstruction of the current state and forecasting of the atmosphere quality. As we do not need a detailed presentation of the hydrodynamic aspect of the model, we give only the formulation of models that describe the convection, diffusion, and reaction processes, which are key elements in formulations of environmental problems:

$$\frac{\partial \pi\varphi_i}{\partial t} + \operatorname{div} \pi(\varphi_i \boldsymbol{u} - \mu_i \operatorname{grad} \varphi_i) + \pi(S\boldsymbol{\varphi})_i - \pi(f_i(\boldsymbol{x}, t) + r_i) = 0. \tag{1}$$

Here $\boldsymbol{\varphi} = \{\boldsymbol{\varphi}_i(x,t),\ i = \overline{1, n_s}\} \in Q(D_t)$ is the part of the vector state functions of the entire set of models that describe the behavior of various substances in a four-dimensional domain D_t, n_s is the number of various constitutents, the functions φ_i are the temperature, components of the hydrological cycle in the atmosphere (water vapor, water in clouds, rain water, snow, and ice crystals), and concentrations of pollutants in the gaseous and aerosol states, $\boldsymbol{Y} \in R(D_t)$ is the vector of model parameters, $\boldsymbol{f} = \{f_i(\boldsymbol{x}, t),\ i = \overline{1, n_s}\}$ are the source functions of heat, moisture, and pollutants, $\boldsymbol{r} = \{r_i(\boldsymbol{x}, t),\ i = \overline{1, n_s}\}$ are the functions that describe uncertainties and errors of the models, and $(S\boldsymbol{\varphi})_i$ are the nonlinear matrix operators that describe local processes of transformation of the corresponding substances and do not contain derivatives of state functions with respect to $\boldsymbol{x}$ and t. The following characteristics of the hydrodynamic background are explicitly included into Eqs. (1): $\boldsymbol{u} = (u_1, u_2, u_3)$ is the velocity vector, $\mu_i = (\mu_1, \mu_2, \mu_3)_i$ is the diagonal tensor of turbulent exchange coefficients for the substance φ_i in the coordinate directions $\boldsymbol{x} = \{x_i\}$, $i = \overline{1,3}$, and π is the function determined via meteo-elements in accordance with the structure of the vertical coordinate in the domain D_t. The function π and the velocity vector satisfy the continuity equation of the carrying medium

$$\frac{\partial \pi}{\partial t} + \operatorname{div} \pi\boldsymbol{u} = 0. \tag{2}$$

The models of the processes, the structure of the domains, and the coordinate systems used in the present work were described in detail in [10, 12].

The initial conditions and model parameters are written in the form

$$\boldsymbol{\varphi}^0 = \boldsymbol{\varphi}^0_a + \boldsymbol{\xi} \quad \text{for} \quad t = 0, \qquad \boldsymbol{Y} = \boldsymbol{Y}_a + \boldsymbol{\zeta}, \tag{3}$$

where the subscript a indicates *a priori* estimates.

The boundary conditions for the models follow from the physical content of the examined problem; these can be the Dirichlet conditions, von Neumann conditions, or mixed conditions of different boundary segments of the domain D_t.

Let us use $\boldsymbol{\Psi}_m$ to denote the group of measurement data on the set $D^m_t \subset D_t$ and determine the ensemble of observation models for the formation of images of the measured quantities in terms of state functions:

$$\boldsymbol{\Psi}_m = [H(\boldsymbol{\varphi})]_m + \boldsymbol{\eta}. \tag{4}$$

Here $[\,\cdot\,]_m$ is the operator of information transfer from the grid $D^h_t \subset D_t$ to the set D^m_t. The grid domain D^h_t is introduced for constructing discrete approximations of the model. The functions $\boldsymbol{r}$, $\boldsymbol{\xi}$, $\boldsymbol{\zeta}$, and $\boldsymbol{\eta}$ in Eqs. (1), (3), and (4) describe the uncertainties and errors of the corresponding objects. In algorithm construction, it is convenient to include not only the internal characteristics of the models as components of the vector of parameters, but also the sources, initial conditions, and inhomogeneities of the boundary conditions.

Let us introduce a set of objective and control functionals necessary to solve problems of estimating the quality of environmental models, monitoring, and diagnostics, ecological forecasting and design. Let us define these objects as functionals of the general form [11]

$$\Phi_k(\boldsymbol{\varphi}, \boldsymbol{Y}) = \int\limits_{D_t} F_k(\boldsymbol{\varphi}, \boldsymbol{Y}) \chi_k(\boldsymbol{x}, t)\, dD\, dt = (F_k, \chi_k), \qquad k = \overline{1, K}, \quad K \geqslant 1. \tag{5}$$

Here $F_k(\boldsymbol{\varphi}, \boldsymbol{Y})$ and $\chi_k(\boldsymbol{x}, t) \geqslant 0$ are the estimated and weight functions; (F_k, χ_k) is the scalar product. Particular forms of all objects in Eq. (5) depend on research goals. We choose functions $F_k(\boldsymbol{\varphi}, \boldsymbol{Y}) \in Q(D_t)$ such that they are summable with respect to the functional arguments $(\boldsymbol{\varphi}, \boldsymbol{Y}) \in \{Q(D_t) \times R(D_t)\}$. The structure of the weight functions is found on the basis of the following considerations.

1. Let $\chi_k(\boldsymbol{x}, t) \in Q^*(D_t)$ in Eq. (5) [$Q^*(D_t)$ be the space of functions adjoint with respect to the space of state functions $Q(D_t)$]. These functions determine the Radon or Dirac measures $\chi_k(\boldsymbol{x}, t)\, dD\, dt$ in D_t. The properties of such measures were studied in detail in [18]. For certainty, we require the normalization condition $\int\limits_{D_t} \chi_k(\boldsymbol{x}, t)\, dD\, dt = 1$ to be fulfilled.

2. We determine the verification domain D_t^v for estimating the functions $F_k(\boldsymbol{\varphi}, \boldsymbol{Y})$ in D_t with the use of a support in which the values $\chi_k > 0$. In particular, in data assimilation problems, the support function χ_k on $D_t^v \subset D_t^m \subset D_t$ describes the scheme of locations of observation points (4) taken into account in functionals.

3. Let us define the intervals of values of χ_k so that the domain D_t^v could be ranged with respect to the degree of the contribution of the function F_k determined in different parts of the estimation domain to the total value of the functional Φ_k.

Variational Principle with Allowance for Uncertainties. To solve the problems, we apply the variational principle [10, 11]. We determine the augmented functional, which unites all elements of the modeling system (1)–(5):

$$\tilde{\Phi}_k^h(\boldsymbol{\varphi}) = [I^h(\boldsymbol{\varphi}, \boldsymbol{Y}, \boldsymbol{\varphi}_k^*)]_{D_t^h} + [\alpha_0 \Phi_k^h(\boldsymbol{\varphi}, \boldsymbol{Y}) + 0.5\alpha_1 (\eta^{\mathrm{t}} W_1 \boldsymbol{\eta})_{D_t^m}]^h$$

$$+ (1/2)[\alpha_2 (\boldsymbol{r}^{\mathrm{t}} W_2 \boldsymbol{r})_{D_t^h} + \alpha_3 (\boldsymbol{\xi}^{\mathrm{t}} W_3 \boldsymbol{\xi})_{D^h} + \alpha_4 (\boldsymbol{\zeta}^{\mathrm{t}} W_4 \boldsymbol{\zeta})_{R^h(D_t^h)}]^h. \tag{6}$$

Here Φ_k is the objective functional of the form (5), the functional $I(\boldsymbol{\varphi}, \boldsymbol{Y}, \boldsymbol{\varphi}_k^*) = 0$ is the integral identity for the description of model (1) in the variational formulation [10], and $\alpha_i \geqslant 0$ ($i = \overline{0, 4}$) are the weight coefficients; the superscript h indicates discrete analogs of the corresponding objects. We determine the last four functionals in Eq. (6) with the help of scalar products of the energetic type. The structure of the functionals in Eq. (6) is described by formulas of the form (5). A particular content of these functionals is determined by specifying the estimated and weight functions in the corresponding scalar products. The third term of Eq. (6), which contains the function $\boldsymbol{\eta}$ from Eq. (4), takes into account all available observation data $\boldsymbol{\Psi}_m$.

We determine the weight matrices W_i in the functionals of Eq. (6) so that the functionals express the energetic norm in the physical space of the corresponding multicomponent functions. With such a method for specifying the weight functions and measures, all functionals for discrete and distributed characteristics are obtained by the same rule that is important in constructing and implementing adaptive algorithms designed for operation in the regime of tracking the space–time dynamics of supports of various information fields.

Universal Algorithm of Forward and Inverse Modeling. Following [11, 13], we construct a scheme of a universal algorithm of forward and inverse modeling with a quantitative assessment of uncertainty functions.

We write the discrete (in time) approximation of the augmented functional (6) with the use of the splitting method:

$$\tilde{\Phi}_k^h(\boldsymbol{\varphi}, \boldsymbol{Y}, \boldsymbol{\varphi}_k^*) = \sum_{j=1}^{J} \Big(\int\limits_D \sum_{\alpha=1}^{p} \Big(\frac{(\boldsymbol{M}_\alpha, \boldsymbol{\psi}_\alpha^{*j})}{\Delta \tau_\alpha^j} + (\boldsymbol{N}_\alpha, \boldsymbol{\varphi}_\alpha^{*j}) + (\boldsymbol{U}, \boldsymbol{\varphi}^{*j}) \Big)\, dD\, \Delta t_j + \Phi_0^{hj} \Big). \tag{7}$$

Here

$$\boldsymbol{M}_\alpha \equiv \boldsymbol{\psi}_\alpha^j - \boldsymbol{\varphi}^{j-1} + \Delta \tau_\alpha^j (L_\alpha^j \boldsymbol{\psi}_\alpha^j - \boldsymbol{f}_\alpha^j - \boldsymbol{r}_\alpha^j) = 0; \tag{8}$$

$$\boldsymbol{N}_\alpha \equiv \boldsymbol{\psi}_\alpha^j - [\sigma_\alpha \boldsymbol{\varphi}_\alpha^j + (1 - \sigma_\alpha) \boldsymbol{\varphi}^{j-1}] = 0; \tag{9}$$

$$\boldsymbol{U} \equiv \boldsymbol{\varphi}^j - \frac{1}{p}\sum_{\alpha=1}^{p} \boldsymbol{\varphi}_\alpha^j = 0, \qquad j = \overline{1,J}, \quad \alpha = \overline{1,p}, \quad p \geqslant 1; \tag{10}$$

Φ_0^{hj} is the decomposition in time of the weighted sum of the functionals included into the augmented functional (6), except for the first one, the superscript j determines the number of the time step, J is the number of time steps, α is the number of the splitting stage, p is the number of splitting stages, Δt_j is the time step, $\Delta\tau_\alpha^j = p\sigma_\alpha\,\Delta t_j$, and $0.5 \leqslant \sigma_\alpha \leqslant 1.0$ are the weight coefficients for two-layer approximations in time. The scheme has the second order of accuracy at $\sigma_\alpha = 0.5$ and the first order at $\sigma_\alpha = 1$. The relations

$$L = \sum_{\alpha=1}^{p} L_\alpha, \qquad \boldsymbol{f} = \sum_{\alpha=1}^{p} \boldsymbol{f}_\alpha, \qquad \boldsymbol{r} = \sum_{\alpha=1}^{p} \boldsymbol{r}_\alpha$$

determine the additive presentations of the spatial operator $L(\boldsymbol{\varphi}, \boldsymbol{Y})$ of model (1) and functions of sources and uncertainties, respectively, in constructing splitting schemes.

The model contains operators of two types: convection-diffusion operators over three spatial coordinate directions and operators of substance transformation. These operators are defined at each grid point D_t^h and at each time step. There are four operators in the scheme; hence, there are four splitting stages. In accordance with these definitions, the first term in Eq. (7) is the approximation of the integral identity functional in model (1) written in terms of the splitting method with the use of aggregates of the type (8) in the variational formulation. The second and third terms in Eq. (7) determine relations (9) and (10) of the images of the state functions $\boldsymbol{\psi}_\alpha^j$ and $\boldsymbol{\varphi}_\alpha^j$ at these splitting stages to the state function of the model $\boldsymbol{\varphi}^j$ at the times t_j; $\boldsymbol{\psi}_\alpha^{*j}$, $\boldsymbol{\varphi}_\alpha^{*j}$, and $\boldsymbol{\varphi}^{*j}$ are the corresponding components of the adjoint state function. The expression for $\boldsymbol{M}_\alpha$ is the result of action of the operator of the two-layer system with respect to time at the splitting stage with the number α. Let us recall that the scalar products in Eq. (7) are determined in accordance with the multicomponent structure of the vector functions in (1). Discretization of the operators and functionals in Eqs. (7) and (8) with respect to spatial variables is performed on the basis of the hybrid method of discrete-analytical approximations [16]. For convection-diffusion operators, this method ensures monotonicity, stability, and transportivity of numerical schemes and their consistency in the main (forward) and adjoint variants.

The use of analytical solutions eliminates the effect of numerical diffusion. It is principally important that the obtained class of schemes does not involve artificial procedures of monotonization and flux correction, which increase the degree of uncertainty of numerical models. The point is that artificial procedures of monotonization generate nonlinear effects of self-limited diffusion, which are not inherent in real transport processes. This can exert a significant effect on the results of forecasting the evolution of multicomponent substances, because a specific self-controlled diffusion situation occurs for each component. As all substances simultaneously participate in reactions described by the transformation operators in model (1), it is not clear which forecast will be obtained.

Without going into details of the computational technology, we present its main elements that ensure the conditions of stationarity of the augmented functional (6) with respect to variations of its functional arguments $\partial\tilde{\Phi}^h/\partial s = 0$ ($s = \boldsymbol{\varphi}$, $\boldsymbol{\varphi}^*$, $\boldsymbol{r}$, $\boldsymbol{\xi}$, $\boldsymbol{\zeta}$). After transformations, we obtain a system of main equations

$$\frac{\partial\tilde{\Phi}^h}{\partial\boldsymbol{\varphi}^*} = 0 \quad \forall\ \boldsymbol{\varphi}^* = (\boldsymbol{\psi}_\alpha^{*j}, \boldsymbol{\varphi}_\alpha^{*j}, \boldsymbol{\varphi}^{*j}) \in Q^{*h}(D_t^h), \tag{11}$$

a system of adjoint equations

$$\frac{\partial\tilde{\Phi}^h}{\partial\boldsymbol{\varphi}} = 0 \quad \forall\ \boldsymbol{\varphi} = (\boldsymbol{\psi}_\alpha^{j}, \boldsymbol{\varphi}_\alpha^{j}, \boldsymbol{\varphi}^{j}) \in Q^{h}(D_t^h); \tag{12}$$

$$\boldsymbol{\varphi}^{*J+1}(\boldsymbol{x}) = 0, \qquad \boldsymbol{x} \in D^h, \tag{13}$$

and a system for uncertainty assessment

$$\frac{\partial\tilde{\Phi}^h}{\partial \boldsymbol{r}} = \alpha_2 W_2 \boldsymbol{r} - \boldsymbol{\varphi}^*(\boldsymbol{x}, t) = 0; \tag{14}$$

$$\frac{\partial\tilde{\Phi}^h}{\partial \boldsymbol{\xi}} = \alpha_3 W_3 \boldsymbol{\xi} - \boldsymbol{\varphi}^*(\boldsymbol{x}, 0) = 0; \tag{15}$$

$$\frac{\partial\tilde{\Phi}^h}{\partial \boldsymbol{\zeta}} = \alpha_4 W_4 \boldsymbol{\zeta} + \Big(\alpha_0 \frac{\partial \Phi_k^h}{\partial \boldsymbol{Y}} + \frac{\partial I^h}{\partial \boldsymbol{Y}}\Big)\Big|_{\boldsymbol{Y}=\boldsymbol{Y}_a} = 0. \tag{16}$$

The superscript asterisk is used to indicate the adjoint (transposed) operators and functions from the adjoint space. System (11) is a set of additively averaged schemes of component-by-component splitting whose properties were described in detail in [19]. These schemes allow independent realization of all splitting stages at each time interval and ensure a parallel structure of calculations as a whole. In Eq. (16), we take into account only those SF components that correspond to parameters for which the uncertainties in the functionals $\tilde{\Phi}_k^h$ and I^h are explicitly taken into account.

After solving problems (11)–(16), we can calculate the sensitivity relations for objective functionals by the algorithm

$$\delta\Phi_k^h(\boldsymbol{\varphi}, \boldsymbol{Y}) = \frac{\partial}{\partial a}\Big[\Phi_k^h(\boldsymbol{\varphi}, \boldsymbol{Y} + a\,\delta\boldsymbol{Y}) + I^h(\boldsymbol{\varphi}, \boldsymbol{Y} + a\delta\boldsymbol{Y}, \boldsymbol{\varphi}_k^*)\Big]\Big|_{a=0} \equiv \Big(\frac{\partial\Phi_k^h}{\partial\boldsymbol{Y}}, \delta\boldsymbol{Y}\Big), \tag{17}$$

where $\delta\boldsymbol{Y}$ are the variations of parameters, a is the real parameter, $\boldsymbol{\varphi}$ is the solution of the basic problem, and $\boldsymbol{\varphi}_k^*$ is the solution of problem (12) generated by the functional Φ_k ($k = \overline{1, K}$). In contrast to Eq. (16), the sensitivity relations (17) take into account all terms with variations of all characteristics, which are model parameters.

Inverse Problems for Identification of Parameters. For solving inverse and optimization problems of design and forecasting in practice, the objective functionals (5) have to be chosen with allowance for the *a priori* information on state functions and model parameters, for instance, by including the parametric part into functional (5):

$$\Phi_k(\boldsymbol{\varphi}, \boldsymbol{Y}) = (F_k, \chi_k) + \frac{1}{2}\int\limits_{D_t}\Big(\sum_{i=1}^{N}\Big[\gamma_1\Gamma_{ip}^{(1)}|\operatorname{grad}(Y_i - \tilde{Y}_i)|^2 + \gamma_2\Gamma_{ip}^{(2)}(Y_i - \tilde{Y}_i)^2\Big]\Big)\,dD\,dt. \tag{18}$$

Here $\tilde{Y}_i$ are the *a priori* values of parameters calculated by the schemes of physical parametrization of models (for example, coefficients of turbulence, characteristics of interaction of substances with inhomogeneities of the Earth's surface, etc.), $\gamma_1 \geqslant 0$ and $\gamma_2 \geqslant 0$ are the weight factors, $\Gamma_{ip}^{(\alpha)}$ are the positive diagonal matrices of the scaling coefficients and weights, constructed by analogy with the matrices W_i in Eq. (6), and N is the total number of parameters.

Following [10], we construct a system of inverse relations equations for identification of parameters on the basis of conditions of minimization of the objective functional and sensitivity relations (17):

$$\frac{\partial Y_i}{\partial t} = -\varkappa\Gamma_i^{-1}\Big(\frac{\partial I^h(\boldsymbol{\varphi}, \boldsymbol{Y}, \boldsymbol{\varphi}^*)}{\partial Y_i} - \gamma_1 \operatorname{div}\Gamma_{ip}^{(1)}\operatorname{grad}(Y_i - \tilde{Y}_i) + \gamma_2\Gamma_{ip}^{(2)}(Y_i - \tilde{Y}_i)\Big). \tag{19}$$

Here $\varkappa$ is the iterative parameter and Γ_i is the diagonal matrix of weights for the formation of the metrics in the space of parameters.

All numerical schemes for problems (11)–(19) were constructed on the basis of the variational principle for assessments of functional (6). The method of generating these schemes provides mutual consistency between all elements of the algorithm. In the general case, the set of problems (11)–(19) is solved by iterative methods. The functionals in Eq. (6) are approximated by decomposition and splitting methods. Equations (19) are also solved by splitting schemes agreed with the overall structure of the algorithm. Note, if the observation data are assimilated via functional (6) and the data assimilation "windows" are assumed to be equal to the discretization intervals of the models in time, then real-time construction of forward (non-iterative) algorithms for solving problems (11)–(19) is possible. Some modifications of such algorithms were described in [13].

Sensitivity and Uncertainty Functions in the Modeling System. For uncertainty assessment, we perform one cycle of calculations by scheme (11)–(16) with *a priori* specified values of input data $\{\boldsymbol{\varphi}_a,\ \boldsymbol{\varphi}_a^0(\boldsymbol{x}),$

$\boldsymbol{Y}_a,\ \boldsymbol{f}_a,\ \boldsymbol{r}_a = 0,\ \boldsymbol{\zeta}_a = 0,\ \boldsymbol{\xi}_a = 0\}$. As the output information, we obtain a set of values of the functions $\{\boldsymbol{\varphi}(\boldsymbol{x},t), \boldsymbol{\varphi}^*(\boldsymbol{x},t), \boldsymbol{r}(\boldsymbol{x},t), \boldsymbol{\xi}(\boldsymbol{x},t), \boldsymbol{\zeta}(\boldsymbol{x},t)\}$ and the total set of sensitivity functions $\{\partial\Phi_k^h/\partial\boldsymbol{Y}\}_i$ $(i = \overline{1,N})$ involved into the sensitivity relation (17). All these functions are determined from the conditions of optimality of the assessment of the response functional (5), (18). The optimality is understood in the sense that the variation of the estimated functional is independent of the variations $\delta\boldsymbol{\varphi}(\boldsymbol{x},t)$ and $\delta\boldsymbol{\varphi}^*(\boldsymbol{x},t)$ in the neighborhood of the current phase trajectory of the process in the domain D_t. The numerical scheme for finding the function $\boldsymbol{\varphi}(\boldsymbol{x},t)$ is constructed so that the values of the variations $\delta\tilde{\Phi}_k^h$ and $\delta I^h(\boldsymbol{\varphi}, \boldsymbol{Y}, \boldsymbol{\varphi}^*)$ of functionals (6), (7) are independent of the variations $\delta\boldsymbol{\varphi}^*$ of the functions $\boldsymbol{\varphi}^*(\boldsymbol{x},t)$ and UF variations. It follows from Eqs. (11) and (14) that the uncertainty functions $\boldsymbol{r}$ of the model are determined, with accuracy to the weight matrices and coefficients, via the solutions of adjoint problems generated by the variational principle for the augmented functional. In the general case, therefore, it suffices to determine the structure of the response functional $\tilde{\Phi}_k$ to estimate the uncertainties by scheme (11)–(16). The solution of the adjoint problem $\boldsymbol{\varphi}_k^*(\boldsymbol{x},t)$ is used in algorithms (17)–(19) for calculating the sensitivity functions $\tilde{\Phi}_k$ to variations $\delta\boldsymbol{Y}$ of parameters $\boldsymbol{Y}$. Recall that the sources $\boldsymbol{f}(\boldsymbol{x},t)$, initial conditions, and inhomogeneities of the boundary conditions are included into the number of model parameters.

Application of UFs and SFs can involve some specific features. In particular, application of SFs is mainly aimed at studying the trends in the behavior of functionals in the space of parameters, which is necessary for identification of parameters, sources, initial and boundary conditions, etc. Indeed, it follows from relations (17) that SFs are partial derivatives of the reponse functionals with respect to model parameters and sources. Depending on research goals and on the character of functionals, SFs can be interpreted as influence, value, risk, vulnerability, or observability functions.

Uncertainty functions provide a quantitative assessment of the errors of the corresponding model elements under conditions of optimality of the forecasted characteristics. Particular values of UFs depend on the choice of the weight matrices $\boldsymbol{W}_i$ and coefficients α_i in Eq. (6). It should be noted that the choice of these elements, which form the metrics in the space of uncertainties, requires a special study and can be a rather complicated task. The proposed algorithm ensures obtaining prognostic estimates under the condition of minimizing the uncertainty functionals in Eq. (6). This is caused by the fact that, by virtue of equalities (14)–(16), the general character of UFs and SFs is determined by the functions $\boldsymbol{\varphi}_k^*(\boldsymbol{x},t)$. The latter are obtained by solving problem (12) with a specified structure of the objective functional and data assimilation functional. To analyze the system as a whole and develop adaptive strategies of monitoring, therefore, all output characteristics of the modeling system (11)–(19) have to be used together. For instance, if the task is to construct an adaptive scheme for locating mobile means of monitoring, aimed at reducing forecast uncertainties, the most suitable areas are the regions with elevated values of the functions $\boldsymbol{\varphi}_k^*(\boldsymbol{x},t)$, UFs, and SFs, because these functions are obtained from conditions of optimality of the assessments of the generalized characteristics of the forecast. Such regions are identified by specified levels of significance of the corresponding functions with respect to their maximum values in D_t^h. The functions $\boldsymbol{\varphi}_k^*(\boldsymbol{x},t)$, UFs, and SFs play the major role in constructing forward and inverse relations between the system parameters and objective functionals. It follows from system (11)–(19) for problems of forecasting and assimilation of observation data.

Various modifications of variational methods of data assimilation involve a scheme first proposed in [9]. In this scheme, the objective functional of the quality is minimized with respect to a function that describes the initial state $\boldsymbol{\varphi}^0(\boldsymbol{x})$. The inverse relation is realized only via the solution of the adjoint problem at $t = 0$: $\boldsymbol{\varphi}^*(\boldsymbol{x},0)$.

Explicit involvement of uncertainty functions into the structure of models and parameters drastically alters the situation. Indeed, in the functions $\boldsymbol{\varphi}^*(\boldsymbol{x},t)$, the adjoint problems (12) accumulate information distributed in D_t about the character of all monitoring data included into the observation functional as the function $\boldsymbol{\eta}$ from Eq. (4) and used to calculate the source functions in system (12). Moreover, it follows from Eq. (14) that the uncertainty function $\boldsymbol{r}$ directly includes the entire four-dimensional phase space of the values of the function $\boldsymbol{\varphi}^*(\boldsymbol{x},t)$ into the inverse regime for system (11), while the uncertainty function of parameters $\boldsymbol{\zeta}$ includes all functions of sensitivity of the objective functional to variations of parameters. The commonly used assimilation scheme includes only Eq. (15) relating the function $\boldsymbol{\xi}$ to $\boldsymbol{\varphi}^*(\boldsymbol{x},t)$ at the initial time $t = 0$ and ensuring a correction of the initial state function in Eq. (3).

When UFs are introduced, the modeling system as a whole acquires a new quality. We mean regularization of computational algorithms. As an example, let us consider the case where the operators of process models and

observation models are linear with respect to the state functions: $L(\boldsymbol{\varphi}, \boldsymbol{Y}) = A(\boldsymbol{Y})\boldsymbol{\varphi}$ and $H(\boldsymbol{\varphi}) = H\boldsymbol{\varphi}$. Such a situation occurs if the operator of transformation of multicomponent mixtures in model (1) is linear (or linearized). Under these assumptions and with $\pi = \text{const}$, system (11)–(14) becomes

$$\Lambda\boldsymbol{\varphi} - \boldsymbol{f} - \boldsymbol{r} = 0, \qquad \Lambda\boldsymbol{\varphi} \equiv \Big(\frac{\partial\boldsymbol{\varphi}}{\partial t} + A(\boldsymbol{Y})\boldsymbol{\varphi}\Big)^h, \tag{20}$$

$$\Lambda^*\boldsymbol{\varphi}^* + \alpha_0 W_0(\boldsymbol{\varphi} - \boldsymbol{\varphi}_a) + \alpha_1 H^{\mathrm{t}} W_1(\boldsymbol{\Psi} - H\boldsymbol{\varphi}) = 0, \qquad \boldsymbol{r} = \alpha_2^{-1} W_2^{-1}\boldsymbol{\varphi}^*.$$

Eliminating the functions $\boldsymbol{\varphi}^*$ and $\boldsymbol{r}$ from these equations and applying some transformations, we obtain the system of equations

$$\Lambda^* W_2 \Lambda\boldsymbol{\varphi} + \alpha_2^{-1}(\alpha_0 W_0 + \alpha_1 H^{\mathrm{t}} W_2 H)\boldsymbol{\varphi} = \Lambda^* W_2 \boldsymbol{f} + \alpha_2^{-1}(\alpha_0 W_0 \boldsymbol{\varphi}_a + \alpha_1 H^{\mathrm{t}} W_2 \boldsymbol{\Psi}). \tag{21}$$

As $\alpha_i \geqslant 0$, Λ is a non-singular monotonic operator, and W_i are the diagonal weight matrices with positive elements, then system (20) and (21) are well posed. It follows from Eq. (21) that, for $\alpha_0 > 0$ and $\alpha_1 > 0$, including a quantitative apparatus for estimating uncertainties into the algorithm exerts a regularization effect similar to Tikhonov's regularization and, thus, improves the properties of convergence of iterative algorithms in solving inverse and optimization problems. Note that system (20) is solved in accordance with the algorithms scheme, while system (21) is derived only to analyze the algorithm as a whole.

Inverse Problem of Estimating Prognostic Functionals. In the present paper, we further develop the forecasting technique described in [10, 11, 15, 18]. Therefore, following the tradition of testing the theoretical postulates of the technique by solving particular problems, as in [14], we consider the scenario of long-term forecasting of the ecological situation in the East Siberian region as an example. This region has a well-developed industrial complex with a high man-caused load on the environment. In addition, this region is located in the Central Asian energy-active zone of the global climate system; the specific features of this zone are the Altai–Sayan cyclogenesis [20] and increased seismic activity. This zone also includes a specially protected territory — Lake Baikal, which is the world-level heritage. For all these reasons, the problem of long-term environmental forecasting and estimating of environmental risks for this territory is very important.

The problem is aimed at long-term assessment (in the time interval from October 1 to October 31, 2005) of the prognostic functional, which is chosen to be of the type (5), with a weight function possessing a non-zero support in a four-dimensional region of the receptor area, which is a three-dimensional area of the atmosphere above the lake, extended in the vertical direction from the water surface to a level corresponding to a pressure level of 10 hPa. The value of this functional is the total amount of pollutants located in the selected region in the indicated time interval. Solving this problem by conventional methods of forward modeling involves many difficulties. Indeed, the field of pollutants is formed in the atmosphere from sources of different natures, which can be located almost anywhere on the Earth's surface, while the quantitative information about the emission of pollutants is unavailable. Air masses carrying the pollutants pass through the region and the receptor area from one boundary to another within a time interval of the order of 24 hours. To solve the problem, we need to estimate the amount of pollutants passing through the domain above the lake during one month. Some part of the pollutants becomes deposited on the underlying surface.

The above-described methods of inverse modeling and methods of organizing prognostic scenarios [17] allow us to obtain necessary assessments acceptable for practical applications without specifying information on emission. The calculations are performed with a set of mathematical models whose general structure was described in [12], with modifications mentioned in the present paper.

The hydrodynamic part of the scenario formed with the use of reanalysis [21] is organized in the same manner as in [14, 15]: the dynamics of four-dimensional fields of meteo-elements is calculated with a 30-min time step in the domain D (over the horizontal variables 47.5° N $\leqslant y \leqslant 60^\circ$ N and 95° E $\leqslant x \leqslant 115^\circ$ E in spherical coordinates) on a latitude–longitude grid with a step of $15'$ in each coordinate direction. The vertical resolution of the grid domain is 19 levels in hybrid p–σ coordinates [12] from the Earth's surface to a level corresponding to a pressure of 10 hPa. The vertical coordinate follows the relief of the underlying surface.

Figure 1 shows one of the main forecasted elements: calculated field of the total (during a month) estimates of the relative contribution of emission of pollutants from acting and potentially possible sources located on the Earth's surface in the region considered to the functional of the atmosphere quality in the receptor area. The

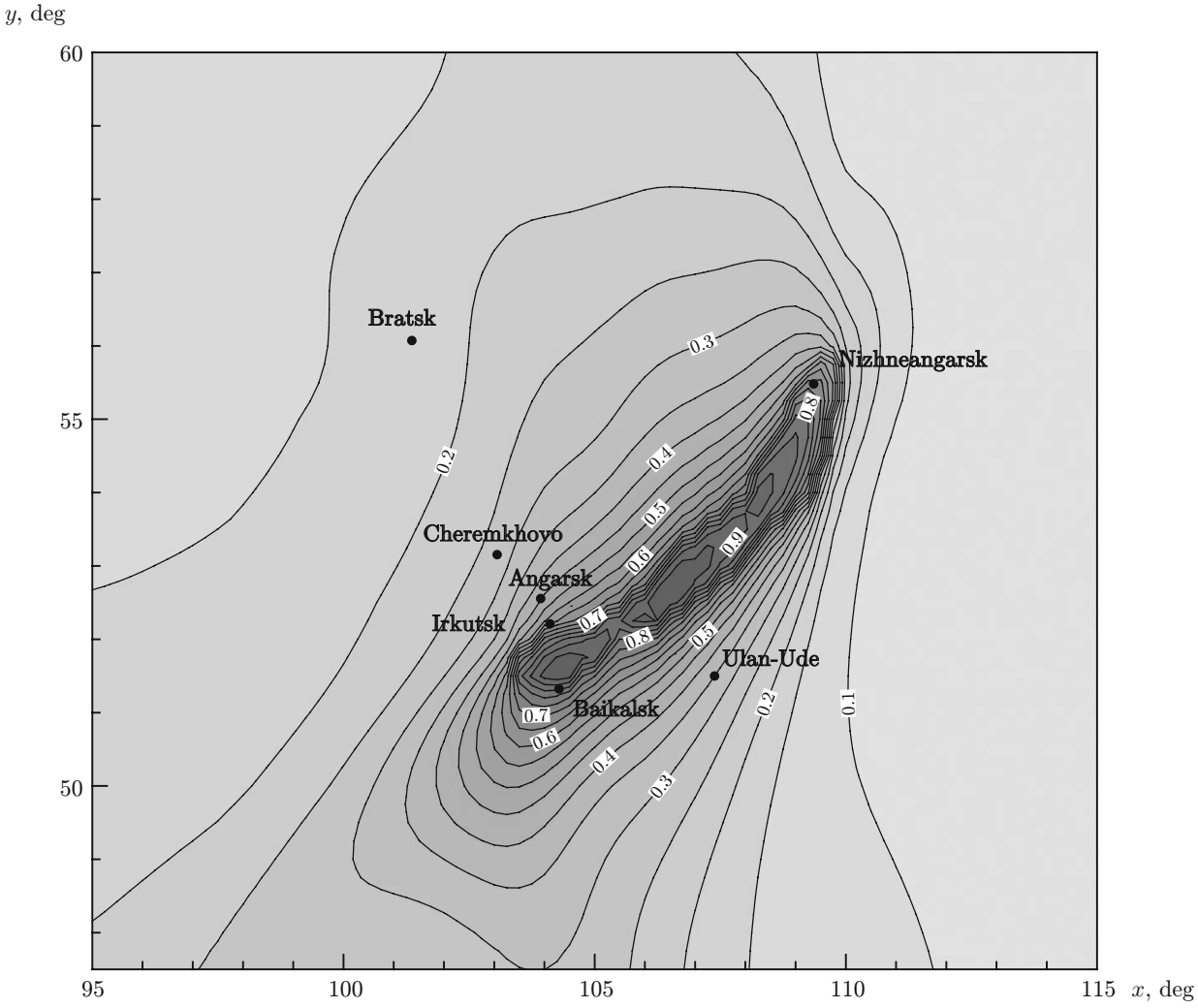

Fig. 1. Total (during a month) estimates of the relative contribution of pollutant emission from acting and potentially possible sources.

sources and their variations are assumed to be stationary in time in the calculations. The forecast fragment in the figure corresponds to the level of the model that coincides with the upper boundary of the surface layer in the coordinate system used. This fragment is a two-dimensional cross section of a three-dimensional function obtained by integration, with respect to time, of a four-dimensional SF of the forecasted functional to variations of the sources of model (1). The values on the isolines are obtained by normalization of the integrated SF to its maximum in the entire three-dimensional domain of the atmosphere in this region. The higher the SF values, the greater the risk of contamination of the receptor area from sources located in areas-carriers of these values.

To estimate the risk of contamination of the receptor area owing to transboundary transport, it is necessary to take into account the information contained in sensitivity functions on the boundaries of the domain D.

An analysis of data plotted in the figure and results calculated for other time intervals confirms the previously made conclusion that almost all cities and industrial areas of the East Siberian region are in the zone of a high environmental risk for Lake Baikal [14]. The city of Baikalsk should be specially noted, because almost all harmful pollutants are found in the atmosphere above the lake.

Generalized information on the degree of environmental risks in long-time intervals obtained by inverse modeling methods is more convenient and, therefore, can be used to make managerial decisions, especially in design of new objects and planning environmentally friendly events.

Conclusions. A variational technique is proposed for constructing optimal long-time forecasts of environment changes. An advantage of this technique is the fact that the results of estimating the objective functional, which is a generalized characteristic of the atmosphere quality, are independent of variations of state functions under conditions of minimizing the total measure of uncertainty functions explicitly included into the formulations of mathematical models. In addition to calculating state functions and estimating prognostic functionals, the algorithms proposed here assimilate all available factual information and allow calculating the functions of environmental risks and vulnerability of areas with respect to acting and potentially possible sources, as well as obtaining quantitative assessments of uncertainties in models and input data.

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REFERENCES

1. G. I. Marchuk, *Adjoint Equations and Analysis of Complex Systems* [in Russian], Nauka, Moscow (1992).
2. R. Buizza and A. Montani, "Targeting observations using singular vectors," *J. Atmosph. Sci.*, **56**, No. 17, 2965–2985 (1999).
3. D. N. Daescu and G. R. Carmichael, "An adjoint sensitivity method for the adaptive location of the observations in air quality modelling," *J. Atmosph. Sci.*, **60**, No. 2, 434–450 (2003).
4. M. Ehrendorfer and J. J. Tribbia, "Optimal prediction of forecast error covariances through singular vectors," *J. Atmosph. Sci.*, **54**, No. 2, 286–313 (1997).
5. R. Gelaro, R. Buizza, T. N. Palmer, and E. Klinker, "Sensitivity analysis of forecast errors and the construction of optimal perturbations using singular vectors," *J. Atmosph. Sci.*, **55**, No. 6, 1012–1037 (1998).
6. H. M. Kim, M. C. Morgan, and E. Morss, "Evolution of analysis error and adjoint-based sensitivities: Implications for adaptive observations," *J. Atmosph. Sci.*, **61**, No. 7, 795–812 (2004).
7. Z. Toth and E. Kalnay, "Ensemble forecasting at NMC: The generation of perturbations," *Bull. Amer. Meteor. Soc.*, **74**, No. 12, 2317–2330 (1993).
8. A. Ebel and T. Davitashvily (eds.), *Air, Water and Soil Quality Modelling for Risk and Impact Assessment*, Springer, Dordrecht (2007).
9. V. V. Penenko and N. N. Obraztsov, "A variational initialization method for the correlation of fields of meteorological elements," *Meteorologiya Gidrologiya*, No. 11, 1–11 (1976).
10. V. V. Penenko, *Methods of Numerical Simulation of Atmospheric Processes* [in Russian], Gidrometeoizdat, Leningrad (1981).
11. V. Penenko, "Some aspects of mathematical modelling using the models together with observational data," *Bull. Novosib. Comp. Center, Ser. Numer. Model in Atmosphere, Ocean Environment. Studies*, **4**, 31–52 (1996).
12. V. V. Penenko and E. A. Tsvetova, "Structure of a set of models for studying interactions in the Baikal Lake — region atmosphere system," *Atmos. Okeanic Opt.*, **11**, No. 6, 586–593 (1998).
13. V. V. Penenko, "Variational data assimilation in real time," *Vychisl. Tekhnol.*, **10**, No. 8, 9–20 (2005).
14. V. V. Penenko and E. A. Tsvetova, "Mathematical models for studying environmental pollution risks," *J. Appl. Mech. Tech. Phys.*, **45**, No. 2, 260–268 (2004).
15. V. V. Penenko and E. A. Tsvetova, "Mathematical models of environmental forecasting," *J. Appl. Mech. Tech. Phys.*, **48**, No. 3, 428–436 (2007).
16. V. Penenko and E. Tsvetova, "Orthogonal decomposition methods for inclusion of climatic data into environmental studies," *Ecol. Model.*, **217**, 279–291 (2008).
17. V. Penenko and E. Tsvetova, "Discrete-analytical methods for the implementation of variational principles in environmental applications," *J. Comput. Appl. Math.* (2008); http://dx.doi.org/ 10.1016/j.cam.2008.08.018.
18. L. Schwartz, *Analyse Mathematique*, Hermann (1967).
19. A. A. Samarskii and P. N. Vabishchevich, *Additive Schemes for Problems of Mathematical Physics* [in Russian], Nauka, Moscow (2001).
20. S.-J. Chen, Y.-H. Kuo, P.-Z. Zhang, and Q.-F. Bai, "Synoptic climatology of ciclogenesis over East Asia, 1958–1987," *Mon. Weather Rev.*, **119**, No. 6, 1407–1418 (1991).
21. E. Kalney, M. Kanamitsu, R. Kistler, et al., "The NCEP/NCAR 40-year reanalysis project," *Bull. Amer. Meteorol. Soc.*, **77**, 437–471 (1996).