## Revealing regions of increased ecological vulnerability: concept and approaches to its realization

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Regions that are ecologically more vulnerable by the anthropogenic load have been revealed with the help of mathematical modeling and analysis of data on the global climate. These regions are characterized by high sensitivity of the atmospheric air quality to variations in the pollution sources. The results presented here were obtained with the use of a technique proposed for solution of interconnected ecological and climate problems. The technique is based on variational principles and combination of direct and inverse modeling procedures, as well as the methods of sensitivity theory. The regional and hemispheric models of pollutant transport and transformation are used. The scenarios of atmospheric circulation are constructed with the help of hydrodynamic models of the informative type, in which the data from Reanalysis NCEP/NCAR are assimilated.

## Introduction

Assessment of the prospects of ecological state of industrial regions subject to anthropogenic impact is now an intensely developed field of integrated interdisciplinary studies. The problems arising in such investigations belong to the class of interconnected ecological and climate problems. They include the problems of the atmospheric air quality, regional manifestations of global changes, ecological designing, prediction of risks from anthropogenic impact, etc. The interest in such investigations is continuously stimulated by the fact that their results are of direct practical significance in the sphere of social and economic relations.

To solve the problems of this class, specialized methods and technologies of modeling based on the combined use of mathematical models and actual data of observation of the processes in the environment are needed. In this paper, the concept of constructing such a technique is discussed. Theoretically, it is based on the variational principles, which, in their turn, give rise to the methods of direct and inverse modeling, as well as the methods of sensitivity theory.<sup>1–4</sup>

Mathematical models consider processes of thermohydrodynamics in a climate system, as well as the processes of pollutant transport and transformation. They allow a detailed pattern of actual situations to be reproduced with a certain degree of accuracy. The data of observations form the basis for constructing "directional" subspaces, which relate models to specific situations and objects, and identifying their parameters.

## Description of the problem. Variational principle

The paper considers the problems of assessing ecological risks associated with the effect of thermal

sources, moisture, and natural and anthropogenic pollutants. The stimuli to statement of these problems are the following.

Studies of the mechanisms of formation of mesoclimate and quality of the atmosphere in towns and industrial regions show that some situations arising under certain conditions can be interpreted as prerequisites of ecological catastrophes.<sup>5,6</sup> These, in particular, are the situations involving formation of inversions and zones of pollutant accumulation in the system "town-suburbs-water-land." The effect of these factors is worsened under conditions of mountainous terrain. Severe situations arise also in regions with open-cast mining objects located in intermountain hollows and deep mines.

In modeling large-scale processes, ecologically unfavorable situations are pronounced not very explicitly. There are many reasons for this, but one of them is rather obvious. It is the model resolution insufficient to take into account and adequately describe the effect of local and mesoscale factors against the background of global ones. Note that the case in point is the resolution not only in the domain of spatiotemporal variables, but also in the domain of admissible values of the parameters.

Within traditional approaches, that use methods of direct modeling, it is rather problematic to estimate the scales of interactions in a climate system with the focus on specific regions, to find the ecologically more vulnerable regions, and to assess the risk from anthropogenic impact for these regions. In such problems, the methods of inverse modeling are still beyond comparison.<sup>2–4</sup> In combination with the methods of direct modeling, they open up new prospects to extending the class of problems and organizing interactive technologies. In their essence, the methods of inverse modeling have diagnostic character. Their value is that they come from a result to its sources and causes. Among the products of inverse modeling, there are sensitivity functions that allow qualitative and quantitative assessment of the system reaction to variations in the external factors.

The modeling technology based on these principles is under development at the Institute of Computational Mathematics and Mathematical Geophysics SB RAS. It was applied in a series of numerical experiments on analyzing the scales of interactions in a climate system and on estimation of the information content of a monitoring system. The scenarios were arranged so that certain regions took part in the climate system both as sources of pollution (Chernobyl Nuclear Power Station,<sup>7</sup> Serbia,<sup>4,8</sup> Norilsk, Novaya Zemlya) and as the recipients of pollutants from other territories (Baikal,<sup>9</sup> Western Siberia,<sup>10</sup> Arctic, Japan). The atmospheric circulation was reconstructed from Reanalysis data<sup>11</sup> with the use of the system proposed in Ref. 12.

Analysis of the results of direct scenario modeling showed that in the Northern Hemisphere there are regions, the distribution of ecologically dangerous sources in which presents a severe potential hazard for vast territories. From scenarios of inverse modeling, it is also seen that there are regions recipients that are ecologically more vulnerable due to the action of pollution sources located on their territories as well as on the other territories. The danger functions calculated for them have far larger space and time scales than for other regions. According to our estimates, one of such regions is the region including Russian Far East and Japan.

Thus, a new problem has arisen: to develop a technique for revealing regions of increased ecological hazard and vulnerability by the anthropogenic impact. The technique should be applicable to assessment of both short-term and climatically significant time intervals. The technique is developed based on the variational approach as applied to heat, moisture, and pollutant transport models in a climate system. To construct information subspaces and modeling scenarios, we use the Reanalysis database.<sup>11</sup>

Consider the set of models in the following form:

$$L \mathbf{\phi} = \left\{ \frac{\partial \pi \varphi_i}{\partial t} + \operatorname{div} \pi (\mathbf{u} \varphi_i - \mu_{\varphi_i} \operatorname{grad} \varphi_i) - R_{\varphi_i} - S_{\varphi_i} - S_{\varphi_i} - \varepsilon_{\varphi_i} = 0 \right\}, \ i = \overline{1, na}, \ na \ge 1,$$
(1)

where  $\mathbf{\varphi} = \{\mathbf{\varphi}_i, i = 1, na\}$  is the vector function of the system state. Its components are scalar functions representing potential temperature, characteristics of humidity, and pollutant fields in the atmosphere; *na* is the total number of the state functions. The functions  $R_{\varphi_i}$  describe rates of local transformations of the corresponding substances. They take into account the divergence of radiative heat fluxes for temperature, microphysical processes of moisture transformation for the characteristics of humidity, and the processes of

photochemical and chemical transformation of substances. The functions  $S_{\varphi_i}$  describe sources and sinks of heat and material substances of natural and anthropogenic origin. Additional terms  $\varepsilon_{\varphi_i}$  are introduced in Eq. (1) to take into account possible errors and uncertainties in the corresponding processes. If models and input data are thought exact, these terms are excluded.

The model (1) is written in sigma-coordinates following the terrain on the spherical Earth, spherical coordinates are taken along the horizontal, and a hybrid coordinate with decomposition of a domain into two subdomains<sup>9</sup> is taken along the vertical; **u** is the velocity vector in this coordinate system;  $\pi$  is the pressure-dependent function, which is defined with the allowance made for the domain decomposition along the vertical. Models are closed by the boundary conditions. At the top of an air mass, the conditions are imposed on the substance fluxes; at the bottom, these are the conditions of interaction of a substance with the surface within the models of surface and boundary layers.<sup>9</sup> To formulate the variational principle and organize the modeling system, we specify the set of functionals

$$\Phi_k(\mathbf{\phi}) = \int_{D_t} F_k(\mathbf{\phi}) \,\chi_k(\mathbf{x}, t) \,\mathrm{d}D \,\mathrm{d}t, \ k = \overline{1, nk}, \ nk \ge 1, \quad (2)$$

which are the generalized estimates of the behavior of the processes under study. In Eq. (2),  $F_k(\mathbf{\varphi})$  are the given functions in the space of values of the state functions;  $\mathbf{\varphi} \in Q(D_t)$ ,  $D_t = D \times [0, \bar{t}]$ , where D is the domain of spatial coordinates;  $[0, \bar{t}]$  is the time interval;  $\chi_k(\mathbf{x}, t) \ge 0$  are weighting functions,  $\chi_k(\mathbf{x}, t) \, dD \, dt$  are the corresponding Radon measures in the domain  $D_t$  (Ref. 13). The functions  $F_k(\mathbf{\varphi})$  are assumed differentiable with respect to  $\mathbf{\varphi}$ . They include the values of the state functions calculated with the use of models (1) and obtained experimentally.

As applied to monitoring and climate and ecological estimates, the carrier of every weighting function  $\chi_k$  in Eq. (2) can be interpreted as a regionrecipient of consequences from the effects arising in the climate system and described through the functions  $F_k(\mathbf{\phi})$ . The effects themselves are specified parametrically through the source functions in Eq. (1), as well as through the boundary and initial conditions. Denote the whole set of the input data, parameters, and sources participating in the models (1) and used in modeling scenarios as  $\mathbf{Y} = \{Y_i, i = \overline{1, N}\}$ . Assume that they belong to the domain of permissible values  $Y \in R(D_t).$ 

The main element of the variational principle is description of the models (1) with the integral identity of the following form:

$$I(\mathbf{\phi}, \mathbf{\phi}^{\star}, \mathbf{Y}) \equiv \int_{D_t} (L\mathbf{\phi}, \mathbf{\phi}^{\star}) \, \mathrm{d}D \, \mathrm{d}t = 0, \qquad (3)$$

where  $\mathbf{\phi}$  are arbitrary sufficiently smooth functions from the space  $Q'(D_t)$  conjugate to the space  $Q(D_t)$ . The scalar product in the integrand in Eq. (3) is constructed so that, if the function  $\mathbf{\phi}$  is selected in a certain way, the energy relation for the model (1) follows from the identity (3).

The main sensitivity relation for the set of functionals (2) is drawn within the framework of the variational principle with the help of the algorithm<sup>3</sup>:

$$\begin{split} \delta \Phi_k^n(\mathbf{\phi}) &= (\operatorname{grad}_{\mathbf{Y}} \Phi_k^n(\mathbf{\phi}), \ \delta \mathbf{Y}) \equiv \\ &\equiv \frac{\partial}{\partial \xi} I^h(\mathbf{\phi}, \ \mathbf{\phi}^{\star}, \ \mathbf{Y} + \xi \delta \mathbf{Y}) \big|_{\xi=0}. \end{split}$$
(4)

In its turn, Eq. (4) gives rise to the algorithm for determining the functions of sensitivity  $\operatorname{grad}_{\mathbf{Y}} \Phi_k^h(\boldsymbol{\varphi})$  to variations  $\delta \mathbf{Y}$  of the  $\mathbf{Y}$  vector of parameters. The superscript h is for the discrete analog, and the symbol  $\delta$  denotes variations of the corresponding objects;  $\xi$  is the real parameter.

The functions  $\boldsymbol{\varphi}$  and  $\boldsymbol{\varphi}'$  in Eq. (4) are considered to be preset. They follow from the solution of the basic and conjugate problems at the unperturbed values of the parameters **Y**. These problems, in their turn, follow from the variational principle and, algorithmically, from the conditions of stationarity of the extended functionals<sup>1,3</sup>

$$\tilde{\Phi}_{k}^{h}(\boldsymbol{\varphi}, \, \boldsymbol{\varphi}^{\cdot}, \, \mathbf{Y}) \equiv \{ \Phi_{k}^{h}(\boldsymbol{\varphi}) + I^{h}(\boldsymbol{\varphi}, \, \boldsymbol{\varphi}^{\cdot}, \, \mathbf{Y}) \}$$
(5)

at arbitrary and independent variations of the functions  $\boldsymbol{\varphi}$ and  $\boldsymbol{\varphi}$  at the nodes of the grid domain  $D_t^h$ , respectively.

The sensitivity functions give a new feature when studying direct relations and feedbacks in the system modeled. Their behavior is characterized by the high variability in space and time. However, from the standpoint of the information content, they introduce significant redundancy into the modeling process. At the same time, analysis should be performed together with the state functions. Therefore, to find the sought dependences in this multicomponent set of multidimensional functions, specialized methods are needed. Toward this end, algorithms of sensitivity theory are combined with the methods of factor analysis. Factor algorithms for the considered class of problems are generally described in Ref. 14. The principal role in them belongs to selecting the scalar product for formation of the Gram matrix for the initial set of multicomponent vectors generated by discrete analogs of the models (1), sensitivity relations (4), and databases on the state of the climate system.

If application of the models is considered from the standpoint of factor analysis, then Eq. (3) contains the definition of the scalar product in the space of the state functions and Eq. (4) introduces the scalar product in the space of the sensitivity functions. The sum of these functionals gives the equation for the scalar product in a combination of both these spaces. Upon definition of the scalar products, the algorithms of factor analysis are realized in a standard way according to the scheme described in Ref. 14.

Then the zones of increased hazard and vulnerability are being sought among the main factors, which are found in the behavior of the state functions of the climate system described by archived data, in the behavior of the state functions of the model (1), and sensitivity functions connecting variations of the studied functionals (2) with the variations of sources and input parameters of the model (1).

# Example of the zone of increased ecological vulnerability

To illustrate the possibility of revealing zones of increased ecological vulnerability, we present here an example of numerical simulation on studying the quality of the atmosphere over Japan as a particular region. This example was mentioned above. The computations have been done by E.A. Tsvetova.

In this case, we estimated the functional of the set (2) with the weighting function, whose carrier of nonzero values is specified by the configuration of Japan Archipelago at the surface level. The scenario has been realized with the model of the type (1) in the mode of inverse modeling since March 24 to April 24 of 1999. The functional was estimated in the time interval of April 14–24 of 1999. The atmospheric circulation was reconstructed from the archived data<sup>11</sup> for this time interval with the model of thermohydrodynamics having the time step of 30 min. The 20-layer version of the model in the "hybrid" vertical coordinates was used.<sup>9,12</sup>

Physically, the main idea of the experiment was to estimate the total pollution coming to the near-ground layer over Japan for 10 days (April 14–24 of 1999) from sources situated in the Northern Hemisphere in the period from March 24 to April 24 of 1999. The ecological risk of pollution from every operating or planned source at this territory was estimated simultaneously.

The problem was solved using the variational principle for the estimated functional (2) with restrictions imposed by the mathematical models (1) and (3). The values of the function of sensitivity to variations in the pollution sources at the places of their location give the sought estimates of the risks, i.e., the relative contribution from every source to the total value of the functional (2). Figure 1 shows the function of sensitivity to ground-based sources in relative units according to the scale of values. The configuration of the region and the distribution of the levels of significance are indicative of the high degree of potential hazard for even far, but powerful emission sources. This ecological situation is caused by the fact that the region is situated in the zone of "continent-ocean" contrast where the atmosphere is characterized by a specific structure of circulation. The pessimistic conclusion on the increased ecological vulnerability of the Japan Archipelago can be somewhat smoothed by the note of some positive moment concerning the atmospheric monitoring.



**Fig. 1.** Normalized sensitivity function for assessment of the ecological risk of pollution of the Japan atmosphere from ground-based sources.

From the position of monitoring, the functional (2) is a result of observations, and the sensitivity function gives the information on the information content of observations and the degree of observability of the pollution sources for their identification from observations.<sup>15</sup> Therefore, it follows from analysis of the results that a monitoring system should be placed in this zone. It provides for tracking specific pollutants from sources situated over a vast territory determined by the configuration of the sensitivity function. The higher are the places of the devices deployment, the larger is the observability domain.

## Conclusion

Thus, the proposed technique allows not only revealing climatically and ecologically significant regions, but also planning the arrangement of the monitoring system that is most efficient from the standpoint of the information content and observability of the anthropogenic pollution sources.

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