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SOME ASPECTS OF SOLVING INTERRELATED PROBLEMS OF ECOLOGY AND CLIMATE

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Special features of interrelated problems of ecology and climate are analyzed. The technique proposed for solving this class of problems is demonstrated by an example of evaluating the atmospheric quality and monitoring and predicting the ecological consequences of man's impact. An approach based on variational principles in combination with methods of splitting and decomposition is developed. The structure of algorithms implementing Eulerian and Lagrangian formulations of the problems is described. Examples of simulation scenarios for particular cases are given.

Introduction. Lately, the solution of interrelated problems of ecology and climate has become the subject of integration studies of specialists in various disciplines. This is a new class of problems, and their solution requires new approaches, models, and methods of simulation, and also special observation experiments of a complex character. From the viewpoint of mathematical simulation, the special features of this class of problems are as follows. Mathematical models and observation data should be used together in the regime of direct and inverse relations. Advanced mathematical models of the climatic system and models of transport and transformation of pollutants in the gaseous and aerosol states are rather complicated, because they should take into account both natural and anthropogenic factors that affect the processes considered. A large body of information on the results of contact and remote (both direct and indirect) observations of the characteristics of the environment has been already accumulated and continues to be accumulated in various databases. Therefore, obtaining new results requires a comprehensive methodical, theoretical, and practical work.

Some aspects of application and development of the simulation technique proposed in [1–7] for studying natural processes and evaluating the scales of interaction in the climatic system are considered in this paper. In particular, Penenko and Tsvetova [1] considered formulations of the problems and offered a description of mathematical models for studying the interaction in the system "Lake Baikal–atmosphere of the region." This is a complicated set of models under development. It consists of basic models of hydrothermodynamics and transport of pollutants in the atmosphere and water, transport and transformation of moisture in the atmosphere, heat conduction and moisture exchange in the soil, and also models of interaction of the media at the water–atmosphere and atmosphere–soil interfaces.

We consider a detailed formulation of the problem, since it contains a typical set of models for the class of problems considered. This class has three basic types of hydrothermodynamic and physicochemical processes: 1) transport and turbulent exchange of substances in the atmosphere and water; 2) dynamic adjustment and mutual adaptation of the fields of pressure, temperature, and velocity of air and water masses; 3) transformation of moisture in the atmosphere (water vapor, cloud and rain water, snow and ice crystals) and pollutants in gaseous and aerosol states.

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Discrete analogs of the models and their algorithms are constructed on the basis of the variational principle combined with methods of splitting and decomposition. In accordance with this simulation methodology, all these processes can be considered formally independent at separate stages of splitting within one rather small step of problem discretization in time. The variational principle ensures the agreement of various elements of the complex so that the models at all stages of computations retain the meaning implied in their initial formulations. The solution of the problems is based on the principles of direct and inverse simulation.

It is impossible to give an extensive description of the simulation technique for the whole set of models within one paper. Therefore, we present the ideas and the main constructional elements by an example of the models of transport and transformation of pollutants. These models include a description of the processes of the first and second types and have a relatively independent significance within the complex. It is assumed that the hydrothermodynamic characteristics of the climatic system described by the remaining elements of the complex are known and prescribed as input information for transport models. The notation in the present paper corresponds to that used in [1].

1. Formulation of the Problems of Transport and Transformation of Pollutants. As in [1, 4], a dual description of the models is used in constructing numerical schemes and their algorithms for direct, adjoint, and inverse problems: (1) in the form of systems of differential equations of transport and transformation of multispecies admixtures, and (2) in the variational formulation with the help of an integral identity.

The basic system of equations of the model is written in the following form:

$$(\Lambda\varphi)_i \equiv \frac{\partial \pi\varphi_i}{\partial t} + L(\pi\varphi_i) + (B(\varphi))_i = f_i, \quad i = \overline{1,n}, \quad n \geqslant 1. \tag{1}$$

Here $\varphi = \{\varphi_i(\boldsymbol{x},t), i = \overline{1,n}\} \in Q(D_t)$ is the vector-function of state, φ_i is the concentration of the ith pollutant, n is the number of different substances, $\boldsymbol{f} = \{f_i(\boldsymbol{x},t),\ i = \overline{1,n}\}$ are the source functions, $L(\pi\varphi_i) = \operatorname{div}[\pi(\boldsymbol{u}\varphi_i - \mu \operatorname{grad}\varphi_i)]$ is the advective-diffusive operator, $\boldsymbol{u} = (u_1, u_2, u_3)$ is the velocity vector, $\mu = \{\mu_1, \mu_2, \mu_3\}$ are the coefficients of turbulent transfer in the direction of the coordinates $\boldsymbol{x} = \{x_i, i = \overline{1,3}\}$, $B(\varphi)$ is the nonlinear matrix operator of an algebraic form, which describes the processes of transformation of the pollutants, π is a function of pressure, whose form depends on the chosen coordinate system, $D_t = D \times [0,\bar{t}]$, D is the domain of variation of the spatial coordinates $\boldsymbol{x}$, $[0,\bar{t}]$ is the time interval, and $Q(D_t)$ is the space of the functions of state, which satisfy the conditions at the boundary of the domain D_t. If the model takes into account the formation of aerosols, the operator $B(\varphi)$ contains one more independent variable, the particle size, and this operator becomes integrodifferential with respect to this variable. The transport operator is made antisymmetric using the continuity equation of [4].

If the model implies the presence of errors, the expressions that describe the latter are formally included into the source functions as additional components.

The operators of transformation of the pollutants are described using an automated system for constructing kinetic models of atmospheric chemistry [3].

The variational formulation of the model has the form

$$I(\varphi, \varphi^*, Y) \equiv \int_{D_t} (\Lambda\varphi - \boldsymbol{f})\varphi^* \, dD\, dt = 0, \tag{2}$$

where $\varphi^* \in Q^*(D_t)$ is a function with rather smooth components, $Q^*(D_t)$ is the space of functions adjoint to $Q(D_t)$, $Y = \{Y_i, i = \overline{1,n}\} \in R(D_t)$ is the vector of parameters of the model, and $R(D_t)$ is the region of their admissible values. The integral functional of identity (2) is constructed taking into account the boundary conditions. The integrand in (2) is made symmetric, which automatically (i.e., without additional operations of differentiation and integration) ensures energy balance of functional (2) with the substitution $\varphi^* = \varphi$ [4].

For the purposes of monitoring, predicting, controlling, designing, and constructing algorithms of inverse simulation, we introduce a set of functionals

$$\Phi_k(\varphi) = \int F_k(\varphi)\chi_k(\boldsymbol{x},t)\, dD\, dt, \qquad k = \overline{1,K}, \quad K \geqslant 1, \tag{3}$$

where $F_k(\varphi)$ are the prescribed functions on the set of the functions of state, which are differentiable with respect to φ, $\chi_k \geqslant 0$ are the weight functions, and $\chi_k\, dD\, dt$ are the corresponding Radon or Dirac measures in D_t. Using a functional of the form of (3) and an appropriate choice of the functions $F_k(\varphi)$ and χ_k, we can find generalized estimates of the behavior of the system, ecological restrictions on the quality of the environment, results of observations of various types, purpose control criteria, criteria of the quality of the models, etc. [5, 6].

The domain D is considered in three variants: a sphere, a hemisphere, and a bounded territory on a sphere. The structure of domains, the choice of the coordinate system, the basic notation, the boundary and initial conditions, the functions of state and parameters, the structure of functionals depending on the objectives of investigation, and also the method of constructing the integral identity are described in [1, 4].

Numerical schemes are constructed using identity (2). Within the framework of the method of splitting, the basic element of discretization of the model is constructed on the basis of relations of the following form [8]:

$$\int\limits_{x_{\alpha-1}}^{x_\alpha} (\Lambda_x\varphi - f)\varphi^*\, dx = \int\limits_{x_{\alpha-1}}^{x_\alpha} \Lambda_x^*\varphi^*\varphi\, dx - (A_x\varphi, \varphi^*)\Big|_{x_{\alpha-1}}^{x_\alpha} - \int\limits_{x_{\alpha-1}}^{x_\alpha} f\varphi^*\, dx. \tag{4}$$

Here φ is a component of φ, x is one of the spatial coordinates, Λ_x is the part of the operator Λ in terms of the method of splitting, which acts in the x direction, $[x_{\alpha-1}, x_\alpha]$ is a cell of the grid region along x, $\alpha = \overline{1, M}$, Λ_x^* is the operator adjoint with respect to Λ_x, and $(A_x\varphi, \varphi^*)$ are the relations at the boundaries of the cells along x; the form of the operator A_x is determined by the structure of the operator Λ_x.

The method of discretization depends on the method of setting the functions φ^* in (4). We choose them in such a way that they are the solutions of local adjoint problems

$$\Lambda_x^*\varphi^* = 0, \qquad x_{\alpha-1} \leqslant x \leqslant x_\alpha, \qquad \alpha = \overline{1, M}. \tag{5}$$

The use of this method yields numerical schemes of the variational-difference type. The construction procedure ensures the monotonicity and transportivity of discrete approximations of the transport operator in terms of spatial variables.

For approximation of identity (2) in time, we use the method of weak approximation with fractional steps in time [4]. The operators of transformation of the pollutant are taken into account on an individual fractional step. The discretization yields a summatory analog of the integral identity (2):

$$I^h(\varphi, \varphi^*, \boldsymbol{Y}) = 0, \quad \varphi \in Q^h(D_t^h), \quad \varphi^* \in Q^{*h}(D_t^h), \quad \boldsymbol{Y} \in R^h(D_t^h). \tag{6}$$

The superscript h here indicates a discrete analog of the corresponding objects. In the grid domain D_t^h, we also construct discrete analogs $\Phi_k^h(\varphi)$ of functionals (3).

Numerical schemes and algorithms are obtained from the stationarity conditions of the functionals $\tilde{\Phi}_k^h(\varphi) = \Phi_k^h(\varphi) + I^h(\varphi, \varphi^*, \boldsymbol{Y})$ to variations of the functions φ^* and φ in nodes of the grid domain D_t^h:

$$\frac{\partial I^h(\varphi, \varphi^*, \boldsymbol{Y})}{\partial \varphi^*} = 0, \qquad \varphi^* \in Q^{*h}(D_t^h) \tag{7}$$

for the direct problem and

$$\frac{\partial I^h(\varphi, \varphi_k^*, \boldsymbol{Y})}{\partial \varphi} + \frac{\partial \Phi_k^h}{\partial \varphi} = 0, \quad \varphi \in Q^h(D_t^h), \quad \varphi_k^*(x, \bar{t}) = 0, \quad k = \overline{1, K} \tag{8}$$

for adjoint problems. The operations of differentiation are performed for all grid components of the function of state and adjoint functions.

The relations of sensitivity for the functionals have the form

$$\delta\Phi_k^h(\varphi) \equiv (\operatorname{grad}_{\boldsymbol{Y}}\Phi_k^h(\varphi), \delta\boldsymbol{Y}) = \frac{\partial}{\partial\xi} I^h(\varphi, \varphi_k^*, \boldsymbol{Y} + \xi\delta\boldsymbol{Y})\Big|_{\xi=0}, \quad k = \overline{1, K}, \tag{9}$$

where the symbol δ indicates variations of the corresponding objects, ξ is a real parameter, $\delta\boldsymbol{Y} = \{\delta Y_i, i = \overline{1, N}\}$ is the vector of variations on the parameters $\boldsymbol{Y}$, and $\operatorname{grad}_{\boldsymbol{Y}}\Phi_k^h(\varphi) \equiv \Gamma_k$ are the functions of sensitivity of

the kth functional to variations of the vector of the parameters. Their explicit form is obtained by operations of differentiation of the expression for the summatory functional

$$\Gamma_{ki} = \frac{\partial}{\partial Y_i} I^h(\varphi, \varphi_k^*, \boldsymbol{Y}), \qquad k = \overline{1,K}, \qquad i = \overline{1,N} \tag{10}$$

for all $\boldsymbol{Y} \in R^h(D_t^h)$ with given φ and φ_k^*.

Since the method of weak approximation with fractional steps and decomposition of the domain D into subdomains is used in the approximation of identity (2), the systems of basic equations (7) and adjoint equations (8) are splitting schemes written for subdomains. The construction of these schemes with the use of (6) ensures their mutual agreement. Their special feature is that the transport processes are performed for each substance separately but over the entire domain D_t^h. The processes of transformation of the pollutants are described by a set of "point" models of chemical kinetics for the entire set of substances at each point of the grid independent of other points [3].

It should be noted that adjoint functions are used in two aspects in this technique. First, they are used in the local aspect as solutions of the sets of local adjoint problems (5), which are chosen as weight functions in constructing discrete analogs of the operators in identity (6). Second, they are used in the global aspect as solutions of global adjoint problems (8), which relate functionals (3) to model (1). These functions are also used for deriving the sensitivity relations (9) and sensitivity functions (10).

Inverse problems and methods of inverse simulation are formulated from the conditions of minimization of functionals of the type of (3) in the space of parameters or from the estimates of sensitivity to variations of these parameters. For this purpose, an algorithm of inverse simulation and its modification are constructed [7]. It includes algorithms for solving problems (7)–(10) and implementation of the feedback from the functionals to the parameters, which follow from relations (9) and (10):

$$\frac{dY_\alpha}{dt} = -\eta_\alpha \Gamma_{k\alpha}, \qquad \alpha = \overline{1,N_\alpha}, \qquad N_\alpha \leqslant N. \tag{11}$$

Here η_α are the coefficients of proportionality, which are found in the course of solving the problem and N_α is the number of refined parameters.

Thus, the structure of the main integral identity of the type of (2) for the description of mathematical models being defined, the use of the variational principle yields all the necessary constructional elements for discretization of the mathematical models themselves and methods of their algorithmic implementation and for their practical use. In other words, with the help of the integral identity, the mathematical model is included into the simulation technology developed by us.

Direct problems are used to study the processes of propagation of perturbations from various sources. These are the so-called source–receptor problems. The spatial-time regions in D_t, where perturbations are observed, play the role of zones–receptors. From the viewpoint of ecological safety, inverse problems of the receptor–source type are of interest, since they allow one to determine the degree of the potential danger of contamination of the zone-receptor by pollutants entering it and to identify sources of this danger. Such problems may be solved by methods of inverse simulation with the use of adjoint problems and sensitivity functions. For prescribed functionals, which are estimates of the atmospheric quality in zones–receptors, the schemes of the algorithms are obtained from sensitivity relations.

In constructing numerical schemes for the transport model, the hydrothermodynamic components of the function of state of the atmosphere are assumed to be known and can be prescribed by different methods. In particular, they can be calculated from the models of atmospheric dynamics, which are integrated simultaneously with the transport models. For diagnostic studies, evaluation of information quality of observation systems, and implementation of scenarios of ecological prospects, transport models may be used together with models of the informational type, which generate characteristics of atmospheric circulation on the basis of retrospective hydrometeorological information [9].

2. Trajectories in Source–Receptor and Receptor–Source Problems. The above-considered methods of simulation are based on the Eulerian description of advective-diffusive processes of transport of

substances. In practice, it is often necessary to calculate the propagation of a pollutant in moving air masses in the Lagrangian approach. These two approaches are not alternatives; they supplement each other. Each approach has its own advantages and drawbacks and application areas. We describe the main elements of the algorithm of "grid–free" simulation of the trajectories of pollutant particles assuming that the fields of hydrometeorological parameters of the atmosphere are specified on a certain grid D_t^h in D_t. In accordance with the definition of the problems of direct and inverse simulation, we construct algorithms for calculation of direct and adjoint (inverse) trajectories.

We build the structure of numerical schemes based on the method of splitting in terms of physical processes. We identify three stages of splitting in the domain D_t^h within rather small time intervals Δt:

1) transport along the trajectories of air masses

$$\frac{d\varphi_i}{dt} = 0; \tag{12}$$

2) turbulent exchange

$$\frac{\partial \pi \varphi_i}{\partial t} - \operatorname{div}(\mu \pi \operatorname{grad} \varphi_i) = 0; \tag{13}$$

3) transformation of pollutants

$$\frac{\partial \pi \varphi_i}{\partial t} + (B(\varphi))_i = f_i, \qquad i = \overline{1,n}, \qquad n \geqslant 1. \tag{14}$$

Note that the third stage in the Eulerian approach is the solution of a system of nonlinear ordinary differential equations in time at each point of the spatial grid within one time step. In Lagrangian schemes, the solution of this problem involves considerable difficulties, since a random set of particles of different components of the pollutant can be formed at each point of the trajectory because of the random character of turbulent exchange, and the reconstruction of the transformation operator for these sets brings the problem of predicting the chemical environment outside the limits of the initial formulations. Therefore, we will use Lagrangian schemes of transport simulation only for conservative admixtures (tracers) at the first and second stages of splitting [2].

In considering source–receptor problems, one has to solve direct problems and simulate trajectories originating from the sources in the direction of increasing time either until they reach the zone-receptor or until a prescribed time moment. For receptor–source problems, by analogy with adjoint problems in the Eulerian formulation (8), one has to simulate adjoint trajectories emanating from the zones–receptors in the inverse direction of time. The splitting in the Lagrangian approach is performed along particle trajectories. At the first stage (12), the solution involves integration of the system

$$\frac{dx_i}{dt} = u_i(\boldsymbol{x}, t), \qquad i = \overline{1,3}, \qquad \boldsymbol{x} = (x_1, x_2, x_3) \in D, \qquad t_j \leqslant t \leqslant t_{j+1}, \tag{15}$$

where $u_i(\boldsymbol{x}, t)$ are the transport velocities in the direction of the coordinates x_i; the component u_3 takes into account the rate of gravitational sedimentation of the particles.

To construct the simulation scheme at the second stage (13), local approximation of the operator of the type of "frozen" coefficients is used [10]. Under these assumptions, each local problem allows separation of variables and, hence, Green's function for it may be represented as a product of Green's functions for one-dimensional equations along the coordinate directions. These functions are identical to the probability density of Gaussian random variables with a zero mean value and a standard deviation $\sigma_i = \sqrt{2\Delta t \mu_i}$ $(i = \overline{1,3})$. As in the Eulerian approach (7), (8), we use second-order schemes in time for the Lagrangian variant.

Introduction of random characteristics into the computational algorithm at the stage of taking into account turbulence requires the use of the technique of statistical simulation over ensembles of particles. If turbulent transfer is ignored, it is possible to calculate direct and adjoint trajectories of individual particles.

Thus, the algorithm of transport is a combination of determinate transport over the trajectories of air masses [see (12)] and the Monte Carlo method for taking into account turbulent transfer [see (13)].

Omitting intermediate calculations, we write the schemes of the algorithms [2]:

$$\frac{\Delta x_\alpha^j}{\Delta t} = u_\alpha^j(\boldsymbol{x}, t) + 0.5 \sum_{k=1}^{3} \frac{\partial u_\alpha^j}{\partial x_k} \Delta x_k^j, \qquad \Delta x_\alpha^j = x_\alpha^{j+1/2} - x_\alpha^j, \qquad \alpha = \overline{1,3} \tag{16}$$

$$x_\alpha^{j+1} = x_\alpha^{j+1/2} + \eta_\alpha^{j+1/2}, \qquad j = \overline{1, J-1} \tag{17}$$

for direct trajectories and

$$x_\alpha^{*j+1/2} = x_\alpha^{*j+1} + \eta_\alpha^{*j+1}, \qquad j = \overline{J-1.1}; \tag{18}$$

$$\frac{\Delta x_\alpha^{*j}}{\Delta t} = u_\alpha^{j+1}(x,t) + 0.5 \sum_{k=1}^{3} \frac{\partial u_\alpha^{j+1}}{\partial x_k} \Delta x_k^{*j}, \quad \Delta x_\alpha^{*j} = x_\alpha^{*j} - x_\alpha^{*j+1/2}, \qquad \alpha = \overline{1,3} \tag{19}$$

for adjoint trajectories. Here $\eta_\alpha^{j+1/2}$ and η_α^{*j+1} are the normally distributed random numbers with zero mean values and standard deviations $\sigma_\alpha^{j+1/2}$ and σ_α^{j+1} within the framework of the method of local approximations for problem (13), respectively, the superscript j indicates the time step, and J is the total number of time steps in the interval $[0, \bar{t}]$. Schemes (16) and (19) approximate Eq. (15) with the second order in time. Near the boundaries, formulas (16)–(19) are constructed taking into account the boundary conditions.

Systems (16) and (19) are solved with respect to coordinate increments by the method of elimination. Direct trajectories are calculated as emanating from the region of distribution of pollutant particles at the moment $t = 0$ or from the coordinates of the sources of pollutants.

Adjoint trajectories are simulated as emanating from "protected" territories of interest for the researcher or from the coordinates of location of observation devices for $t = \bar{t}$ in the backward direction in time. As the solution of adjoint problems (8), adjoint trajectories have an informational meaning in terms of the theory of sensitivity. They may be defined as a Lagrangian analog of adjoint problems. They provide information about the prehistory of pollutants entering the "protected" territory or the region of location of observation devices.

3. Two Simulation Scenarios for the Siberian Region. The above-described simulation technique is designed for solving problems of evaluation of the ecological prospects and safety for different variants of man's impact on the climatic system. We give two scenarios of inverse simulation: (1) evaluation of the information quality of the monitoring system and the danger of contamination of the zone-receptor, and (2) calculation of adjoint trajectories for interpretation of the observation results for particular contaminants of the environment. In both cases, we use hemispherical basic models for transport of pollutants in the atmosphere in the hybrid coordinate system described in [1], which is isobaric in the free atmosphere and relief-following in the lower layers of the atmosphere. The first scenario is calculated in the Eulerian formulation, and the second one in the Lagrangian statement. To increase the reliability of calculations, the hydrometeorological situations are reconstructed on the basis of the actual information from the Reanalysis NCEP/NCAR USA database [11] using the system described in [9]. The receptor is a local region near the city of Novosibirsk. Observations are performed here from a flying laboratory aircraft at several horizontal levels up to 7 km. The reference point for formation of the observation functional in the form of (3) has the coordinates 54°23′ N and 82°09′ E and the pressure $p = 700$ mbar. One observation lasts for about 30 minutes.

The calculations were performed during 30 days with a step of 30 min in the inverse direction of time starting at the end of observations. Leaving aside the explanation of the physical essence of the observation experiments, we give two calculation results.

A fragment of the first scenario is depicted in Fig. 1, which shows a two-dimensional section at the level of the Earth's surface for the sensitivity function of the atmospheric quality functional (or the observation functional) in the zone-receptor to variations of the power of sources of pollution located at the Earth's surface. The sensitivity is given in relative units in accordance with the scale in Fig. 1, which shows the weight contribution of each source located in this region to the variation of the quality functional. From the viewpoint of monitoring, the sensitivity function characterizes the observability of the sources from the zone-receptor for determining their power and location.

Figure 2 shows a fragment of the second scenario. There are 11 adjoint trajectories originating at the zone-receptor. Their behavior characterizes the prehistory of the air masses that bring pollutants to

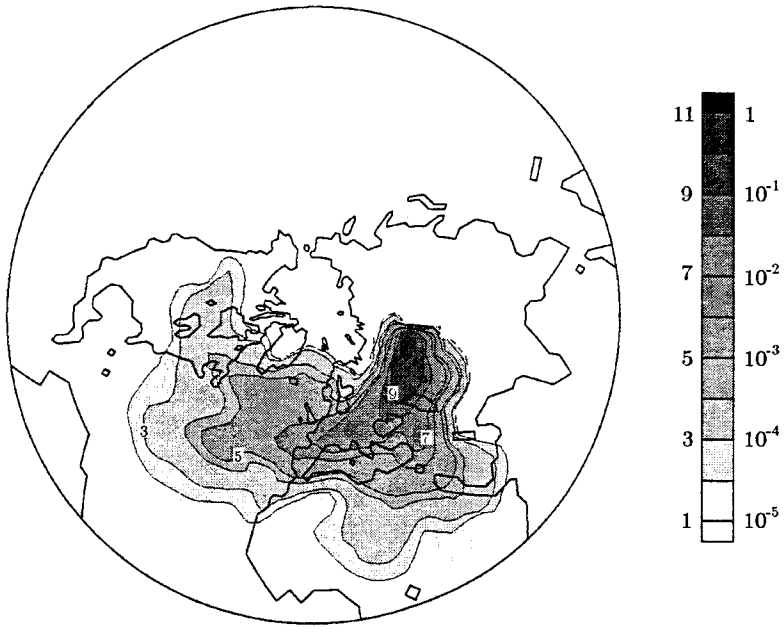

Fig. 1. Sensitivity function (two-dimensional section at the height of the Earth's surface relief) of the atmospheric quality functional in the zone-receptor to variations of the source of pollutants located on the Earth's surface.

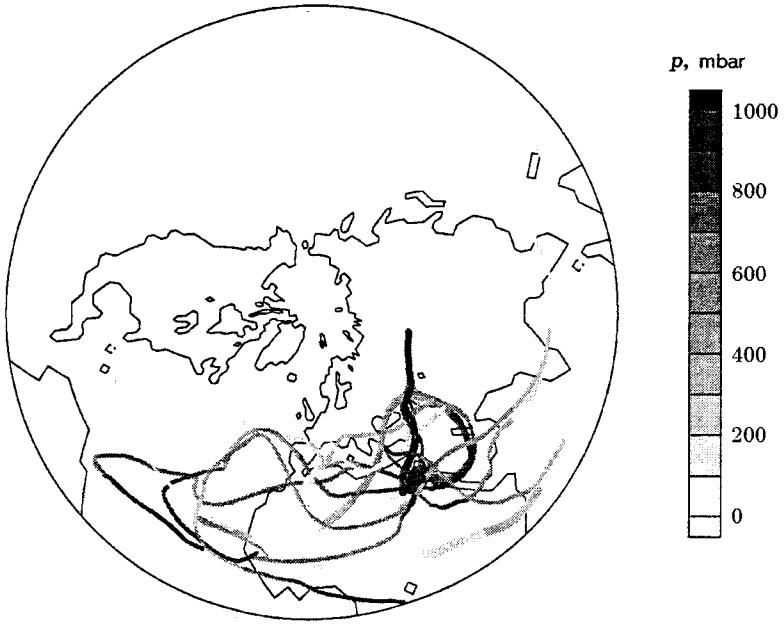

Fig. 2. Adjoint trajectories for studying the prehistory of transport of air masses and pollutants to the zone-receptor.

the region examined. The scale is the altitude in isobaric coordinates. The pattern plotted in Fig. 2 is a complicated spatial-time structure in which different parts of trajectories are located at different altitudes in accordance with the motion of air masses.

An analysis of calculation results for both scenarios shows that they supplement each other in the informational aspect, characterizing the results of observation experiments and the process of formation of the quality of the atmosphere in the zone-receptor depending on ecological and hydrothermodynamic situations in the local environment. This allows us to draw certain conclusions concerning the direction wherefrom the adverse action should be expected and the scale of this action. Actually, the scenarios trace the processes that develop for a month before the observations from the viewpoint of their potential danger for a chosen territory.

Conclusions. The methodology of solving interrelated problems of ecology and climate is actively developed, and the development is directed to extension of both informational and physical contents of the basic models and methods of their implementation and practical applications. The approach described in the present paper, which is based on the principles of direct and inverse simulation, extends the capabilities of the multifunctional set of models created by us for diagnosing and predicting the processes in the climatic system and for planning and evaluating the information quality of observations. The chosen methods for constructing discrete approximations and algorithms take into account the difference in spatial-time scales of the examined phenomena and ensure the optimal use of actual information.

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