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MATHEMATICAL MODELS FOR THE STUDY OF INTERACTIONS IN THE SYSTEM LAKE BAIKAL–ATMOSPHERE OF THE REGION

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The structure of mathematical models for studying the processes of thermodynamics and transfer of pollutants in a climatic system involving the atmosphere of an industrial region and a lake is presented. These models are used to solve the problems of climatic and ecological monitoring and prediction. The problems of constructing numerical schemes and simulation methods are discussed. An example for estimating the effect of pollutants from sources located in the northern hemisphere of the Earth on the Baikal region is given.

Introduction. Mathematical models have become a multifunctional tool for studying processes in the atmosphere and water objects. In particular, for solving the problems of evaluation of the prospects of industrial regions with anthropogenic actions imposed on natural climatic and ecological factors, mathematical simulation is, apparently, the only means for obtaining information.

The immediate effect of anthropogenic loads is primarily manifested in regions of local and mesoregional scales; therefore, it is important to study the possible preconditions for the appearance of ecologically unfavorable situations in each region that are caused mainly by its climatic conditions. From the viewpoint of monitoring and climatic-ecological prediction, Siberian industrial regions are not only interesting but also strategically important objects of investigation since their activity is mainly connected with raw materials.

The Baikal region plays a specific role in the formation of climatic conditions and ecological environment in the south of Siberia. Taking into account this circumstance, we chose this region as a basic object for the development and application of ecologic-climatic models. The specific feature of the Baikal region is that Lake Baikal is a powerful climate-forming factor in the south of Siberia. The importance of this factor is amplified by the fact that this region is in the influence zone of the summer Sayan–Altai cyclogenesis and the winter Asian anticyclone. The interaction of background and local atmospheric processes forms unique "Baikal" mesoclimates, which, in turn, have a determining effect on the formation of mesoclimates and the quality of atmosphere in industrial zones of this region. The contrast of water–land temperatures, which is always observed in the open-water period, is a source of instability in the climatic system and leads to the fact that the zone of immediate influence of Lake Baikal, which was preliminarily estimated as 100–200 km from the coast line [1], becomes a potential accumulator of pollution not only from the territory of the region, but also from other territories of the northern hemisphere: Siberia, China, and Mongolia. All these processes should be studied to understand the ecological prospects of the region and the lake.

Thus, forming a concept of studying climatic changes in the system lake–atmosphere, we do not confine ourselves to the scale of direct interaction of water and atmosphere, but consider mesoregional processes together with hemispherical phenomena, and do not separate the hydrothermodynamics of the system from the processes of transportation of hazardous pollutants. This is necessary to evaluate the role of transboundary transfer and external processes and sources for the region. Hemispherical models give a correlated description of the processes in the lake and in the atmosphere of the region, which have the corresponding characteristic time scales.

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This work continues the studies performed by the Provisional scientific group on the task of the Presidium of the Siberian Division of the USSR Academy of Sciences for evaluating the anthropogenic effect on the lake and surrounding region [1]. The present work is conceptually a continuation of the research cycle [2–10].

It should be noted that the first principal discussion of the problems of mathematical simulation as applied to the problems of investigation and defense of Lake Baikal took place in August 1967 at the "Baikal" Workshop with participation of the leading scientists of the USSR Academy of Sciences. At this Workshop, L. V. Ovsyannikov formulated for the first time the fundamental theoretical principles of the mathematical model of the lake as a model of dynamic convection of variable-density water in bounded water reservoirs such as seas or deep lakes [11].

Structure of the Domains and Coordinate Systems. First, we describe the domains and coordinate systems for the basic models. In the horizontal directions, we use a universal coordinate system (x, y) with parametrically specified scale factors m and n, which can be used to obtain spherical, polar, Cartesian coordinates, or coordinates of cartographic projections depending on the purpose of investigation. For atmospheric models, we consider two types of domains: the northern hemisphere and the limited areas of the region. The region occupied by the lake is described parametrically in a chosen system of horizontal coordinates.

For the vertical description of the models, we use the principle of decomposition into domains and conventionally divide the atmosphere into two layers: the free atmosphere D_1 ($p_T \leqslant p \leqslant p_B$) and the boundary layer D_2 ($p_B \leqslant p \leqslant p_s$), where p is the pressure and $p_s = p_s(\boldsymbol{x}, t)$, p_T, and p_B are the pressures on the Earth surface, the upper boundary of the atmosphere, and the interface between the layers $[\boldsymbol{x} = (x, y)]$. We introduce the following hybrid coordinate system, which allows one to combine the advantages of realization of the models in isobaric coordinates in the free atmosphere (in the case of constant p_T and p_B) and the conveniences of the σ-coordinates following the Earth relief:

$$\text{in } D_1\text{:} \quad \sigma = (p - p_T)/\pi_1, \qquad \text{in } D_2\text{:} \quad \sigma = (p - p_B)/\pi_2 + \epsilon, \quad 0 \leqslant \epsilon \leqslant 1; \tag{1}$$

$$\pi_1 = (p_B - p_T)/\epsilon, \quad \pi_2 = (p_s - p_B)/(1 - \epsilon). \tag{2}$$

The parameter ϵ is introduced so that the surface $\sigma = \epsilon$ is higher than the level of the "model" relief of the Earth surface. In accordance with the definition of (1) and (2), we write the following relations for the vertical velocities $\omega = dp/dt$ and $\dot{\sigma} = d\sigma/dt$ in the domains D_{it} ($i = 1, 2$) and the boundary conditions for them:

$$\omega = \frac{d_s \chi_i}{dt} + \pi_i \dot{\sigma}, \quad \frac{d_s}{dt} = \frac{\partial}{\partial t} + mu\frac{\partial}{\partial x} + nv\frac{\partial}{\partial y}, \quad \frac{d}{dt} = \frac{d_s}{dt} + \dot{\sigma}\frac{\partial}{\partial \sigma}; \tag{3}$$

$$\chi_1 = \sigma\pi_1 + p_T, \quad \chi_2 = (\sigma - \epsilon)\pi_2 + p_B, \quad \dot{\sigma} = 0 \quad \text{for} \quad \sigma = 0 \quad \text{and} \quad \sigma = 1; \tag{4}$$

$$\omega\Big|_{\epsilon^-} = \omega\Big|_{\epsilon^+}, \qquad \pi_1\dot{\sigma}\Big|_{\epsilon^-} = \pi_2\dot{\sigma}\Big|_{\epsilon^+} \quad \text{for} \quad \sigma = \epsilon. \tag{5}$$

We define the models in the time–space domain $D_t \equiv D \times [0, t_k]$, where $[0, t_k]$ is the range of variation of the time t and $D = \bigcup_{i=1}^{4} D_i$ is the range of variation of the spatial coordinates: $D_1 = S \times [0 \leqslant \sigma \leqslant \epsilon]$, $D_2 = S \times [\epsilon \leqslant \sigma \leqslant 1]$, $D_1 \cup D_2 = D_a$, $D_3 = \{\boldsymbol{x} \subset S_c, 0 \leqslant z \leqslant h_c(\boldsymbol{x})\}$, and $D_4 = \{\boldsymbol{x} \subset S_b, 0 \leqslant z \leqslant h_w(\boldsymbol{x})\}$, where $S = \{0 \leqslant a \leqslant x \leqslant b \leqslant 2\pi, 0 \leqslant c \leqslant y \leqslant d \leqslant \pi\}$. Here S is the region on the Earth surface, a, b, c, and d are the parameters that determine the horizontal size of the region S ($S = S_c \cup S_b$, where S_c and S_b are the areas of the regions occupied by land and water), and $h_c(\boldsymbol{x})$ and $h_w(\boldsymbol{x})$ are functions that describe the depth of the active layer of the soil and the bottom relief of the water object, respectively. The z axis is directed downward. The lateral boundaries of the domains D_i are denoted by Ω_i and their overall boundaries in the three-dimensional space are denoted by $\bar{\Omega}_i$. The subscript t indicates everywhere the variation in time.

The state functions are denoted by $\varphi = \{\varphi_i, i = \overline{1, r}\} \in Q(D_t)$, where $Q(D_t)$ is the corresponding functional space on D_t, φ_i are the components of the vector-function of state, and r is the number of components. The structure of these objects and their properties are determined by the functional content of the basic models. The space of conjugate functions $\{\varphi^* \in Q^*(D_t)\}$ is constructed in a similar manner.

In the domain D_t, we introduce the following scalar product for the state functions:

$$(\varphi_1, \varphi_2) = \sum_{k=1}^{4} \int_{D_{kt}} \Big(\sum_{i=1}^{r} \varphi_{1i}\varphi_{2i}æ_i\Big)\gamma_k \, dD_k \, dt. \tag{6}$$

Here $dD_k = dz_k\, dx\, dy/(mn)$, $dz_1 = dz_2 \equiv d\sigma$, $dz_3 = dz_4 \equiv dz$, $\gamma_1 = \pi_1$, $\gamma_2 = \pi_2$, $\gamma_3 = \rho_n$, and $\gamma_4 = \rho_0$ (γ_k are the map scale factors in decomposed domains); ρ_n and ρ_0 are the densities of soil and water, respectively. The dimensional factors $æ_i$ are chosen with account of the physical meaning of the corresponding components, and γ_k ($k = \overline{1, 4}$) are chosen depending on the coordinate system and the method of decomposition of the domain D_t into subdomains D_{kt}.

Basic Models of the Atmosphere and the Lake. The complex contains the models of several system levels. The first basic level is formed by the models that describe the processes in the climatic system and its parts. These are the models of hydrothermodynamics and transfer of pollutants in the atmosphere and water, and also the processes of direct interaction of various media. The second system layer is formed by the models for solving optimization problems of controlling, planning, and ecological design using the basic-level models. The study of atmospheric processes requires models of three types, which differ in time–space scales of the processes and in dimensions of the domains:

(A1) The model with characteristic horizontal scales of about 100 km for studying mesoclimates of industrial regions and cities;

(A2) The mesoregional model with a characteristic horizontal scale of 100–1000 km;

(A3) The model of the atmosphere for the northern hemisphere designed to study the long-term interaction between the lake and the atmosphere.

In the vertical direction, the model A1 operates mainly in the domain D_{2t}, whereas the models A2 and A3 work in the domain $D_{at} = D_{1t} \cup D_{2t}$ in the regime of decomposition.

For the lake, we use models of two types:

(B1) The model of global circulation of the lake;

(B2) The models for parts of the lake and local regions.

These models have identical structure but different boundary conditions and space–time resolutions of discrete approximations. The models of direct interaction of the atmosphere and the lake are organized on the basis of the models A2 and B1.

Hydrodynamics of Atmospheric Processes. The governing equations of the model are written with regard for decomposition of the domain D_{at} relative to the vertical coordinate into D_{it} ($i = 1, 2$):

$$\frac{du}{dt} - lv + m\Big[\frac{\partial \Phi}{\partial x} - \frac{1}{\pi_i}\frac{\partial \Phi}{\partial \sigma}\frac{\partial \chi_i}{\partial x}\Big] - F_u = 0; \tag{7}$$

$$\frac{dv}{dt} + lu + n\Big[\frac{\partial \Phi}{\partial y} - \frac{1}{\pi_i}\frac{\partial \Phi}{\partial \sigma}\frac{\partial \chi_i}{\partial y}\Big] - F_v = 0; \tag{8}$$

$$\frac{\partial \Phi}{\partial \sigma} + \frac{RT\pi_i}{\chi_i} = 0; \tag{9}$$

$$\frac{dT}{dt} - \omega A_i - F_T = Q_T, \quad A_i = -\frac{1}{c_{pm}\pi_i}\frac{\partial \Phi}{\partial \sigma} = \frac{RT\pi_i}{\chi_i c_{pm}}; \tag{10}$$

$$\frac{\partial \pi_i}{\partial t} + L(\pi_i) = 0. \tag{11}$$

Here u and v are the components of the velocity vector $\boldsymbol{u}$ in the x and y directions, respectively; l is the Coriolis parameter, Φ is the geopotential, R is the universal gas constant, T is the virtual temperature, Q_T is the source of heat, and c_{pm} is the specific heat at constant pressure for moist air. The operator of the transfer of substances η over the trajectories of air particles in a divergent form is

$$L(\pi_i\eta) = mn\Big[\frac{\partial}{\partial x}\Big(\frac{\pi_i\eta u}{n}\Big) + \frac{\partial}{\partial y}\Big(\frac{\pi_i\eta v}{m}\Big)\Big] + \frac{\partial \pi_i\eta\dot{\sigma}}{\partial \sigma}, \tag{12}$$

and the operators of turbulent exchange $F_\eta \equiv F_\eta^s + F_\eta^v$ are

$$F_\eta^s = \frac{mn}{\gamma_i}\Big[\frac{\partial}{\partial x}\Big(\frac{\gamma_i \mu_{\eta x}}{n}\frac{\partial \eta}{\partial x}\Big) + \frac{\partial}{\partial y}\Big(\frac{\gamma_i \mu_{\eta y}}{m}\frac{\partial \eta}{\partial y}\Big)\Big], \qquad F_\eta^v = \frac{1}{\gamma_i}\frac{\partial}{\partial \sigma}\Big(\gamma_i \nu_\eta \frac{\partial \eta}{\partial \sigma}\Big). \tag{13}$$

For $\sigma = 1$, we have $\Phi = \Phi_s \equiv gZ_s$, where g is the acceleration of gravity and Z_s is a function that describes the Earth surface relief. In addition to conditions (3) and (4) at the upper boundary, we assume the absence of turbulent fluxes of the substances to close the models. At the lower boundary we prescribe parametric values of the heat flux and momentum, and the heat balance equation on the Earth surface. The conditions of approaching the background values are set at the lateral boundaries of the limited area, and the conditions of periodicity are set for the sphere.

Transport and Transformation of Moisture in the Atmosphere. The lake serves as a powerful accumulator and a source of moisture and heat for the atmosphere. In turn, strong winds induce significant spatial reconstructions in the flow fields and water temperature. As a result of interaction between the lake and the atmosphere, the signs of the temperature contrasts water–air–land are subjected to seasonal and daily changes; therefore, it is very important to study the character of the energy and mass exchange processes in the system atmosphere–lake in different situations and to trace the feedback from the atmosphere to the lake and alleviation of the consequences of intense actions. This study requires a rather exact reproduction of the hydrological cycle in the atmosphere. The influence of moisture should be also taken into account in the equations of heat transfer in the atmosphere and the heat balance on the underlying surface when calculating radiative heat fluxes and the speed of elimination of pollutants from the atmosphere.

We determine the components of the state function φ, which take part in the models of the hydrological cycle. We denote them by $\boldsymbol{q} = \{q_k,\ k = \overline{1,6}\} \equiv \{q_v, q_c, q_r, q_{ic}, q_s, q_g\}$, where q_k are the mixing ratios for water vapor q_v, cloud water q_c, rain water q_r, cloud ice q_{ic}, snow q_s, and ice crystals q_g.

As a basic model, we take the model with the first three components of the hydrological cycle, i.e., q_v, q_c, and q_r:

$$\frac{\partial \pi_i q_k}{\partial t} + \tilde{L}(\pi_i q_k) - R_{qk} - Q_{qk} = 0. \tag{14}$$

Here $k = \overline{1,3}$, $i = 1, 2$, R_{qk} are the rates of variation of q_k due to microphysical processes of moisture transformation, Q_{qk} are functions that describe the sources, and $\tilde{L}(\pi_i q_k)$ is the advective-diffuse operator

$$\tilde{L}(\pi_i q_k) = L(\pi_i q_k) - \pi_i F_{qk} + \pi_i DF_{qk}, \tag{15}$$

where $DF_{qk} = g\partial(\rho\omega_T q_k q_3)/\pi_i \partial\sigma$ is the diffusion flux for the components of moist air, which is caused by the relative motion of moist air relative to dry air, ω_T is the mean velocity of rain drops, and the first two expressions have the form of (12) and (13).

To close the model, we assume the absence of fluxes at the upper boundary, and a flux of water vapor is prescribed at the lower boundary depending on the "moisture capability" of various portions of the Earth surface. This model is applicable to situations with a hydrological cycle including warm rain water. To describe the processes with low temperatures related to the formation of snow and ice, the basic model is supplemented by additional equations for the account of transfer and transformation of the corresponding components [12].

Transport of Pollutants in the Atmosphere. The complex contains various modifications of the models with account of the specific features of the objects of investigation. Formally, the basic equations have the same structure as the model of moisture transfer (14) and (15) [3, 9]:

$$\frac{\partial \pi_i c_k}{\partial t} + \tilde{L}(\pi_i c_k) - R_{ck} - Q_{ck} = 0. \tag{16}$$

Here $i = 1$ and 2, c_k are the concentrations of pollutants, $k = \overline{1, n_a}$, where n_a is the number of different substances, R_{ck} are the speed of changing concentrations c_k because of chemical transformation of the pollutants, and Q_{ck} are the sources of pollutants. Gaseous and aerosol substances are considered. The advective-diffusion operator $\tilde{L}$ is determined by an expression of the form (15) in which the velocity of gravitational deposition of particles is added to the vertical velocity $\dot{\sigma}$. In contrast to [3, 9], this model takes into account the diffusion flux of pollutants with rain water. The boundary conditions at the upper boundary are prescribed fluxes of pollutants, and the background concentrations are set at the lateral boundaries. At the lower boundary, we use the equation of balance of pollutants for different land-use categories with account of dry and moist deposition of particles, turbulent flow, aerodynamic lifting of particles from the Earth surface, and the sources of admixtures of natural and anthropogenic origin.

Hydrothermodynamics and Transport of Pollutants in Lake Baikal. The governing equations of the models are

$$\frac{du}{dt} - lv + \frac{m}{\rho_0}\frac{\partial p}{\partial x} - F_u = 0; \tag{17}$$

$$\frac{dv}{dt} + lu + \frac{n}{\rho_0}\frac{\partial p}{\partial y} - F_v = 0; \tag{18}$$

$$\alpha\left(\frac{dw}{dt} - F_w\right) + \frac{1}{\rho_0}\left(\frac{\partial p}{\partial z} + g\rho\right) = 0; \tag{19}$$

$$\frac{\alpha}{\rho_0}\frac{\partial \rho}{\partial t} + \frac{mn}{\rho_0}\left[\frac{\partial}{\partial x}\left(\frac{\rho_0 u}{n}\right) + \frac{\partial}{\partial y}\left(\frac{\rho_0 v}{m}\right)\right] + \frac{1}{\rho_0}\frac{\partial \rho w}{\partial z} = 0; \tag{20}$$

$$\frac{d\eta_k}{dt} - F_{\eta k} - Q_{\eta k} = 0, \qquad k = \overline{1, 2 + n_w}; \tag{21}$$

$$\rho = \rho(p, T, S_l). \tag{22}$$

Here $\{\eta_k\} = \{T, S_l, c_i, i = \overline{1, n_w}\}$, T is the temperature, S_l is the salinity, c_i are the concentrations of pollutants in water, n_w is the number of pollutants, u, v, and w are the components of the velocity vector $\boldsymbol{u}$ in the x, y, and z directions, respectively, p is the pressure, $\rho = \rho_0 + \rho'$ is the density, ρ_0 is the prescribed distribution of the relative density, $Q_{\eta k}$ are the sources of heat, salt, and pollutants, and α is a parameter determining the structure of the model (for example, for the hydrostatic model $\alpha = 0$). The operators of transport and turbulent exchange are determined by expressions of the form (12) and (13) in the coordinate system adopted in the domain D_{4t}. In addition, the function w in the equations of pollutant transport takes into account the velocities of gravitational deposition of buoyancy of the pollutants. The following conditions are prescribed at the free surface $z = \zeta$, which is the interface water–air:

$$\nu\rho_0\frac{\partial u}{\partial z} = -\tau_x, \qquad \nu\rho_0\frac{\partial v}{\partial z} = -\tau_y, \qquad \nu_\eta\rho_0 c_p\frac{\partial \eta_k}{\partial z} = -H^s_{\eta k}; \tag{23}$$

$$w = \frac{d_s\zeta}{dt}, \qquad p = p_s. \tag{24}$$

At the bottom for $z = h_w(x,y)$, we have $u = 0$, $v = 0$, $w = 0$, and $\partial\eta_k/\partial N = H^N_{\eta k}$; at the solid lateral boundaries, we have $u = 0$, $v = 0$, and $\partial\eta_k/\partial N = H^N_{\eta k}$; at river inlets, we have $u = u_{\text{riv}}$, $v = v_{\text{riv}}$, and $\partial\eta_k/\partial N = U_{\text{riv}}(\eta_k - (\eta_k\rho)_{\text{riv}}/\rho)$; in the mouths of outflow rivers, we have $u = u_{\text{riv}}$, $v = v_{\text{riv}}$, and $\partial\eta_k/\partial N = 0$. Here τ_x and τ_y are the components of wind stress on the surface, $H^s_{\eta k}$ and $H^N_{\eta k}$ are the fluxes of heat, salt, and admixtures at the interface and solid boundaries, c_p is the heat capacity of water at constant pressure, the subscript riv denotes functions that refer to rivers, and $\partial/\partial N$ is the co-normal derivative. In solving the problems for parts of the lake, conditions exist for the functions of state to reach their background values on the side of "free water."

Parametrization of Turbulent Exchange. The basic variants of the models of the atmosphere and water are supplemented by operators of turbulent exchange of the form (13) with second-order partial derivatives. The coefficients of turbulent exchange in the horizontal directions μ_x and μ_y are calculated using a nonlinear parametrization scheme similar to [3] with account of the horizontal deformation of the velocity field, stratification of the atmosphere and water, and the characteristics of the cell size of the grid domains.

Depending on particular situation, one of two schemes is used to calculate the vertical coefficients of turbulence. The first scheme is simplified: the coefficient is calculated as a function of the local Richardson number and the characteristic vertical scale of vortices. This scheme is convenient and effective in application, but it does not possess "memory" in passing from one space–time cell to another. This drawback becomes significant in the case of sudden reconstruction of the fields.

The second scheme is based on the solution of two equations for the kinetic energy of turbulence E and dissipation ε in the atmosphere and water [13, 14]. The (E–ε)-equations for the atmosphere and water are joined under the assumption of continuity of the energy fluxes and dissipation at the interface between the media.

Heat Budget on the Surface. To close and unite the models for different media at the interfaces atmosphere–water–land, we can write the equation of heat budget

$$c_{pm}\rho_a\frac{\partial T}{\partial t} = R_n - H_m - H_s - L_vE_s, \tag{25}$$

where R_n is the net radiation on the surface, H_m is the heat flow into the substrate or the turbulent heat flux in water, H_s and L_vE_s are the fluxes of perceptible and latent heat to the atmosphere, L_v is the latent heat of vaporization, $H_s = \rho_a c_{pm}C_uC_\Theta(T_s - T_\Theta)V$, $E_s = \rho_aC_uC_\Theta M(q_{vs}(T_s) - q_{va})V$, C_u and C_Θ are the exchange coefficients, T_s is the surface temperature, $V = (v_a^2 + v_c^2)^{1/2}$ (v_c is the convective velocity), ρ_a, v_a, T_a, and q_{va} are the values of meteor elements at the first level of calculation, and $q_{vs}(T_s)$ is the saturation mixing ratio of water vapor on the surface at the temperature T_s. The exchange coefficients and the fluxes in Eqs. (23) are calculated using the parametrization models of the ground layer with account of atmosphere stratification and the properties of the underlying surface. The net radiation is the sum of the long-wave and short-wave radiation. Based on the requirements of efficiency of model application, the value of R_n is calculated in two variants depending on the state of the atmosphere: for "clear sky" without regard for clouds and for cloudy sky. In both cases, account is taken of the influence of pollutants on the radiation balance on the surface.

The vertical distribution of heat addition in the atmosphere is modeled with account of solar radiation and realization of latent heat due to phase transformations of moisture. The model for calculation of radiation heat fluxes is based on the system of radiation transfer equations in Eddington's two-flux approximation [15]. The structure of a radiative block is described in detail [10].

Variational Formulation of the Models. We determine the basic functional identity, which is a variational formulation of the atmospheric model (7)–(16):

$$\begin{aligned}
I_a(\varphi,\varphi^*) = \sum_{i=1}^{2}\Big\{\int_{D_{it}}\Big[\Big(\frac{du}{dt} - F_u\Big)u^* + \Big(\frac{dv}{dt} - F_v\Big)v^* + c_{pm}\Big(\frac{dT}{dt} - F_T\Big)T^* + l(u^*v - v^*u)\\
+(\boldsymbol{u}^*\mathrm{grad}\Phi - \boldsymbol{u}\,\mathrm{grad}\,\Phi^*) - \frac{1}{\gamma_i}\frac{\partial\Phi}{\partial\sigma}\Big(\frac{d_s^*\chi_i}{dt} - T^*\frac{d_s\chi_i}{dt}\Big) - \frac{\partial\Phi}{\partial\sigma}(T^*\dot\sigma - \dot\sigma^*) - c_pQ_TT^*\\
+\frac{1}{\pi_i}\Big(\frac{\partial\Phi}{\partial\sigma} + \Phi^*\Big)\frac{\partial\pi_i}{\partial t} + \sum_{j=1}^{3+n_a}\frac{1}{\gamma_i}\Big(\frac{\partial\pi_i\phi_j}{\partial t} + \tilde L(\pi_i\phi_j) - R_{\phi j} - Q_{\phi j}\Big)\phi_j^*\ae_j\Big]\gamma_i dD_i dt\\
+\int_{\Omega_{it}} u_n\Phi^*\,d\Omega_i\,dt\Big\} + \int_{D_{1t}}\frac{\partial\Phi}{\partial\sigma}\frac{\partial p_T}{\partial t}\,dD_1\,dt + \int_{D_{2t}}\frac{\partial\Phi}{\partial\sigma}\frac{\partial}{\partial t}(p_B - \epsilon\pi_2)\,dD_2\,dt = 0,
\end{aligned} \tag{26}$$

where $\varphi = (u, v, \dot\sigma, T, \Phi, \phi_j)$; $\varphi^* = (u^*, v^*, \dot\sigma^*, T^*, \Phi^*, \phi_j^*)$; $\{\phi_j\} \equiv \{q_k, k = \overline{1,3}, c_i, i = \overline{1, n_a}\}$; u_n is the normal component of the velocity vector $\boldsymbol{u}$ to the domain boundaries,

$$\frac{d_s^*\chi}{dt} \equiv \frac{\partial\chi}{\partial t} + mu^*\frac{\partial\chi}{\partial x} + nv^*\frac{\partial\chi}{\partial y},$$

and φ^* are vector-functions with arbitrary, sufficiently smooth components, which belong to the space $Q^*(D_t)$.

The integral identity for the lake models (17)–(24) has the form

$$I_w(\varphi,\varphi^*) = \int_{D_{4t}}\Big\{\Big(\frac{du}{dt} - F_u\Big)u^* + \Big(\frac{dv}{dt} - F_v\Big)v^* + \alpha\Big(\frac{dw}{dt} - F_w\Big)w^* + \frac{\alpha}{\gamma_4}\frac{\partial\rho}{\partial t}p^*$$

$$+l(u^*v - v^*u) + \frac{1}{\gamma_4}[(\boldsymbol{u}^*\operatorname{grad} p - \boldsymbol{u}\,\rho \operatorname{grad} p^*) + g\rho w^*]$$

$$+ \sum_{j=1}^{2+n_w} \Big(\frac{d\phi_j}{dt} - F_{\phi j} - Q_{\phi j}\Big)\phi_j^* \text{æ}_j\Big\}\gamma_4 dD_4 dt + \int_{\Omega_{4t}} \rho u_n p^* d\bar{\Omega}_4\, dt = 0, \tag{27}$$

where $\varphi = (u, v, w, p, \phi_j)$, $\varphi^* = (u^*, v^*, w^*, p^*, \phi_j^*)$, $\{\phi_j\} \equiv \{T, S, c_i, i = \overline{1, n_w}\}$, u_n is the normal component of the velocity vector to the boundary $\bar{\Omega}$ of the domain D_{4t}, and $d\bar{\Omega}_i = \{dx\,dy/(mn), dy\,dz_i/n, dx\,dz_i/m\}$ $(i = \overline{1, 4})$.

The integral identity for the heat-transfer model in the soil is

$$I_n(T, T^*) = \int_{D_{3t}} \Big(\frac{\partial T}{\partial t} - F_T^n\Big) T^* \text{æ}\gamma_3\, dD_3\, dt. \tag{28}$$

The operator F_T^n describes the heat-transfer processes in the soil, and its structure is similar to (13) with a scale factor γ_3. The structure of the functionals in (26)–(28) is chosen in accordance with the scalar product (6) and the balance equation for the total energy of the system.

For the system as a whole we obtain

$$I(\varphi, \varphi^*) = I_a(\varphi, \varphi^*) + I_w(\varphi, \varphi^*) + I_n(\varphi, \varphi^*) = 0. \tag{29}$$

All the closure conditions are taken into account and controlled through the integrals over the boundaries of the corresponding domains. The models of direct interaction of the media enter identity (29) through the integrals over the inner interfaces. Particular representations of the models are obtained after the transformation using integration by parts of expressions containing the operators of transport and turbulent exchange under the assumption of continuity of the corresponding components of the function φ^* and the fluxes of the state functions across the interfaces. Collecting all integrals over the surface S_t for $\sigma = 1$ with account of the equations of heat balance (25) and admixtures on this surface, we obtain the relations for the fluxes at the interfaces atmosphere–water and atmosphere–soil. Similarly, from the integrals over the boundary Ω_3 between the domains D_3 and D_4 we obtain the conditions of interaction between the lake and the land.

Functionals for Design and Control Problems. Based on the research objectives, identities (26)–(29) are supplemented by the functionals on $Q(D_t)$ differentiated with respect to φ, and a number of adjoint and optimization problems are formulated for them [4, 6].

The functionals are determined as

$$\Phi_k(\varphi) = \int_{D_t} F_k(\varphi)\chi_k(\boldsymbol{x}, t) dD dt, \tag{30}$$

where $F_k(\varphi)$ are certain prescribed differentiated functions of φ, $\chi_k(\boldsymbol{x}, t)$ are non-negative weight functions defined in D_t or on a discrete set of points $D_t^m \subset D_t$ containing at least one point, and $\chi_k(\boldsymbol{x}, t)dDdt$ are the corresponding Radon or Dirac measures in D_t. We can classify functionals of the following types: generalized description of the system behavior, quality (they characterize the deviations between the calculated and measured values of the state functions), observations, constraints on the functions of state, and objective functionals (for formulating optimization problems of planning, control, and ecological design). The formal structure of all these functionals is described by expressions of the form (30) setting the corresponding functions F_k and χ_k and measures in the domain D_t. Using identities, discrete analogs of the basic and adjoint equations are constructed in the form of splitting schemes, and also formulas for calculation of the functions of sensitivity to variations of the input parameters and external actions and the relations of the theory of sensitivity for functionals (30) using the basic models separately and for the system as a whole. The technology of these constructions and organization of the algorithms of direct and inverse modeling based on these constructions are well developed [1–9]. The key element in them is the main relationship of the sensitivity theory for functionals of the form (30)

$$\delta\Phi_k(\varphi) = (\operatorname{grad}_{\boldsymbol{Y}} \Phi_k(\varphi), \delta \boldsymbol{Y}) \tag{31}$$

and the algorithms for their realization. Here $\boldsymbol{Y}$ is the vector of the input parameters of the model and external actions, $\delta \boldsymbol{Y}$ is the vector of variation of these quantities, and $\mathrm{grad}_{\boldsymbol{Y}} \Phi_k$ is the set of sensitivity functions.

Numerical Experiment on Evaluation of the Danger of Contamination of the Region. The complex of models is an open system under development for providing climatic and ecological monitoring and prediction. This complex has a wide spectrum of applications. In the present work, we confine ourselves to one example of calculation using the hemispherical model of the atmosphere, which is a part of this complex. Following the chosen concept, we consider the problem of contamination of the region and the lake by anthropogenic sources of the northern hemisphere of the Earth. One of the most dangerous phenomena (from the viewpoint of intensity and scale of pollution of the natural environment) of the 20th century in the northern hemisphere was the Chernobyl' catastrophe, which led to the discharge of significant amounts of radioactive wastes into the atmosphere. Using the developed model of propagation and transformation of pollutants in the hemispherical variant, we demonstrate here the possibility of evaluating the contamination of the territory of the Baikal region and, hence, the lake itself from distant sources.

Figure 1 shows the danger function of contamination of the region by the sources of wastes, which operated from April 26 to May 5, 1986, i.e., in the period of intense outburst of radionuclides from the Chernobyl' atomic station (the scale is in relative units with normalization to the maximum value of the function in the three-dimensional domain D). We describe the information content of this function in terms of (30) and (31). It is a sensitivity function of the observation functional of the type (30) to variations of the power of the sources under the following conditions: the function $F_k = \varphi$, the weight function $\chi_k(\boldsymbol{x}, t)$ is other than zero only in the nodes of the grid domain, which belong to the Baikal water area, and within the time interval corresponding to the period of observation from May 3 to May 13, 1986, i.e., the functional is the estimate of the total contamination that enters the chosen region during the chosen time. Because of the linearity of the observation functional, the values of the danger function at each point of the region yield the relative contribution of the discharge from a source located at this point to the total amount of wastes represented by the value of this functional under the conditions described above.

To improve the reliability of the estimates, the real information about the atmospheric circulation from the data of Reanalysis NCEP/NCAR (U.S.A.) [16] for April–May 1986 was used in the calculations rather than the model data. For working with this information, we developed a special software system including algorithms of data assimilation and "hydrodynamic" interpolation in regimes specified by the corresponding basic model. In this case, the grid domain contained 144×39 points over the horizontal coordinates with cell size $2.5 \times 2.5°$ and ten vertical levels ($p_T = 10$ mbar, $p_B = 500$ mbar, and $\epsilon = 0.45$), among which there were six isobaric levels in D_{1t} and four σ-levels in the domain D_{2t}. The regions of observations and Chernobyl' are marked by circles. In solving the direct and adjoint problems of waste transport, the time steps were chosen automatically from the approximation conditions of the splitting schemes.

Analysis of the calculated danger function allows us to conclude that the high-danger zone (marked by red color) has a rather complicated structure. Not only wastes from the CIS countries, but also pollutants from the territories of China and Mongolia, enter the Baikal region. It is seen that the west-east transport is still rather strong in May, but the effect of the summer East-Asian cyclogenesis is already increasing, which can cause the contamination of Lake Baikal by transboundary transfer from Asian countries. The figure also illustrates the scales of interaction in the climatic system and the possibilities of zoning the territories depending on the level of danger of anthropogenic action. A response to events that took place thousands of kilometers away from the point of observation can be obtained in a comparatively short time. The danger function shows that traces of the Chernobyl' catastrophe could be found in the Baikal region in the period of May 3–13, 1986. Thus, the calculations confirm one of the basic principles of the concept: a global system of information or a global model should be used to describe the interaction between Lake Baikal and the atmosphere of the region.

Conclusion. The climatic system involving the regional atmosphere and lake Baikal is unique from the viewpoint of the combination of natural and anthropogenic factors. To describe the processes occurring in this system, a special complex of models of different space–time scales with a variable developed structure is constructed. The concept and methodology of modeling that we propose for solving research and applied problems of climatic and ecological directions are based on the joint use of the results of measurements and mathematical models. Constructionally, this is realized by the methods of direct and inverse modeling, which are based on variation and optimization principles.

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