STRUCTURE OF A COMPLEX OF MODELS FOR INVESTIGATION OF THE INTERACTIONS IN THE "LAKE BAIKAL – REGIONAL ATMOSPHERE" SYSTEM

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We formulate here some idea and main principles of constructing a complex of models for the "Lake – Regional atmosphere" system. Following this concept, we propose the structure of the complex of four models: a lake model, mesoregional and hemispheric models of the atmosphere, and the model of the immediate interaction of the lake and the atmosphere. The agreement of the descriptions of the functional content of all the models and processes, as well as the construction of numerical schemes and computation algorithms, is performed using the variational principle in a combination the splitting and decomposition techniques.

It is a specific feature of Baikal region that the Lake Baikal is a powerful climate forming factor in the South of Siberia. This factor is strengthened by that the region is in the influence zone of summer Sayan-Altay cyclic genesis and winter Asian anticyclone. The Lake Baikal, on the background of these atmospheric processes, forms a unique Baikal mesoclimate, which in turn, essentially affects both the mesoclimate and the quality of the atmosphere over industrial areas of the region.

The constant temperature contrast between the water and land during the season of open water with the seasonal changes in the heat fluxes is a source of instability in the climate system. It leads to that the zone of Lake Baikal influence (we beforehand have estimated this zone in Ref. 1 being approximately equal to 100–200 km outside from the coastal line), especially in the atmospheric layer adjacent to the water surface, is the potential accumulator of pollution, coming here not necessarily only from the nearby region only, but also from the vast territories of Northern hemisphere: Siberia, China, and Mongolia. All these processes have to be investigated for understanding the ecological prospects of the region and the lake. Therefore, forming the conception of the investigation into the climatic changes in the "Lake – Atmosphere" system, we are not limited only by the water – atmosphere interactions. We consider the mesoregional processes in combination with the hemispherical ones, and do not separate out the system hydrothermodynamics from the processes of the pollutants' dispersal. This is needed when estimating the role of transboundary pollution transfer as well as of the processes and sources which are external with respect to the region under study.

In this paper we present a development of the complex study on assessing the anthropogenic influence on Lake Baikal and the region nearby.[1] These investigations have been carried out by a temporary scientific group under the auspices of the Presidium of Siberian Branch of the Russian Academy of Sciences. The main idea of this work continues that developed in the cycle of investigations, presented earlier in Refs. 2 and 9.

1. COORDINATE SYSTEM AND DECOMPOSITION OF THE AREAS

First, let us describe the solution domain and the coordinate system for basic models. We use the universal coordinate system (x, y) for horizontal directions with the scale factors m and n that are set parametrically to obtain the spherical, polar, and Cartesian coordinates, or the coordinates of cartographic projections, depending on the purpose of the investigations. For atmospheric models we shall consider two types of the solution domain that is the Northern hemisphere and a limited territory of the region. The area of the lake is described parametrically in a selected system of horizontal coordinates.

To describe the model representations along vertical direction, we make use of the principle of decomposition into the regions and conditionally divide the atmosphere into two layers: the free atmosphere, D_1 $(p_t \le p \le p_b)$, and the boundary atmospheric layer, D_2 $(p_b \le p \le p_s)$. Here p is the air pressure, $p_s = p_s(\mathbf{x}, t)$, p_t and p_b are the pressure on the Earth's surface, at top boundary of the atmosphere, and at the boundaries of the layers, $\mathbf{x} = (x, y)$, accordingly. Let us introduce a hybrid coordinate system to combine the advantages of using isobaric coordinates in the free atmosphere (in the case, when p_t and p_b are constants) with the conveniences of sigma-coordinates for the representing the Earth's terrain

$$\text{for } D_1 \text{ layer } \sigma = \varepsilon \frac{p - p_t}{p_b - p_t},$$

$$\text{for } D_2 \text{ layer } \sigma = (1 - \varepsilon) \frac{p - p_b}{p_s - p_b} + \varepsilon, \quad 0 \le \varepsilon \le 1. \qquad (1)$$

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The parameter ε is introduced so that the surface $\sigma = \varepsilon$ be always above the level of the model Earth's terrain. According to definition (1), we can write relations for vertical velocities $\omega = \mathrm{d}p/\mathrm{d}t$, and $\dot{\sigma} = \mathrm{d}\sigma/\mathrm{d}t$ in the areas D_{it} ($i = 1, 2$) and their boundary conditions

$$\omega = \alpha_i \left(\frac{\mathrm{d_s}\, \chi_i}{\mathrm{d}t} + \pi_i\, \dot{\sigma} \right),$$

$$\frac{\mathrm{d_s}}{\mathrm{d}t} = \frac{\partial}{\partial t} + mu \frac{\partial}{\partial x} + nv \frac{\partial}{\partial y},$$

$$\frac{\mathrm{d}}{\mathrm{d}t} = \frac{\mathrm{d_s}}{\mathrm{d}t} + \dot{\sigma} \frac{\partial}{\partial \sigma}, \quad (2)$$

$$\chi_1 = \sigma\pi_1 + \varepsilon\, p_\mathrm{t}, \quad \pi_1 = p_\mathrm{b} - p_\mathrm{t}, \quad \alpha_1 = 1/\varepsilon,$$

$$\chi_2 = \sigma\pi_2 + p_\mathrm{b} - \varepsilon\, p_\mathrm{s}, \quad \pi_2 = p_\mathrm{s} - p_\mathrm{b},$$

$$\alpha_2 = 1/(1 - \varepsilon),$$

$$\dot{\sigma} = 0 \ \text{ at } \ \sigma = 0 \text{ and } 1, \quad (3)$$

$$\omega|_{\varepsilon^-} = \omega|_{\varepsilon^+}, \quad \alpha_1\, \pi_1\, \dot{\sigma}|_{\varepsilon^-} = \alpha_2\, \pi_2\, \dot{\sigma}|_{\varepsilon^+} \ \text{ at } \sigma = \varepsilon. \quad (4)$$

We determine the models in spatiotemporal region $D_t \equiv D\times[0, t_k]$, where $[0, t_k]$ is the time interval, and $D = \cup_{i=1}^{4} D_i$ is the domain of spatial coordinates variation,

$$D_1 = S\ [0 \le \sigma \le \varepsilon],$$

$$D_2 = S\ [\varepsilon \le \sigma \le 1],\ D_1 \cup D_2 = D_a,$$

$$D_3 = \{\mathbf{x} \subset S_\mathrm{l},\ 0 \le z \le h_\mathrm{l}(\mathbf{x})\},$$

$$\text{and } D_4 = \{\mathbf{x} \subset S_\mathrm{w},\ 0 \le z \le h_\mathrm{w}(\mathbf{x})\},$$

$$S = \{0 \le a \le x \le b \le 2\pi,\ 0 \le c \le y \le d \le \pi\},$$

where S is the area of Earth's surface, a, b, c, and d are the parameters determining the horizontal size of the area S, $S = S_\mathrm{l} \cup S_\mathrm{w}$, where S_l and S_w are the parts of the surface areas occupied by land and water, $h_\mathrm{l}(\mathbf{x})$, $h_\mathrm{w}(\mathbf{x})$ are the functions describing the active depth of soil and the bottom relief of the aqueous object, accordingly. The axis z is directed downwards. The side boundaries of the domains D_i we denote as Ω_i and their full boundaries in three-dimensional space as $\bar{\Omega}_i$. Everywhere the subscript t denotes the time variability.

Let us denote the functions of a state as

$$\varphi = \{\varphi_i\ (i = \overline{1, n}\ \} \in Q(D_t),$$

where $Q(D_t)$ is the appropriate functional space on D_t, φ_i are the components of the vector function of state, n is the number of components. The structure of these objects is determined by a functional content of the basic models. The space of conjugated functions $\{\varphi^* \in Q^*(D_t)\}$ is constructed similarly.

Let us introduce the scalar product for the functions of state in the domain D_t

$$(\varphi_1, \varphi_2) = \sum_{k=1}^{4} \alpha_k \int_{D_{kt}} \left(\sum_{i=1}^{n} \varphi_{1i}\, \varphi_{2i}\, æ_i \right) \gamma_k\, \mathrm{d}D_k\, \mathrm{d}t, \quad (5)$$

where $\mathrm{d}D_k = \mathrm{d}z_k\, \mathrm{d}x\, \mathrm{d}y/(mn)$, $\mathrm{d}z_1 = \mathrm{d}z_2 \equiv \mathrm{d}\sigma$, $\mathrm{d}z_3 = \mathrm{d}z_4 \equiv \mathrm{d}z$, $\gamma_1 = \pi_1$, $\gamma_2 = \pi_2$, $\alpha_3 = \alpha_4 = 1$; $\gamma_3 = \rho_\mathrm{s}$, $\gamma_4 = \rho_0$, α_k are the weighting parameters of the decomposition, γ_k are the metric parameters in the regions decomposed, ρ_s and ρ_0 are the density of the soil and water, respectively. The dimensional factors $æ_i$ were selected depending on the physical meaning of the corresponding components, and α_k and γ_k at $k = \overline{1, 4}$ depends both on the coordinate system, and on the way of the decomposition of the domain D_t into the sub-regions D_{kt}.

2. BASIC MODELS OF THE ATMOSPHERE AND THE LAKE

Let us consider the basic models of the hydrothermodynamic processes and the processes of the pollutants transfer in the “Atmosphere – Lake” system. We use the models of three types for the investigation into the atmospheric processes. These models are different both in the spatial and time scales of the processes, and in the sizes of the regions considered. The model A_1 with the characteristic horizontal scales about 100 km is used for investigating mesoclimate of the industrial regions and cities; A_2 is the mesoregional model with the characteristic horizontal scales of 100–1000 km; A_3 is the model of the atmosphere for the Northern hemisphere, destined for investigation into the long-term interactions of the lake with the atmosphere. The model A_1 is mainly used in the vertical domain D_{2t}. The models A_2 and A_3 are used in the area $D_{at} = D_{1t} \cup D_{2t}$ in the decomposition mode.

We introduced two types of models for the lake: B_1 and B_2. The model B_1 is the model of general lake circulation and the model B_2 may be used for parts of the lake and for local zones. These models have identical structure, while differ by the boundary conditions and spatiotemporal resolutions of the discrete approximations. The models of interaction between the atmosphere and the lake are organized on the basis of the models A_2 and B_1.

2.1. Models of the hydrothermodynamics of atmospheric processes

The basic equations are being written with the account of the domain D_{at} decomposition over vertical coordinate into the sub-regions D_{it} ($i = 1, 2$) as follows:

$$\frac{\mathrm{d}u}{\mathrm{d}t} - lv + m\left[\frac{\partial \Phi}{\partial x} - \frac{1}{\pi_i} \frac{\partial \Phi}{\partial \sigma} \frac{\partial \chi_i}{\partial x} \right] - F_u = 0, \quad (6)$$

$$\frac{dv}{dt} + lu + n\left[\frac{\partial\Phi}{\partial y} - \frac{1}{\pi_i}\frac{\partial\Phi}{\partial\sigma}\frac{\partial\chi_i}{\partial y}\right] - F_v = 0, \quad (7)$$

$$\frac{\partial\Phi}{\partial\sigma} + \frac{RT\pi_i}{\chi_i} = 0, \quad (8)$$

$$\frac{dT}{dt} - \omega A_i - F_t = Q_t,$$

$$A_i = -\frac{1}{c_p\,\pi_i\,\alpha_i}\frac{\partial\Phi}{\partial\sigma} = \frac{RT\,\pi_i}{\alpha_i\,\chi_i\,c_{pm}}, \quad (9)$$

$$\frac{\partial\pi_i}{\partial t} + L(\pi_i) = 0. \quad (10)$$

Here u, v, and $\dot{\sigma}$ are the components of the velocity vector $\mathbf{u}$ along the directions x, y, and σ, respectively, Φ is the geopotential, T is the virtual temperature, c_{pm} is the specific heat capacity of the moist air at a constant pressure, R is the universal gas constant, l is the Coriolis parameter, Q_t are the heat sources.

The transfer operator of the substances η along the trajectories of air particles in the divergent form is as follows:

$$L(\pi_i\,\eta) = mn\left[\frac{\partial}{\partial x}\left(\frac{\pi_i\,\eta\,u}{n}\right) + \frac{\partial}{\partial y}\left(\frac{\pi_i\,\eta\,v}{m}\right)\right] + \frac{\pi_i\,\eta\,\dot{\sigma}}{\partial\sigma}, \quad (11)$$

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

$$F_\eta^s = \frac{mn}{\gamma_i}\left[\frac{\partial}{\partial x}\left(\frac{\gamma_i\,\mu_{\eta x}}{n}\frac{\partial\eta}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{\gamma_i\,\mu_{\eta y}}{n}\frac{\partial\eta}{\partial y}\right)\right],$$

$$F_\eta^v = \frac{1}{\gamma_i}\frac{\partial}{\partial\sigma}\left(\gamma_i\,\nu_\eta\frac{\partial\eta}{\partial\sigma}\right). \quad (12)$$

At $\sigma = 1$ $\Phi = \Phi_s \equiv gZ_s$, where g is the acceleration of gravity, Z_s is the Earth's surface terrain. To close the models, we assume, besides the conditions (3) and (4), the absence of turbulent fluxes of substances through the top boundary. The parametric values of the heat fluxes, the kinetic momentum, and the equation of the heat balance on the Earth's surface are set on the bottom boundary. The conditions of passing to the background process are set on the side boundaries of a limited territory, and the condition of periodicity on the sphere.

2.2. The model of moisture transfer and transformation in the atmosphere

The hydrological cycle plays an essential role in the processes of the energy and mass exchange in the "Atmosphere – Lake" system. For the atmosphere the lake is a powerful accumulator and source of moisture and heat with the seasonal and daily variations in the sign of temperature contrast in the "Water–Air–Land" system and with sharp variations in the surface-layer temperature under the effect of high winds. Therefore to study the variability of the atmosphere under the action of the lake in various situations, it is extremely important, both to observe the feedback from the atmosphere to the lake and relaxation of the intense effects. To do this, one needs for full reconstruction of the hydrological cycle in the atmosphere. The presence of water vapor must also be taken into account in the equations of heat transfer in the atmosphere and in the equations of heat balance on the underlying surface. The influence of moisture is very important when calculating both the radiation heat influx and the removal of pollutants from the atmosphere.

Let us determine the components of the function of state, φ, that enter the models of the hydrological cycle. For a convenience of the below treatment we denote these components as

$$\mathbf{q} = \{\mathbf{q}_k,\ k = \overline{1, 6}\} \equiv \{q_v, q_c, q_r, q_{ic}, q_c, q_g\},$$

where q_k are the mixing ratios of water vapor (q_v), cloud water (q_c), rain water (q_r), cloud ice (q_{ic}), snow (q_s), and ice crystals (q_g).

We take the model that involves the first three components of the hydrological cycle q_v, q_c, and q_r as the basic model.

$$\frac{\partial\pi_i\,q_k}{\partial t} + \tilde{L}(\pi_i\,q_k) - R_{qk} - Q_{qk} = 0, \quad (13)$$

where $k = \overline{1, 3}$, $i = 1, 2$, R_{qk} are the rates of the concentration q_k change due to microphysical processes of the moisture transformations: $R_{q1} = \pi_i\,(P_{re} - P_{con})$, $R_{q2} = -\pi_i\,(P_{ra} + P_{re} - P_{con})$, $R_{q3} = \pi_i(P_{ra} + P_{rc} - P_{re}) - g\partial(\rho\omega_t q_k)/\partial\sigma$, P_{ra} is the rate of the growth of rain droplets from the cloud particles, P_{rc} is the rate of auto conversion of cloud particles into the rain droplets, P_{re} is the rate of evaporation of rain water, P_{con} is the rate of condensation of water vapor or of the cloud particles evaporation, Q_{qk} are the functions describing the sources, ω_t is the average rate of the rain droplets fall, $\tilde{L}(\pi_i\,q_k)$ is the operator of advective diffusion

$$\tilde{L}(\pi_i\,q_k) = L(\pi_i\,q_k) - \pi_i\,F_{qk} + \pi_i\,DF_{qk}, \quad (14)$$

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, due to the movement of moist air relative to the dry air. The first two expressions have the view like that of the Eqs. (11) and (12).

To close the model, we suppose the absence of fluxes through the top boundary, and set the flux of water vapor on the low boundary depending on the "moisture ability" of different areas of the Earth's surface. This model is implemented for investigations of situations, when the hydrological cycle involves warm rain water. To describe the processes at low temperatures, connected with the formation of ice and snow, we added into the structure of the basic model additional equations of transfer and transformation of the corresponding components.[12]

2.3. Model of the admixture transfer in the atmosphere

We formulate here, by analogy with Ref. 3, the models of transfer of an admixture and the basic problems that are being achieved with the help of these models. We include, into the model complex, the modifications of these models adapted to specific features of the objects under study. The basic equations have the same structure as the moisture transfer model, Eqs. (13) and (14),

$$\frac{\partial \pi_i c_k}{\partial t} + \tilde{L}(\pi_i c_k) - R_{ck} - Q_{ck} = 0, \quad (15)$$

where $i = 1, 2$, $k = \overline{1, n_{\text{a}}}$, c_k are the pollution concentration, n_{a} is the number of substances, R_{ck} are the rates of the concentrations c_k change due to chemical transformations of the pollutants, Q_{ck} are sources of pollutants. Here we consider the gaseous and aerosol substances. The advective diffusion operator $\tilde{L}$ is defined by expression (14), in which the vertical rate σ is adding the rate of the gravitational sedimentation of particles. We also consider here (in contrast to Ref. 3) the diffusion flux of the rain water pollutants. As the boundary conditions we suppose the absence of fluxes of pollutants through the top boundary and the presence of pollutants at the background concentration level on side boundaries. At the low boundary we use the equation of the pollutants balance for various categories of land tenure and allow for the dry and moisture sedimentation of particles, turbulent flux, aerodynamic rise of particles from Earth's surface, and the pollutants sources of natural and anthropogenic origin.

2.4. Models of hydrothermodynamics and transfer of pollutants in the Lake Baikal

Let us write the basic equations of the models as

$$\frac{du}{dt} - lv + \frac{m}{\rho_0}\frac{\partial p}{\partial x} - F_u = 0, \quad (16)$$

$$\frac{dv}{dt} + lu + \frac{n}{\rho_0}\frac{\partial p}{\partial y} - F_v = 0, \quad (17)$$

$$\frac{1}{\rho_0}\left(\frac{\partial p}{\partial z} + g\rho\right) = 0, \quad (18)$$

$$\frac{mn}{\rho_0}\left[\frac{\partial}{\partial x}\left(\frac{\rho_0 u}{n}\right) + \frac{\partial}{\partial y}\left(\frac{\rho_0 v}{m}\right)\right] + \frac{1}{\rho_0}\frac{\partial \rho w}{\partial z} = 0, \quad (19)$$

$$\frac{d\eta_k}{dt} - F_{\eta k} - Q_{\eta k} = 0, \quad k = \overline{1, 2 + n_{\text{w}}}, \quad (20)$$

$$\rho = \rho\,(p, T, S_l). \quad (21)$$

Here $\{\eta_k\} = \{T, S_l, c_i\ (i = \overline{1, n_{\text{w}}})\}$, T is temperature, S_l is the salinity, c_i are the pollutants' concentrations in water, n_{w} is their amount, u, v, and w are the components of the velocity vector **u** along the directions x, y, and z, respectively, p is the pressure, ρ is the density, ρ_0 is the set distribution of the relative density, $Q_{\eta k}$ are the sources of heat, salt, and pollutants. The operators of transfer and turbulent exchange are determined by following expressions:

$$\frac{d}{dt} = \frac{d_s}{dt} + w\,\frac{\partial}{dz}, \quad F_{\eta k} = F^s_{\eta k} + F^v_{\eta k}.$$

The operators $F^s_{\eta k}$ has the form (12) at $i = 4$, and

$$F^v_{\eta k} = \frac{1}{\gamma_4}\frac{\partial}{\partial z}\left(\gamma_4\, \nu_{\eta k}\,\frac{\partial \eta_k}{dz}\right), \ \eta_k = u, v, T, S_l, c_i, \quad (22)$$

here ν_η are the coefficients of turbulent exchange along the vertical direction. In the function w entering the transfer equation for pollutants we have also included the rate of the gravitational sedimentation or float up of the pollutants to surface. On the free surface $z = \zeta$, which is the water-air interface,

$$\nu\rho_0\,\frac{\partial u}{\partial z} = -\,\tau_x,\ \nu\rho_0\,\frac{\partial v}{\partial z} = -\,\tau_y,$$

$$\nu_\eta\,\rho_0\,c_p\,\frac{\partial \eta_k}{\partial z} = -\,H^s_{\eta k}, \quad (23)$$

$$w = \frac{d_s\zeta}{dt}, \quad p = p_{\text{s}}. \quad (24)$$

At the bottom of the lake ($z = h_{\text{w}}(x, y)$) $u = 0$, $v = 0$, $w = 0$, and $\partial\eta_k/\partial N = H^N_{\eta k}$. On the hard side boundaries $u = 0$, $v = 0$, and $\partial\eta_k/\partial N = H^N_{\eta k}$. In places where the rivers flow into the lake $u = u_{\text{riv}}$, $v = v_{\text{riv}}$, and $\partial\eta_k/\partial N = U_{\text{riv}}(\eta_k - (\eta_k\rho)_{\text{riv}}/\rho)$. In places where rivers flow out from the lake $u = u_{\text{riv}}$, $v = v_{\text{riv}}$, 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 heat fluxes and the salt and pollutant fluxes through the interface and hard boundaries, c_p is heat capacity of water at constant pressure. The index "riv" denotes the values of functions referring to the rivers, $\partial/\partial N$ is the derivative with respect to the co-normal. When solving the problem for parts of the lake we form the conditions when the function of the state approaches the background values from the side of open water.

2.5. Parametrization of the turbulent exchange

In the basic models of the atmosphere and water we introduce the operators of turbulent exchange with partial derivatives of the second order. The coefficients of turbulent exchange along horizontal directions μ_x and μ_y are calculated following a nonlinear parametric scheme similar to that used in Ref. 3 with the account for the horizontal deformation of velocity field, stratification of the atmosphere and water, sizes of the grid cells.

To calculate the vertical coefficients of turbulence, we use one of the below schemes, depending on situation. The first of these is a simplified scheme when the coefficient is calculated as a function of local Richardson number and characteristic vertical scale of vortices. This scheme is very convenient and effective in application, but has no "memory" at transitions from one spatiotemporal point of the domain to the other. This disadvantage becomes critical when fields rapidly vary.

The second scheme is based on solving two equations for the kinetic energy of turbulence, E, and for the dissipation energy ε in the atmosphere and water.[10,11] The matching of equations for E and ε at the atmosphere–water interface is performed assuming the continuity of energy and dissipation fluxes at the boundary between the two media.

2.6. The heat balance equation on the surface

To close and join the models for various media at the boundaries within the atmosphere–water–land system, we can write the condition of heat balance in the following form:

$$c_{p\mathrm{m}}\,\rho_\mathrm{a}\frac{\partial T}{\partial t} = R_\mathrm{n} - H_\mathrm{m} - H_\mathrm{s} - \mathrm{L_v}\,E_\mathrm{s}, \tag{25}$$

where R_n is the radiation balance on surface, H_m is the molecular heat flux in the soil or the turbulent thermal flux in water, H_s and $L_\mathrm{v}\,E_\mathrm{s}$ are the fluxes of explicit and latent heat to the atmosphere, L_v is the latent heat of vaporization

$$H_\mathrm{s} = \rho_\mathrm{a}\times c_{p\mathrm{m}}C_\mathrm{u}C_\Theta(T_\mathrm{s} - T_\Theta)V,$$

$$E_\mathrm{s} = \rho_\mathrm{a}C_\mathrm{u}C_\Theta\,M(q_\mathrm{vs}(T_\mathrm{s}) - q_\mathrm{va})V,$$

where C_u, C_Θ are the exchange coefficients, T_s is the surface temperature, $V = (v_\mathrm{a}^2 + v_\mathrm{c}^2)^{1/2}$, v_c is the convective velocity, ρ_a, v_a, T_a, and q_ca are the values of meteorological quantities at the first calculation level, $q_\mathrm{vs}(T_\mathrm{s})$ is the saturation ratio of mixture for a water vapor on the surface at temperature T_s. The coefficients of exchange are calculated by the parametrization models of the near-ground layer with the account for stratification of the atmosphere and properties of the underlying surface. The radiation balance of heat is the sum of long-wave and short-wave radiation. From the requirements of model efficiency, the R_n value is calculated in two variants depending on the state of the atmosphere: for clear sky without the consideration of cloudiness and for the case of a cloudy sky. In both variants the influence of pollutants on the radiation balance of the surface is being taken into account.

The vertical distribution of the heat influx in the atmosphere is simulated with the allowance for solar radiation and the release of latent heat at the phase transitions of moisture. The model for calculation of radiation fluxes of heat is based on a complex of equations of the radiation transfer in the two-flux Eddington approximation.[13] A detailed description of the radiation block structure may be found in Ref. 9.

3. VARIATIONAL FORMULATION OF THE MODELS

Let us define the functional of the basic identity in the variational formulation of the atmospheric model (6)–(15)

$$I_\mathrm{a}(\varphi, \varphi^*) = \sum_{i=1}^{2}\Bigg\{\alpha_i\int_{D_{it}}\Bigg[\left(\frac{\mathrm{d}u}{\mathrm{d}t} - F_u\right)u^* +$$

$$+\left(\frac{\mathrm{d}v}{\mathrm{d}t} - F_v\right)v^* + c_{p\mathrm{m}}\left(\frac{\mathrm{d}T}{\mathrm{d}t} - F_t\right)T^* + l(u^*v - v^*u) +$$

$$+(\mathbf{u}^*\,\mathrm{grad}\,\Phi - \mathbf{u}\,\mathrm{grad}\,\Phi^*) - \frac{1}{\gamma_i}\frac{\partial\Phi}{\partial\sigma}\left(\frac{\mathrm{d}_s^*\,\chi_i}{\mathrm{d}t} - T^*\frac{\mathrm{d}_s\,\chi_i}{\mathrm{d}t}\right) -$$

$$-\frac{\partial\Phi}{\partial\sigma}(T^*\,\dot\sigma - \dot\sigma^*) - c_p\,Q_T\,T^* + \frac{1}{\pi_i}\left(\frac{\partial\Phi}{\partial\sigma}\sigma + \Phi^*\right)\frac{\partial\pi_i}{\partial t} +$$

$$+\sum_{j=1}^{3+n_a}\frac{1}{\gamma_i}\left(\frac{\partial\pi_i\,\phi_j}{\partial t} + \tilde{L}(\pi_i\,\phi_j) - R_{\phi j} - Q_{\phi j}\right)\phi_j^*\,æ_j\Bigg]\times$$

$$\times\,\gamma_i\,\mathrm{d}D_i\,\mathrm{d}t + \int_{\Omega_{it}}u_\mathrm{n}\,\Phi^*\,\mathrm{d}\Omega_i\,\mathrm{d}t\Bigg\} +$$

$$+\,\alpha_1\int_{D_{1t}}\frac{\partial\Phi}{\partial\sigma}\,\varepsilon\,\frac{\partial p_t}{\partial t}\,\mathrm{d}D_1\,\mathrm{d}t +$$

$$+\,\alpha_2\int_{D_{2t}}\frac{\partial\Phi}{\partial\sigma}\frac{\partial}{\partial t}(p_\mathrm{b} - \varepsilon p_\mathrm{s})\,\mathrm{d}D_2\,\mathrm{d}t = 0, \tag{26}$$

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 $\mathbf{u}$ to the domain boundaries.

$$\frac{\mathrm{d}_s^*\,\chi_i}{\mathrm{d}t} \equiv \frac{\partial\chi}{\partial t} + mu^*\frac{\partial\chi}{\partial x} + nv^*\frac{\partial\chi}{\partial y},$$

φ^* are the vector-functions with arbitrary while sufficiently smooth components belonging to the space $Q^*(D_t)$.

An integral identity for lake models (16)–(24) is as follows:

$$I_{\rm w}(\varphi,\varphi^*) = \int_{D_{4t}} \Big\{ \left(\frac{{\rm d}u}{{\rm d}t} - F_u\right) u^* + \left(\frac{{\rm d}v}{{\rm d}t} - F_v\right) v^* +$$

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

$$+ \sum_{j=1}^{2+n_{\rm w}} \left(\frac{{\rm d}\phi_j}{{\rm d}t} - F_{\phi j} - Q_{\phi j}\right)\phi_j^* \,æ_j \Big\} \gamma_4 \,{\rm d}D_4\, {\rm d}t +$$

$$+ \int_{\Omega_{4t}} u_{\rm n}\, p^*\, \gamma_4 \,{\rm d}\bar{\Omega}_4\, {\rm d}t = 0, \qquad (27)$$

where $\varphi = (u, v, w, p, \phi_j)$, $\varphi^* = (u^*, v^*, w^*, p^*, \phi_j^*)$, $\{\phi_j\} \equiv \{T, S_l, c_i, i = \overline{1, n_{\rm w}}\}$, $u_{\rm n}$ is the normal component of the velocity vector to the boundary $\bar{\Omega}$ of the area D_{4t},

$${\rm d}\bar{\Omega}_i = \left\{\frac{{\rm d}x{\rm d}y}{(mn)}, \frac{{\rm d}y{\rm d}z_i}{n}, \frac{{\rm d}x{\rm d}z_i}{m}\right\},\ i = \overline{1, 4}\ .$$

An integral identity for the model of thermal exchange in soil is

$$I_{\rm n}(T, T^*) = \int_{D_{3t}} \left(\frac{\partial T}{\partial t} - F_{\rm t}^n\right) T^* \,æ\, \gamma_3 \,{\rm d}D_3\, {\rm d}t. \qquad (28)$$

The operator $F_{\rm t}^n$ describes the processes of thermal exchange in soil and has a structure similar to that of Eq. (22) with the scale factor γ_3. The structure of functionals in Eqs. (26)–(28) is selected according to definition of the scalar product (5) and the balance equation of the total energy of the system.

For the system as a whole we can obtain

$$I(\varphi, \varphi^*) = I_{\rm a}(\varphi, \varphi^*) + I_{\rm w}(\varphi, \varphi^*) + I_{\rm n}(\varphi, \varphi^*) = 0. \quad (29)$$

All the closure conditions are being taken into account and controlled via the integrals over the boundaries of the corresponding domains. The models of direct interaction among the media are concluded into the identity (29) as integrals over internal boundaries. One can obtain their concrete representations, after certain transformations, by integrating by parts the expressions

$$\int_{D_{kt}} \left(\frac{\partial \varphi}{\partial t} - F_\varphi\right) \varphi^* \,{\rm d}D_k\, {\rm d}t,$$

$$\int_{D_{kt}} \left(\frac{\partial \pi_i \varphi}{\partial t} - \tilde{L}(\pi_i\, \varphi)\right) \varphi^* \,{\rm d}D_k\, {\rm d}t \qquad (30)$$

in the assumption of continuity of the relevant components of the function $\boldsymbol{\varphi}^*$ and fluxes of functions of the state through the boundaries. Collecting all integrals over surface S_t at $\sigma = 1$, and having in view the equations of heat balance (25) and fluxes of pollutants on this surface, we can obtain relations for the fluxes through the water–atmosphere and the atmosphere–soil boundaries. Similarly, from the integrals over the boundary Ω_3 between the domains D_3 and D_4 we obtain the conditions of the lake and continent interaction.

Keeping in view the purposes of investigations, let us add the set of functionals, to identities (26)–(29), differentiated with respect to $\boldsymbol{\varphi}$ in space $Q(D_t)$, and formulate the number of the conjugated problems, for these functionals as in Refs. 4 and 6. Using these identities, we construct discrete analogs of the basic and conjugate equations in the form of the splitting schemes. The formulas for calculating the functions of sensitivity and the relations of theory of sensitivity for basic models are also constructed both for separate models and the whole system. The techniques of making such constructions and arranging on their basis of the computing algorithms of direct and inverse simulations are well developed (see, e.g., Refs. 1–9).

CONCLUSIONS

The concept of constructing of the complex of models of the atmosphere–lake system presented is based on a fruitful idea of using the variational formulation of the task for the system as a whole. It allows one to create numerical schemes and algorithms based on a unified conception that enables coordination at all stages of the simulation with an automatic control of the processes of the energy and mass exchange in the system. Besides, on the basis of the variational approach one can arrange the intercomparison of the models with data of observations.

Recently, the Lake Baikal has become an object for international investigations from the positions of global changes of the environment and climate. The lake–atmosphere model should become a tool for these investigations, to help checking the validity of the hypotheses proposed as well as the field experiments and interpretation of the results of such experiments.

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