Bull. Nov. Comp. Center, Num. Model. in Atmosph., etc., 4 (1996), 31–52

Some aspects of mathematical modeling using the models together with observational data*

V.V. Penenko

The methods of the solution of optimization problems on the basis of variational principle are described. They use numerical models together with observational data. In particularly, the problems of sensitivity investigations and data assimilation are considered. The algorithmic advantages of the proposed approach based on the adjoint problems and sensitivity functions as compared with the Kalman filtering methods are discussed.

Introduction

The present paper describes some applications of mathematical models and numerical methods for the investigation of climate and for the solution of environmental problems. There is a wide range of problems connected with mathematical simulation of the atmosphere and ocean and with estimation of the industrial effect for the environment. With the industrial development the man's influence on the climatic system becomes apparent in variations of basic parameters characterizing the atmospheric state. It means that human impact could be interpreted as one of the factors in the climatic system and estimation of this factor is one of the applications of the models sensitivity theory. To solve such problems a special mathematical method is needed. It should be based on variational principles, methods of perturbation, optimization and identification theory. Since we discuss here the behaviour of the model and its stability to variations of input data. Practical realization of numerical algorithms is of particular importance.

Variational principles together with splitting-up methods can serve as methodological base of computational algorithms. Splitting-up methods provide economic and stable numerical algorithms for realization of the models and optimization theory. The variational principle guarantees mutual concordance of values at different steps of computation. It allows us to formulate methods for determining functions of the model's sensitivity and to consider them from the viewpoint of perturbation theory as methods of esti-

*Supported by the Russian Fondation of Basic Research under Grant 94–05–16105 and INTAS–93–1176.

mation of functional variations depending on variations of input data. Also important are the inverse problems, i.e., estimation of the input parameters by means of measured data of meteorological fields being simulated.

Perturbation and optimization methods as applied to numerical simulation of atmospheric and oceanic processes make it possible to analyze qualitatively the model, estimate relative contribution of various factors, rationally design numerical experiments, formulate a series of new problems of analysis and prediction of hydrometeorological fields and environmental situations including inverse problems of identification of the model's parameters, estimate space and time scales of the domains of influence of parameter variations and sources etc.

The questions concerned the specification of input parameters and initial data for mathematical models always arise when solving different problems related to the physics of atmosphere, ocean and environmental protection. The information obtained from observations in real conditions is usually used for this purpose.

Let us formulate the problem in a more general way and consider mathematical models together with observational data. In this case mathematical models will be used for the estimation of initial fields, reconstruction of the field time- spatial structure and more precise definition of the parameters for the models themselves with the help of the measured data. Diagnostic quality estimation of the model will be made simultaneously with assimilation of observations.

For the solution of this problem it is convenient to use optimization methods, combined with methods for investigation of the model sensitivity. Such a combination results in the closed formulation of the problems and in the clear organization of interaction between the mathematical model and the actual information. Adjoint problems play an essential role in the realization of this approach.

At present a considerable experience has been gained in the application of optimization methods and adjoint equations in different fields of science and technology [2-12]. Problems of analysis and assimilation of observations using numerical models offer wide possibilities for the utilization of these methods. The detailed review of different applications of variational methods in meteorology is given in [15]. This paper is the development of the results of the works described in [11-21].

Data assimilation with optimization makes it possible to use simultaneously all the available data in such a form which is obtained from measurements.

Three types of basic elements must be defined in order to represent the methods for the assimilation of observations and the diagnosis of the model quality:

- mathematical models of investigated processes,
- mathematical models of "measurements",
- criteria for the model quality and assimilation of observations.

Models of the processes are well-known. Models of observations describe the transformation in which state functions correspond to the set of observed quantities. Observations can be contact, indirect and remote. Their sense determines the structure of the corresponding model. For example, if contact measurements give the state function values, then the appropriate interpolation procedure is a model of such observations. In this case interpolation must be carried out from the simulated fields, i.e., the state functionvalues, calculated with the models, are transferred to the set of points where measurements are made.

1. Statement of the problem and construction of the discrete approximations

Major definition in the description of mathematical models are state functions and parameters. Their physical meaning and the difference between them depend on the specific formulation of the model.

In the problems of geophysical hydrothermodynamics and environment, velocity vector components, temperature, pressure, density, humidity and concentrations of pollutants refer to the state functions. These functions determine the system behaviour at every point of the model integration domain. The values of turbulent coefficients, integration domain characteristics, coefficients of equations and boundary conditions, the source characteristics, etc., will be given as parameters. The fields of initial values can also be referred either to the unknown parameters or to the state functions.

For the convenience of the further description let us give advantage of the operational notations. Let us write the model equations in the form

$$
\begin{gathered}
B\frac{\partial \vec{\varphi}}{\partial t} + G(\vec{\varphi}, \vec{Y}) - \vec{f}(\vec{x}, t) = \vec{r}(\vec{x}, t), \\
\vec{\varphi} \in Q(D_t), \quad \vec{Y} \in R(D_t).
\end{gathered}
\tag{1}
$$

The following notations are used here: $\vec{\varphi}$ is a state vector, $\vec{Y}$ is a parameter vector, B is a diagonal matrix, some diagonal elements of which can be zero, $G(\vec{\varphi}, \vec{Y})$ is a nonlinear matrix operator depending on the state function and parameters, $\vec{f}$ is a function of sources, $\vec{r}$ is a function of the model errors, $D_t = D \times [0, \bar{t}\ ]$, D is a domain of spatial variables $\vec{x}$, $[0, \bar{t}\ ]$ is the time interval, $Q(D_t)$ is the space of state functions satisfying the boundary conditions, $R(D_t)$ is the range of admissible parameter values. For the considered class of problems, the operator $G(\vec{\varphi}, \vec{Y})$ is defined by the hydrothermodynamic equations of the "atmosphere-water-earth" system, transport and transformation of pollutants, and by the relations at the interface boundaries. It includes all the terms of equations except the time derivatives. With respect to the components of the state function $\vec{\varphi}$, this is a nonlinear matrix operator with partial derivatives. In the stationary case, B-matrix is zero.

The initial conditions at $t = 0$ and the model parameters can be written in the form

$$\vec{\varphi}^0 = \vec{\varphi}_a^0 + \vec{\xi}_0(\vec{x}), \tag{2}$$

$$\vec{Y} = \vec{Y}_a + \vec{\zeta}(\vec{x}, t). \tag{3}$$

Here, $\vec{\varphi}_a^0$ and $\vec{Y}_a$ are the given *a priori* estimates of the initial fields $\vec{\varphi}^0$ and the parameters' vector $\vec{Y}$; $\vec{\xi}_0(\vec{x})$, $\vec{\zeta}(\vec{x}, t)$ are the errors of the initial state and parameters. If we suppose that the model and input data are exact, the error terms in (1)–(3) should be omitted. The boundary conditions for the closure of the model are the consequences of the physical content of the problem under investigation.

1.1. Variational description of the model

For the construction of the algorithms of the direct and inverse modeling, it is necessary to have both the differential and variational formulations of the models. Let us give the variational form of the model (1)–(3) by means of the integral identity [4, 5]

$$\begin{gathered} I(\vec{\varphi}, \vec{Y}, \vec{\varphi}^*) = \left(B\frac{\partial \vec{\varphi}}{\partial t} + G(\vec{\varphi}, \vec{Y}) - \vec{f} - \vec{r}, \vec{\varphi}^* \right) = 0, \\ \vec{\varphi} \in Q(D_t), \quad \vec{\varphi}^* \in Q^*(D_t), \quad \vec{Y} \in R(D_t). \end{gathered} \tag{4}$$

Here, $\vec{\varphi}^*$ is an arbitrary sufficiently smooth function, $Q^*(D_t)$ is the space of sufficiently smooth functions defined in D_t. The functional $I(\vec{\varphi}, \vec{Y}, \vec{\varphi}^*)$ in (4) is formed so that all the equations of model (1), initial and boundary conditions, conditions at the interface boundaries and external sources are included in it simultaneously.

The form of the functional and scalar product in (4) are generated from the form of the total energy balance equation for model (1).

1.2. The model of observational data

Now let us describe one more essential element of the investigation. Here we mean the data of measurements. In order to include them into the model processing, it is necessary to formulate the functional relationship between the measurements themselves and the state functions. Let this relation take the form

$$\vec{\Psi}_m = \vec{H}(\vec{\varphi}) + \vec{\xi}(\vec{x}, t), \tag{5}$$

Here $\vec{\Psi}_m = \{\vec{\Psi}_m(\vec{x}_k,\ k = \overline{1, K_0}\}$ is the set of observed values; $\vec{H}(\vec{\varphi})$ is the set of measurement models; $\vec{\xi}(\vec{x}, t)$ are the errors of these models, K_0 is a number of measurements. The values of $\vec{\Psi}_m$ are defined on the set of points $D_t^m \in D_t$.

1.3. Generalized characteristics of the processes

From the point of view of the computational technology, the methods of inverse modeling and sensitivity investigations are more suited to the work with global (integral) characteristics of the models and processes than to the work with the local ones. That is why we determine the set of such objects in the form

$$\Phi_k(\vec{\varphi}) = \int_{D_t} F_k(\vec{\varphi}(\vec{x}, t))\chi_k(\vec{x}, t) dDdt, \quad k = \overline{0, K}. \tag{6}$$

Here $F_k(\vec{\varphi})$ are some functions of $\vec{\varphi}$, $\chi_k(\vec{x}, t)dDdt$ is the Radon measure in the region D_t, and $\chi_k(\vec{x}, t)$ are non-negative weight functions.

In particular, the functions $\chi_k(\vec{x}, t)$ can have a finite support in D_t. For the functionals defined on the discrete set of points in D_t the measure $\chi_k(\vec{x}, t)dDdt$ is the Dirac measure located on unique point or on the set of points $D_t^m \in D_t$ [22]. Relations (5) have a local nature. Therefore, it is not convenient to include them into the modeling process directly. For these purposes, it is better to construct with their use the functional of the form (6)

$$\Phi_0(\vec{\varphi}) = \left(\left(\vec{\Psi}_m - \vec{H}(\vec{\varphi}) \right)^T \chi_o S \left(\vec{\Psi}_m - \vec{H}(\vec{\varphi}) \right) \right)_{D_t^m}, \tag{7}$$

where the index T denotes the operation of transposition. The vectors are arranged in columns. Functional (7) has the form of a scalar product with the positive definite weight matrix S and the weight function χ_0. They are defined in the domain D_t^m. If we choose the function χ_0 as a measure of a special type, the functional (7) can be rewritten in the integral form (6). Functional (7) is the quality functional of the model.

2. Discrete approximations of the models and functionals

Variational formulation (4) is used for the construction of the discrete approximations of the model. For these purposes, a grid D_t^h is introduced into the domain D_t and the discrete analogs $Q^h(D_t^h)$, $Q^{*h}(D_t^h)$, $R^h(D_t^h)$ of the corresponding functional spaces are defined on it. Then the integral identity (3) is approximated by its sum analog

$$I^h(\vec{\varphi}, \vec{Y}, \vec{\varphi}^*) = 0, \quad \vec{\varphi} \in Q^h(D_t^h), \quad \vec{\varphi}^* \in Q^{*h}(D_t^h), \quad \vec{Y} \in R^h(D_t^h). \tag{8}$$

The superscript h denotes the discrete analog of the corresponding object. Numerical schemes for the model (1) are obtained from the stationarity conditions of the functional $I^h(\vec{\varphi}, \vec{Y}, \vec{\varphi}^*)$ at arbitrary and independent variations of the grid functions $\vec{\varphi} \in Q^h(D_t^h)$ and $\vec{\varphi}^* \in Q^{*h}(D_t^h)$ at the grid nodes D_t^h [12].

Constructively, these conditions are realized by the operations

$$\frac{\partial}{\partial \vec{\varphi}^*} I^h(\vec{\varphi}, \vec{Y}, \vec{\varphi}^*) = 0, \quad \vec{\varphi}^* \in Q^{*h}(D_t^h). \tag{9}$$

The set of equations adjoint to (10) is obtained similarly

$$\frac{\partial}{\partial \vec{\varphi}} I^h(\vec{\varphi}, \vec{Y}, \vec{\varphi}^*) + \vec{\eta}(\vec{x}, t) = 0, \quad \vec{\varphi} \in Q^h(D_t^h). \tag{10}$$

Here $\vec{\eta}(\vec{x}, t)$ is some given function. Its form is defined with the specific use of the adjoint problem. This will be considered later. Differentiation in (9)–(10) is realized with respect to the function grid components at every grid point.

Boundary conditions in (9)–(10) are taken into account by the coefficients and parameters of discrete equations. This is a consequence of the sum functional.

If fractional time steps and decomposition into subdomains are used in the construction of identity (8), equations (9) and (10) are the numerical splitting schemes.

The number of the splitting stages is determined by the assignment of the number of fractional steps in time and the number of subdomains, and also by the type of quadrature formulas in time and in space. Description of specific approximations and methods for the realization of splitting-up schemes is given in [4, 5, 10, 12]. Note only, that the stability of computational algorithms in this way of the numerical model construction is provided by the property of energetic balance inherent in the identity (4). The numerical model is constructed using this property. The set of adjoint equations is a consequence of approximations of the basic model.

Investigation of the model sensitivity to the variations of input parameters is a necessary step in the solution of the numerical simulation problems. This is especially necessary in studying the real physical system behaviour with the help of numerical models. In this case sensitivity functions play a substantial role. In accordance with their definition they represent partial derivatives of the investigated state function characteristics with respect to model parameters. If the model is considered together with the observational data, then the sensitivity functions make it possible to realize interrelations between observations and models. Actually, algorithmically the sensitivity investigation gives numerical values of the gradients, that are required for the realization of optimization methods. By the way, we pose the problem of data assimilation by the models as a problem of optimization. The construction of the main sensitivity relation is made according to the algorithm

$$\delta I^h(\vec{\varphi}, \vec{\varphi}^*, \vec{Y}) = \frac{\partial}{\partial \xi} I^h(\vec{\varphi}, \vec{\varphi}^*, \vec{Y} + \xi \delta \vec{Y}) \mid_{\xi=0} \equiv R^h(\vec{\varphi}, \vec{\varphi}^*, \delta \vec{Y}), \tag{11}$$

where $\vec{\varphi}, \vec{\varphi}^*$ are the solution of (35) and (42) with the unpertubed values of $\vec{Y}$.

The calculation of the sensitivity function is made by the formula

$$\frac{\partial I^h}{\partial Y_i} = \frac{\partial}{\partial \delta Y_i} R^h(\vec{\varphi}, \vec{\varphi}^*, \delta \vec{Y}), \qquad i = \overline{1, N}. \tag{12}$$

3. Governing equations of basic model

Let us write governing system of equations of atmospheric hydrodynamics: the equations of motion

$$\frac{\partial \pi u}{\partial t} + M(\pi u) - f \pi v + m \pi \left[\frac{\partial \Phi}{\partial x} + \frac{RT}{\pi + p_T/\sigma} \frac{\partial \pi}{\partial x} \right] - D(u) = 0, \tag{13}$$

$$\frac{\partial \pi v}{\partial t} + M(\pi v) + f \pi u + m \pi \left[\frac{\partial \Phi}{\partial y} + \frac{RT}{\pi + p_T/\sigma} \frac{\partial \pi}{\partial y} \right] - D(v) = 0, \tag{14}$$

the thermodynamic equation

$$\frac{\partial \pi T}{\partial t} + M(\pi T) - D(T) - Q_T - \frac{RT}{c_p(\sigma + p_T/\pi)} \left[\pi \dot{\sigma} + \sigma \left(\frac{\partial \pi}{\partial t} + m \left(u \frac{\partial \pi}{\partial x} + v \frac{\partial \pi}{\partial y} \right) \right) \right] = 0, \tag{15}$$

the water vapour continuity equation

$$\frac{\partial \pi q}{\partial t} + M(\pi q) - D(q) - Q_q = 0, \tag{16}$$

the continuity equation

$$\frac{\partial \pi}{\partial t} + m^2 \left[\frac{\partial}{\partial x} \left(\frac{\pi u}{m} \right) + \frac{\partial}{\partial y} \left(\frac{\pi v}{m} \right) \right] + \frac{\partial \pi \dot{\sigma}}{\partial \sigma} = 0, \tag{17}$$

the hydrostatic equation

$$\frac{\partial \Phi}{\partial \sigma} + \frac{RT}{\sigma + p_T/\pi} = 0, \tag{18}$$

the equation for the surface pressure variations

$$\frac{\partial \pi}{\partial t} + m^2 \int_0^1 \left(\frac{\partial}{\partial x}\left(\frac{\pi u}{m}\right) + \frac{\partial}{\partial y}\left(\frac{\pi v}{m}\right)\right) d\sigma = 0. \tag{19}$$

The latter equation is the result of vertical integration of the continuity equation. The sigmadot ($\dot{\sigma}$) equation is also obtained by vertical integration of the continuity equation

$$\pi\dot{\sigma} + \int_0^\sigma \left(\frac{\partial \pi}{\partial t} + m^2 \left(\frac{\partial}{\partial x}\left(\frac{\pi u}{m}\right) + \frac{\partial}{\partial y}\left(\frac{\pi v}{m}\right)\right)\right) d\sigma' = 0. \tag{20}$$

The formula

$$\Phi(\sigma) = \Phi_s + \int_0^1 \frac{RT}{\sigma' + p_T/\pi} d\sigma' \tag{21}$$

is used to calculate Φ, where Φ_s is the surface geopotential. The operators $D(\varphi)$, in which φ denotes u, v, T or q, are the turbulent exchange operators, Q_T is the diabatic heating rate, Q_q is the source term in the water vapour equation,

$$M(\varphi) = m^2 \left(\frac{\partial}{\partial x}\left(\frac{u\varphi}{m}\right) + \frac{\partial}{\partial y}\left(\frac{v\varphi}{m}\right)\right) + \frac{\partial}{\partial \sigma}(\varphi\dot{\sigma}), \tag{22}$$

where $\varphi = \pi u$, πv, πT, πq; $\sigma = (p - p_T)/\pi$, $\pi = p_s - p_T$, p is pressure, p_s is a surface pressure, p_T is the pressure at the top of the model atmosphere, u, v, $\dot{\sigma}$ are the components of vector velocity $\vec{u}$, Φ is geopotential, T is temperature, f is the Coriolis parameter, R is the gas constant for the dry air, m is the map scale factor, c_p is a specific heat at a constant pressure.

3.1. The structure of the state functions and adjoint functions

Let us define the state function vector for the system (13)–(22) and introduce some auxilary notations which we shall need later on

$$\begin{aligned}
&\vec{\varphi} = \{\varphi_i,\ i = \overline{1,8}\} \equiv \{u, v, T, q, \dot{\sigma}, \chi, \Phi, \pi\} \in Q(D_t),\\
&\vec{\varphi}^* = \{\varphi_i^*,\ i = \overline{1,8}\} \equiv \{u^*, v^*, T^*, q^*, \dot{\sigma}^*, \chi^*, \Phi^*, \pi^*\} \in Q^*(D_t),\\
&\vec{\psi} = \{\psi_i,\ i = \overline{1,8}\} \equiv \{U, V, \tilde{T}, \tilde{q}, \dot{\Sigma}, \chi, \Phi, \pi/m\} \in Q(D_t),\\
&\vec{\psi}^* = \{\psi_i^*,\ i = \overline{1,8}\} \equiv \{U^*, V^*, \tilde{T}^*, \tilde{q}^*, \dot{\Sigma}^*, \chi^*, \Phi^*, \pi^*\} \in Q^*(D_t),\\
&\delta\vec{\varphi} = \{\delta\varphi_i,\ i = \overline{1,8}\}, \quad \delta\vec{\psi} = \{\delta\psi_i,\ i = \overline{1,8}\},\\
&\{\psi_i, \psi_i^*\} \equiv \{\pi\varphi_i/m, \pi\varphi_i^*/m\}, \quad i = \overline{1,5},\\
&\delta\psi_i = (\pi\delta\varphi_i + \varphi_i\delta\pi)/m, \quad \delta\varphi_i = (m\delta\psi_i - \varphi_i\delta\pi)/\pi, \quad i = \overline{1,5},\\
&\vec{c} = \{c_i, (i = \overline{1,8})\} \equiv \{1, 1, c_p, c_q, 1, 1, 1, 1\}.
\end{aligned} \tag{23}$$

Here $Q(D_t)$ is the space of sufficiently smooth functions $\vec{\varphi}$ which satisfy the boundary conditions; χ is the auxiliary function of the same structure as $\dot{\sigma}$; $\vec{\varphi}^*$ is a vector-function with sufficiently smooth components ("trial" functions), which are introduced for the formal definition of the main integral identity corresponding to the origin problem; $Q^*(D_t)$ is the space of the trial functions. Both vectors $\vec{\varphi}$ and $\vec{\varphi}^*$ are of the same time-space structure. $\vec{\psi}$ and $\vec{\psi}^*$ are the auxiliary definitions for the state and trial functions; $\delta\vec{\varphi}$ and $\delta\vec{\psi}$ are the variations of the state functions; c_i $(i = \overline{1,8})$ are the coefficients which serve to equalize the physical dimensions of different terms in the inner product; $D_t = D \times [0, \bar{t}\ ]$; $S_t = S \times [0, \bar{t}\ ]$; $\Omega_t = \Omega \times [0, \bar{t}\ ]$; $D = S \times [0 \le \sigma \le 1]$; $S = \{a \le x \le b, c \le y \le d\}$; Ω is the lateral boundary of D, $[0, \bar{t}\ ]$ is the time interval. The functions $\vec{\varphi}$ and $\vec{\psi}$ and their variations $\delta\vec{\varphi}$ and $\delta\vec{\psi}$ are one-to-one interrelated by the formulas of the variations in the vicinity of unperturbed values of the state vector.

Besides the state functions, the definition of the parameter vector and its variations is introduced

$$\begin{aligned}
&\vec{Y} = \{Y_i,\ i = \overline{1,N}\} \in R(D_t),\\
&\delta\vec{Y} = \{\delta Y_i,\ i = \overline{1,N}\}, \quad \vec{Y} + \zeta\delta\vec{Y} \in R(D_t),
\end{aligned} \tag{24}$$

where N is a number of the given parameters and $R(D_t)$ is a range of their admissible values, ζ is a real parameter. The vector-function of the initial state $\vec{\varphi}^0(\vec{x})$, source functions Q_T, Q_q, coefficients of the equations, boundary values of the state function and other prescribed values are included in the parameter vector. The variations of the parameters are considered in the vicinity of the prescribed unperturbed values of the $\vec{Y}$.

The specific feature of the σ-coordinate model is in the fact that there is some redundancy in the system (13)–(20). First, as the continuity equation (17) as the two its consiquences (19), (20) are used. Second, the time differtial operators are applied to the product of the state functions. To take this into account and to simplify the algorithmic realization, we introduce the dual definitions of the state and trial functions in (23) and include auxiliary components in them.

3.2. Boundary conditions

The boundary conditions for the state functions are defined by the physical closure of the model. For $\dot{\sigma}$ it is

$$\dot{\sigma} = 0 \quad \text{at} \quad \sigma = 0, 1. \tag{25}$$

The condition of the continuous approach to the background processes is used in the limited area models. In global models, the periodic conditions are involved. The interaction between the air and underlaying surface is taken into account at the low boundary in the frames of the boundary or surface layer parameterizations. The conditions of the interaction with the higher atmospheric layers are exploited at the upper boundary. The form of these conditions are dependent on the description of the turbulent exchange operators. The boundary conditions for $\vec{\varphi}^*$ are given in the connection with the conditions for the state functions. They are the consequences of both the variational formulation of the model and the structure of evaluable functionals (6).

4. Formulation of integral identity

First of all, it is necessary to introduce the scalar product in the space of the state functions

$$(\vec{\varphi}_1, \vec{\varphi}_2) = \int_{D_t} \sum_{i=1}^{7} c_i(\varphi_{1i}\varphi_{2i})\, dD\, dt + c_8 \int_{S_t} \pi_1 \pi_2\, dS\, dt, \tag{26}$$

where $\vec{\varphi}_1$, $\vec{\varphi}_2 \in Q(D_t)$, $dD = dS\, d\sigma$, $dS = dx\, dy/m^2$.

Let $G_i \equiv G_i(\vec{\varphi})$, $i = \overline{1,8}$, be the left-hand sides of the equations (13)–(16), (18), (20), (17), (19), accordingly, except the time derivatives. Then, using the operator notations, let us rewrite the system (13)–(20) in the operator form

$$B\frac{\partial \vec{\psi}}{\partial t} + \vec{G}(\vec{\psi}) = 0, \tag{27}$$

where $G(\vec{\psi}) \equiv \{G_i,\ i = \overline{1,8}\}$, B is the (8×8) square matrix defined by the local time structure of the model: $B = \{b_{ii} = 1$, for $i = \overline{1,4}, 8$; $b_{ii} = 0$, for $i = \overline{5,7}$; $b_{78} = 1$; the rest $b_{ij} = 0$, for $i, j = \overline{1,8}$, $i \neq j\}$.

The next point is to construct the main integral identity for the model. To this aim, the equations (27) are scalar multiplied by the arbitrary sufficiently smooth functions $\vec{\varphi}^* \in Q(D_t)$ in accordance with (26)

$$I(\vec{\varphi},\vec{\varphi^*})\equiv\Big(B\frac{\partial\vec{\psi}}{\partial t}+G(\vec{\psi}),\vec{\varphi^*}\Big)=\int_{D_t}\Big\{\sum_{i=1}^{4}c_i\Big(\frac{\partial\psi_i}{\partial t}+G_i(\vec{\psi})\Big)\varphi_i^*$$

$$+c_5G_5\dot{\sigma}^*+c_6G_6\chi^*+c_7\Big(\frac{\partial\pi/m}{\partial t}+G_7\Big)\Phi^*\Big\}dD\,dt$$

$$+\int_{S_t}c_8\Big(\frac{\partial\pi/m}{\partial t}+G_8\Big)\pi^*m\,dS\,dt=0. \qquad (28)$$

After substitution the expressions for G_i and c_i ($i=\overline{1,8}$) into (28), the identity can be transformed to the form which is more convinient for the construction of the discrete approximations and derivation of the main relations of the sensitivity theory of the mathematical models [18].

$$\begin{aligned}I(\varphi,\varphi^*) = \int_{D_t}&\Big\{\sum_{i=1}^{4}c_i\Big(\frac{\partial\psi_i}{\partial t}+M(\psi_i)+D(\psi_i)\Big)\varphi_i^*+\\
&f(Uv^*-Vu^*)-(C_p\pi Q_TT^*+\pi C_qQ_qq^*)/m+\\
&\frac{R\tilde{T}m}{\pi(\pi+p_T/\sigma)}\tau^*+\Big(\Phi^*-\Phi\frac{\partial\sigma T^*}{\partial\sigma}\Big)\frac{\partial}{\partial t}(\pi/m)+\\
&\Big[\dot{\Sigma}+\int_0^\sigma N(\sigma')d\sigma'-\sigma\int_0^1N(\sigma')d\sigma'\Big]\chi^*+\\
&\Big[m\Big(U^*\frac{\partial\Phi}{\partial x}+V^*\frac{\partial\Phi}{\partial y}\Big)+\dot{\Sigma}^*\frac{\partial\Phi}{\partial\sigma}\Big]-\\
&\Big[m\Big(U\frac{\partial\Phi^*}{\partial x}+V\frac{\partial\Phi^*}{\partial y}\Big)+\dot{\Sigma}\frac{\partial\Phi^*}{\partial\sigma}\Big]\Big\}md D dt+\\
\int_{S_t}&\Big\{\Big(\frac{\partial}{\partial t}(\pi/m)+\int_0^1N(\sigma')d\sigma'\Big)\Big\}\pi^*m\,dS\,dt+\\
\int_{\Omega_t}&U_n\Phi^*m\,d\Omega\,dt+\int_{S_t}\Phi_sT^*\frac{\partial}{\partial t}(\pi/m)m\,dS\,dt=0,\end{aligned} \qquad (29)$$

where

$$M(\psi_i)=m\Big[\frac{\partial}{\partial x}\Big(U\psi_i\frac{m}{\pi}\Big)+\frac{\partial}{\partial y}\Big(V\psi_i\frac{m}{\pi}\Big)+\frac{\partial}{\partial\sigma}\Big(\dot{\Sigma}\psi_i\frac{m}{\pi}\Big)\Big],$$

$$\tau^*=(\pi/\sigma)(\dot{\Sigma}^*-\dot{\Sigma}T^*)+m(U^*-UT^*)\frac{\partial\pi}{\partial x}+m(V^*-VT^*)\frac{\partial\pi}{\partial y},$$

$$N(\sigma)=m\Big(\frac{\partial U}{\partial x}+\frac{\partial V}{\partial y}\Big);$$

U_n is the normal components of the vectors $\vec{U}_s=(U,V)$, $d\Omega=\{dxd\sigma/m;\ dyd\sigma/m\}$.

As it is seen, in the first integrand the group of terms is organized posessing the antisymmetric character with respect to the functions $\vec{\psi}$ and $\vec{\varphi}^*$. These terms are responsible for the mutial energy exchange between the different parts of the model. The forms $(M(\psi_i), \varphi^*)$, $i = \overline{1,4}$, correspond to the transport operators, and $(D(\psi), \varphi^*)$ is the symmetric integral form of the diffusive operators. It is seen from (20), (21) that the functions $\dot{\sigma}$ and Φ are expressed by the other components of the state function and that is why they can be excluded from the system. Unfortunately, such procedure makes the formulas more complicated. To avoid these undesirable consequences, the three components with their multipliers $\dot{\sigma}^*$, χ^*, Φ^* are additionary included in (29).

The transport operators $M(\psi_i)$ posess the properties of antisymmery and energy balance:

$$\int_{D_t}\Big(\frac{\partial\psi_i}{\partial t}+M(\psi_i)\Big)\varphi_i^* m\, dDdt = -\int_{D_t}\Big(\frac{\partial\psi_i^*}{\partial t}+M(\psi_i^*)\Big)\varphi_i m\, dDdt + A(\psi_i, \varphi_i^*), \quad (30)$$

$$\int_{D_t}\Big(\frac{\partial\psi_i}{\partial t} + M(\psi_i)\Big)\varphi_i m\, dD\, dt = 0.5A(\psi_i, \varphi_i), \quad (31)$$

$$A(\psi_i, \varphi_i^*) = \int_D \psi_i\varphi_i\big|_0^{\bar{t}} m\, dD + \int_{\Omega_t} U_n\psi_i\varphi_i^* m^2\pi\, d\Omega\, dt, \quad i = \overline{1,4}.$$

The turbulent operators $D(\psi_i)$, $(i = \overline{1,4})$, are defined at the surfaces $\sigma = const$ in such a way that they are divergent, symmetric with respect to the ψ_i, φ_i and non-positive in D_t. In particular,

$$D(\psi_i) = m\, \mathrm{div}_s\, \mu_i\, \mathrm{grad}_s\, \psi_i + \frac{\partial}{\partial\sigma}\nu_i\frac{\partial\psi_i}{\partial\sigma}, \quad (32)$$

where μ_i, ν_i are the turbulent coefficients, s marks the horizontal operators. To complete the statement of the problem with turbulence, let us take the following boundary conditions

$$k_i\frac{\partial\psi_i}{\partial n} = r_i, \quad (\vec{x}, t) \in \Omega_t, \quad (33)$$

$$\nu_i\frac{\partial\psi_i}{\partial\sigma} = 0 \text{ at } \sigma = 0; \qquad \nu_i\frac{\partial\psi_i}{\partial\sigma} = \tau_i \text{ at } \sigma = 1. \quad (34)$$

The functions r_i in (33) are defined from the real conditions of the approach of the corresponding fields to their background values. τ_i in (34) are calculated with the help of the boundary or the surface layer models, which describe the regimes of the interaction of the atmosphere with the underlaying surface.

In the absence of turbulent exchange operators and external sources, after the substitution $\vec{\varphi}^* = \vec{\varphi}_a \equiv \{u, v, 1, q, \dot{\sigma}, 0, \Phi, 0\}$ into the integral identity (29), it turns to the energy balance equation

$$I(\vec{\varphi},\vec{\varphi}_a) = \left[\frac{1}{2}\int_D \pi(u^2+v^2+2c_pT+c_qq^2)dD + \int_S \Phi_s\pi dS\right]\Big|_0^{\bar{t}} + \frac{1}{2}\int_{\Omega_t}\pi u_n(u^2+v^2+2c_pT+c_qq^2+2\Phi)d\Omega\, dt = 0. \qquad (35)$$

The same property of energy balance should posess both the discrete analoque of (29) and the numerical model constructed on its basis.

5. The adjoint problem and sensitivity functions for the model in σ-coordinates

The specific character of the presentation of the hydrodynamical model in σ-coordinates is aslo seen in the structure of the ajoint equations. To take this into account, the insertion of the integral identity (29) to the general scheme of the variational principles of discretization and sensitivity investigations, described in Sections 3 and 4, is made with the help of the dual presentation of the state and trial function and their variations.

The main functional of the model in (29)

$$I(\vec{\varphi},\vec{\varphi}^*) \equiv I(\vec{\varphi},\vec{Y},\vec{\varphi}^*)$$

has got the rather complicated dependence on its arguments. That is why, for convinience, we shall describe all formulas in the differential form keeping in mind that all operations are carried out in the discrete form. First, let us extract three groups of the terms connected with (1) the transport operators, (2) turbulence operators, (3) the energy exchange in the system. Then, after linearization and variation procedures, the results are reorganized in two groups: (1) terms with the variations $\delta\vec{\psi}$ and (2) terms with the variations $\delta\vec{Y}$. Finally, the first group generates the adjoint problems (10), and the second one – the main sensitivity relation (11) and the sensitivity functions themselves (12).

5.1. The adjoint system

In accordance with (10), the conditions of the independence of the variations of the functional $\delta I(\vec{\varphi},\vec{\varphi}^*)$ on the variations of the components of the state function $\delta\vec{\psi} = \{\delta\psi_i,\ i=\overline{1,8}\}$ give us the system of adjoint equations [18]

$$-\frac{\partial u^*}{\partial t} + M^*u^* + fv^* - m\left(\frac{\partial\Phi^*}{\partial x} + aT^*\frac{\partial\pi}{\partial x} + \frac{\partial}{\partial x}\left(\int_\sigma^1 \chi^* d\sigma' - \int_0^1 \sigma'\chi^* d\sigma'\right)\right) - \sum_{i=1}^4 c_i\left(\frac{m^2}{\pi}\right)\psi_i\frac{\partial\varphi_i^*}{\partial x} - D(u^*) + \eta_1 = 0, \qquad (36)$$

$$-\frac{\partial v^*}{\partial t} + M^*v^* - lu^* - m\Big(\frac{\partial \Phi^*}{\partial y} + aT^*\frac{\partial \pi}{\partial y} + \frac{\partial}{\partial y}\Big(\int_\sigma^1 \chi^* d\sigma' - \int_0^1 \sigma'\chi^* d\sigma'\Big)\Big) -$$
$$\sum_{i=1}^{4} c_i\Big(\frac{m^2}{\pi}\Big)\psi_i\frac{\partial \varphi_i^*}{\partial y} - D(v^*) + \eta_2 = 0, \tag{37}$$

$$-\frac{\partial T^*}{\partial t} + M^*T^* + \frac{Rm}{\pi(\pi + p_1/\sigma)}\tau^* - D(T^*) + \eta_3 = 0, \tag{38}$$

$$-\frac{\partial q^*}{\partial t} + M^*q^* - D(q^*) + \eta_4 = 0, \tag{39}$$

$$m\Big(\frac{\partial U^*}{\partial x} + \frac{\partial V^*}{\partial y}\Big) + \frac{\partial \dot\Sigma^*}{\partial \sigma} + \frac{\partial \sigma T^*}{\partial \sigma}\frac{\partial}{\partial t}\Big(\frac{\pi}{m}\Big) - \eta_5 = 0, \tag{40}$$

$$\chi^* - \frac{a\pi T^*}{\sigma} - \frac{\partial \Phi^*}{\partial \sigma} - \sum_{i=1}^{4} c_i\psi_i\frac{\partial \varphi_i^*}{\partial \sigma} + \eta_6 = 0, \tag{41}$$

$$\Phi^* - \pi a T^* + \eta_7 = 0, \tag{42}$$

$$\frac{\partial}{\partial t}(\pi^*/m) + \frac{a(2\pi + p_T/\sigma)}{\pi(\pi + p_T/\sigma)}\tau^* + \frac{a}{\sigma}(\dot\Sigma^* - \dot\Sigma T^*) +$$
$$m\Big(\frac{\partial}{\partial x}a(U^* - UT^*) + \frac{\partial}{\partial y}a(V^* - VT^*)\Big) +$$
$$\frac{1}{\pi^2}\sum_{i=1}^{4} m^2 c_i\psi_i\Big(\vec{U}_s\,\mathrm{grad}_s\,\varphi_i^* + (\dot\Sigma/m)\frac{\partial \varphi_i^*}{\partial \sigma}\Big) - \eta_8 = 0, \tag{43}$$

$$a \equiv (RT)/(\pi + p_T/\sigma).$$

The conditions

$$u^* = 0, \quad v^* = 0, \quad T^* = 0, \quad q^* = 0, \quad \pi^* = 0, \quad \text{at } t = \bar{t} \tag{44}$$

are obtained from the same reasons. The discrete analog of the ajoint equations and the scheme of their solution are the consequences of both the integral identity and the scheme of realization of the direct problem. The equations (40)–(42) are axiliary. The time integration, starting with $t = \bar{t}$, is made in the inverse direction.

The components $\vec{\eta} = \{\eta_i,\ i = \overline{1,8}\}$ are introduced into the system to solve the problems of the sensitivity for the dynamical model. The concrete form of this vector is obtained by the gradients of the quality functional. The vector-gradient is calculated with respect to the components $\vec{\psi}$.

5.2. Dependence of variations on the input parameters and sensitivity functions

If to suppose that the function $\vec{\varphi}^*$ satisfies the homogenious system (36)–(43) (i.e., at $\vec{\eta} = 0$), and the condition (44), it is obtained

$$\delta I(\vec{\varphi}, \vec{Y}, \vec{\varphi}^*) = \left(\frac{\partial I(\vec{\varphi}_i, \vec{\varphi}^*)}{\partial \vec{Y}}, \delta \vec{Y}\right) \equiv R(\vec{\varphi}, \vec{\varphi}^*, \delta \vec{Y})$$

$$= \int_{D_t} (c_3 \delta Q_T T^* + c_4 \delta Q_q q^*) dD\, dt + \int_D \sum_{i=1}^{4} c_i \delta \psi_i \varphi_i^* |_{t=0} m\, dD +$$
$$R_1(\vec{\varphi}, \vec{\varphi}^*, \delta \vec{Y}) + R_2(\vec{\varphi}, \vec{\varphi}^*, \delta \vec{Y}) + R_3(\vec{\varphi}, \vec{\varphi}^*, \delta \vec{Y}), \tag{45}$$

where R_1, R_2, R_3 are given by

$$R_1(\vec{\varphi}, \vec{\varphi}_i^*, \delta \vec{Y}) \equiv \int_{\Omega_t} \Big\{ \delta U_n \sum_{i=1}^{4} c_i \psi_i \varphi_i^* \frac{m^2}{\pi} + \sum_{i=1}^{4} c_i U_n \delta \psi_i \varphi_i^* \frac{m^2}{\pi} -$$
$$\frac{\delta \pi}{\pi^2} \sum_{i=1}^{4} m^2 c_i U_n \psi_i \varphi_i^* \Big\} d\Omega\, dt. \tag{46}$$

$$R_2(\vec{\varphi}, \vec{\varphi}_i^*, \delta \vec{Y}) \equiv \sum_{i=1}^{4} c_i \Big\{ \int_{D_t} \Big[\delta \mu_i \operatorname{grad}_s \psi_i \operatorname{grad}_i \varphi_i^* + \frac{\delta \nu_i}{m} \frac{\partial \psi_i^*}{\partial \sigma} \frac{\partial \varphi_i^*}{\partial \sigma} \Big] m^2\, dD dt +$$
$$\int_{\Omega_t} \delta r_i \varphi_i^* m\, d\Omega\, dt + \int_{S_t} \delta \tau_i \varphi_i^* m\, dS\, dt \Big\}, \tag{47}$$

$\delta \mu_i$, $\delta \nu_i$, δr_i, $\delta \tau_i$ $(i = \overline{1,4})$ are the variations of $\vec{Y}$.

$$R_3(\vec{\varphi}, \vec{\varphi}^*, \delta \vec{Y}) \equiv \int_{\Omega_t} \{ \Phi^* \delta U_n + U_n^* \delta \Phi + (U_n^* - U_n T^*) \delta \pi - \pi T^* \delta U_n \} m\, d\Omega\, dt -$$
$$\int_S (T^* \delta(\Phi_s \pi) + \pi^* \delta \pi)|_{t=0} dS. \tag{48}$$

The variations of functionals

$$\delta \Phi_k(\vec{\varphi}) = (\operatorname{grad}_{\vec{Y}} \Phi_k(\vec{\varphi}), \delta \vec{Y}), \quad k = \overline{1,K}, \tag{49}$$

are used as the measure of the model sensitivity, where

$$\operatorname{grad}_{\vec{Y}} \Phi_k(\vec{\varphi}) = \Big\{ \frac{\partial \Phi_k(\vec{\varphi})}{\partial Y_i}, \quad i = \overline{1,N} \Big\}$$

is the set of the sensitivity functions of (6) to the variations of the parameters $\delta \vec{Y}$ in the vicinity of undisturbed their values $\vec{Y}$.

The algorithm for the calculation of variations consists of some steps [13]:

1. The direct problem with the undisturbed values of the parameter vector is solved in the discrete form (9). As a result, the solution $\vec{\varphi}$ is obtained.

2. The set of the vectors are calculated

$$\vec{\eta}_k = \frac{\partial \Phi_k^h(\vec{\varphi})}{\partial \vec{\psi}} \equiv \left\{\eta_{ki} = \frac{\partial F_k^h(\vec{\varphi})}{\partial \vec{\psi}_i} \chi_k(\vec{x}, t),\ i = \overline{1,8}\right\}, \quad k = \overline{1,K}. \tag{50}$$

3. The set of the adjoint problems (36)–(44) with the source term $\{\vec{\eta}_k,\ k = \overline{1,K}\}$ are solved. The result is $\{\vec{\varphi}_k^*,\ k = \overline{1,K}\}$.

4. With the use of $\{\vec{\varphi}, \vec{\varphi}_k^*,\ k = \overline{1,K}\}$, the sensitivity formulas are constructed as

$$\delta\Phi_k^h(\vec{\varphi}) = R^h(\vec{\varphi}, \vec{\varphi}_k^*, \delta\vec{Y}), \quad k = \overline{1,K}, \tag{51}$$

where $R^h(\vec{\varphi}, \vec{\varphi}_k^*, \delta\vec{Y})$ is obtained from (11) and (45) by the substitution of the values $\vec{\varphi}^* = \vec{\varphi}_k^*,\ k = \overline{1,K}$.

To find out the expressions for the sensitivity functions, the coefficients with the same components of the vector of variations $\delta\vec{Y}$ in (49), (45) and (51) are equated with each other. This action is equivalent to the calculations of

$$\operatorname{grad}_{\vec{Y}} \Phi_k^h(\vec{\varphi}) = \left\{\frac{\partial}{\partial \delta Y_i} R^h(\vec{\varphi}, \vec{\varphi}_k^*, \delta\vec{Y}),\ i = \overline{1,N}\right\}, \quad k = \overline{1,K}. \tag{52}$$

The differentiation in (52) is carried out on the whole set of the components of $\delta\vec{Y}$ in its discrete form. If to subsitute the concrete values of $\{\vec{\varphi}, \vec{\varphi}_k^*,\ k = \overline{1,K}\}$ into the formulas, the numerial values of the sensitivity functions are obtained.

6. The basic algorithm of data assimilation, diagnostics of the model and inverse modeling

Let us use the ideas of the optimization theory and the variational technique for the statement of the inverse problems and for the construction of methods for their solution. In this case, all approximations are defined by the structure of the quality functional and by the way of its minimization on the set of values of the state functions, parameters and errors of the discrete formulation of the model [13, 21].

The basic functional is formulated so that all the available real data, errors of the numerical model and input parameters are taken into account:

$$\Phi(\vec{\varphi}) = 2\Phi_k(\vec{\varphi}) + \left(\vec{r}^T M_2 \vec{r}\right)_{D_t^h} + \left(\left(\vec{\varphi}^0 - \vec{\varphi}_a^0\right)^T M_o \left(\vec{\varphi}^0 - \vec{\varphi}_a^0\right)\right)_{D^h} + \left(\left(\vec{Y} - \vec{Y}_a\right)^T M_1 \left(\vec{Y} - \vec{Y}_a\right)\right)_{R^h(D_t^h)} \quad 2I^h(\vec{\varphi}, \vec{Y}, \vec{\varphi}^*). \tag{53}$$

Here the first term is given by (6), (7), the second term takes into account the model errors, the third term describes errors in the initial data, the fourth term is responsible for the errors of the parameters, and the fifth one is a numerical model of the processes in a variational form. M_0, M_1, M_2 are weight matrices. The stationarity conditions for the functional (53) gives us the system of equations [21]

$$B\Lambda_t\vec{\varphi} + G^h(\vec{\varphi}, \vec{Y}) - \vec{f} = \vec{r}, \tag{54}$$

$$(B\Lambda_t)^T\vec{\varphi}_k^* + A^T(\vec{\varphi}, \vec{Y})\vec{\varphi}_k^* + \vec{\eta}_k = 0, \tag{55}$$

$$\vec{\varphi}_k^*(\vec{x})\,|_{t=\bar{t}} = 0, \tag{56}$$

$$\vec{\eta}_k(\vec{x}, t) = \mathrm{grad}_{\vec{\varphi}}\,\Phi_k^h(\vec{\varphi}) \equiv \frac{\partial\Phi_k^h(\vec{\varphi})}{\partial\vec{\varphi}}, \tag{57}$$

$$\vec{\varphi}^0 = \vec{\varphi}_a^0 + M_0^{-1}\vec{\varphi}_k^*(0), \qquad t = 0, \tag{58}$$

$$\vec{r}(\vec{x}, t) = M_2^{-1}(\vec{x}, t)\vec{\varphi}_k^*(\vec{x}, t), \tag{59}$$

$$\vec{Y} = \vec{Y}_a + M_1^{-1}\vec{\zeta}_k, \tag{60}$$

$$\vec{\zeta}_k = \frac{\partial}{\partial\vec{Y}} I^h(\vec{\varphi}, \vec{Y}, \vec{\varphi}_k^*), \tag{61}$$

$$A(\vec{\varphi}, \vec{Y})\vec{\varphi}' = \frac{\partial}{\partial\alpha}\left[G^h(\vec{\varphi} + \alpha\vec{\varphi}', \vec{Y})\right]|_{\alpha=0}, \tag{62}$$

where Λ_t is a discrete approximation of time differential operator, $\vec{\zeta}_k$ are the functions of model sensitivity to the variations of parameters, and α is a real parameter. For the purposes of diagnosis of the models, data assimilation, identification of parameters, index k is set equal to zero and this means that the functional $\Phi_0^h(\vec{\varphi})$ participates in (53) and (57).

System of equations (54)–(62) is solved with respect to $\vec{r}$, $\vec{\varphi}^0$, $\vec{Y}$ by the iterative procedures beginning with the initial approximations for the sought functions

$$\vec{r}^{(0)} = 0; \qquad \vec{\varphi}^{0(0)} = \vec{\varphi}_a^0; \qquad \vec{Y}^{(0)} = \vec{Y}_a. \tag{63}$$

Three basic elements are necessary for the realization of the method:

(1) algorithm for the solution of the direct problem (9), (54);

(2) algorithm for the solution of the adjoint problem (10), (55);

(3) algorithm for the calculation of sensitivity functions $\vec{\zeta}_k$ with respect to the variations of the parameters (11), (12), (60). Let us note that the

second term in the quality functional (53), which takes into account the errors of the model, additionally playes the role of regulator of calculations.

Iterations are not carried out for the investigation of model sensitivity. First, one cycle of calculations is made for each functional $\Phi_k^h(\vec{\varphi})$, $k = \overline{0, K}$ to find the functions $\vec{\varphi}$,$\vec{\varphi}_k^*$,$\vec{\zeta}$. Then the main sensitivity relationsis constructed:

$$\delta\Phi_k(\vec{\varphi}) = (\vec{\zeta}_k, \delta\vec{Y}) = \frac{\partial}{\partial\alpha} I^h(\vec{\varphi}, \vec{Y}_a + \alpha\delta\vec{Y}, \vec{\varphi}_k^*) \,|_{\alpha=0} \,. \tag{64}$$

If to exclude adjoint function $\vec{\phi}^*$ from the system of equations (54)–(61), the result will be the procedure of the Kalman–Bucy type [1]. Indeed, if matrix B is nonsingular one and $k = 0$, then after simple operations the following system of equations are obtained from (54)–(59) [13, 16]

$$B\frac{\partial\vec{\varphi}}{\partial t} + G^h(\vec{\varphi}, \vec{Y}) - \vec{f} = BPB^{-1}\Big(\frac{\partial\vec{H}(\vec{\varphi})}{\partial\vec{\varphi}}\Big)^T \chi_o S(\vec{\Psi}_m - \vec{H}(\vec{\varphi})), \tag{65}$$

$$B\frac{\partial P}{\partial t} + AP + BPB^{-1}\Big(A^T + \Big(\frac{\partial\vec{H}(\vec{\varphi})}{\partial\vec{\varphi}}\Big)^T \chi_o S \frac{\partial\vec{H}(\vec{\varphi})}{\partial\vec{\varphi}} P\Big) = M_2^{-1}, \tag{66}$$

$$\vec{\varphi} = \vec{\varphi}_a^0, \qquad P(\vec{x}, 0) = M_0^{-1}B, \quad \text{at} \quad t = 0, \tag{67}$$

where $P = P(\vec{x}, t)$ is $n \times n$ weight matrix, n is dimension of the functions $\vec{\varphi}$ and $\vec{\varphi}^*$ in discrete form. The system (65)–(67) is the scheme of the first order extended Kalman filtering. In the case when $B = E$ and operators $G^h(\vec{\varphi}, \vec{Y})$ and $\vec{H}(\vec{\varphi})$ are linear with respect to $\vec{\varphi}$, the system of equation (54)–(59) is algebraically identical to the scheme of Kalman filtering (65)–(67). And it is not surprising because both types of procedures are generated by the same quality functional (53). If to keep in mind the dimensions of matrices and vectors and to compare the computational costs of realizations of the algorithms, the following conclusion can be done. For the problems of oceanic and atmospheric dynamics, the filtering of the Kalman type has not adventage over the algoritm of data assimilation with the use of the adjoint problems and sensitivity functionals. It is essential that ajoint problems and sensitivity functions for all functionals can be simultaniously and parallelly calculated. It is due to the fact that the problems (55) differ just by the right-hand sides. The solution of the system (54) is the usual stage of the direct modeling. Its result is the reconstruction of the space-time behavior of the state function $\vec{\varphi}$ in the grid domain D_t^h. It is worth to mention that the algorithm (54)–(62), while working for the data assimilation, is typical algorithm of computing tomography of the natural object with respect to observational data.

7. Design of observational experiment

State function plays an important role in the understanding of physical processes in the climatic system. But it is difficult to estimate the observed system behaviour only with this function. In particular, this is due to the fact that not all the characteristics of the investigated processes can be measured directly. Introduction of adjoint problems allows to relate mathematical models with observations. Using them sensitivity and influence functions for the evoluated functional can be calculated and optimal plans for observations can be constructed. Calculation of the influence functions is especially useful for the solution of problems on the limited territory. In this case estimates for the influence domains for the considered territory help us to understand how to treat boundary conditions on the lateral boundaries and how to realize interaction between models of different scales. The design of observational experiments with the help of sensitivity functions was described in [12, 16]. The model of pollutants' transport in the atmosphere was taken there as an example. Here we consider one more approach connected with the problems of data assimilation.

The functionals of the type (7) are defining ones at the stage of data assimilation. To construct them all kinds of available data are taken into account. The points of observation are proposed to be fixed.

While the problem of design is solved the locations of the points $\vec{x_k}$ will be changed according to the given criterion. As usual, this criterion is the condition of obtaining the acceptable accuracy of estimations of desired parameters [23]. Due to nonlinearity of the models we shall use the ideas of successive design of observations [23]. Let us suppose that the law of the moving of the observational points can be parameterized by

$$x_{\vec{k}\tau} = \vec{x_k} + \tau\vec{V}(\vec{x_k}), \qquad x_{\vec{k}\tau}, \vec{x_k} \in D_t, \tag{68}$$

where $\vec{x_k}$ and $x_{\vec{k}\tau}$ are starting and planning observational points, $\vec{V}(\vec{x_k})$ is the "rate" in the space of design, τ is a parameter. In the contrary of the data assimilation problem where the influence domains of all observations could be supperposed the design problem demands to separate the influence domains of each observation. To this goal we write the result of each observation from (5) as a functional

$$\Psi_m(\vec{x_k}) = H(\vec{\varphi}) \mid_{\vec{x}=\vec{x_k}} = \int_{D_t} H(\vec{\varphi})\chi(\vec{x} - \vec{x_k})dDdt, \quad \vec{x_k} \in D_t^m, \tag{69}$$

where $\chi(\vec{x} - \vec{x}_k)dDdt$ is the Dirac measure in the point $\vec{x_k}$. The sensitivity functions with respect to the variations of the evaluated model parameters and the coordinates of the observational points $\vec{x_k}$ are calculated for the functionals. For these aims the modification of the basic algorithm from the previous item is constructed. Using it, the problem of minimizing of the goal functional with respect to the parameters $\vec{V}(\vec{x_k})$ and τ of the equations (6) is solved. It should be mentioned that the solution of the optimization problems, particularly the problems of the experimental design, is not easy to obtain. Iterative techniques demand the interactive procedures for choosing the parameters influencing on the behavior and convergence of algorithms. In such cases the sensitivity functions give us the auxiliary information for the organization of the interactive calculations.

8. Conclusion

The use of models together with observational data expands the possibilities of mathematical modeling for the estimation of climatic changes and for the solution of ecological problems. For these goals it is necessary to develop the methods of direct and inverse modeling. The variational methods of optimization can be used as an instrument for the realization of the inverse modeling and diagnostic investigations.

The algorithms for the solution of the inverse and optimizational problems are closed in the sense that all stages of calculations in them are mutually agreed. Nevertheless, the trouble with the rate of convergence of iterations as well as the difficulties with the choose of the appropriate weight matrices in the functional (53) and of the *a priori* estimations for the desirable functions may occur. It is due to nonlinearity of the models, the presence of limitations, the huge number of internal and external degrees of freedom in the discrete presentation of the models, etc. For the efficient realization of the goals we need the interactive methods of modeling. From this point of view the methods of calculation of sensitivity functions for the model of complicated structure and the differential functionals of general form are the most advanced parts of the investigations. The adjoint problems allow us to exclude the internal degrees of freedom in the external cycles of optimization methods. The sensitivity functions give us the constructive basis for the interactive analysis and control the calculations.

References

[1] K.E. Kalman, *A new approach to linear filtering and prediction problems*, ASME J. Basic Eng., **82**, 1960, 127–139.

[2] J.L. Lions, *Optimal control of systems governed by partial differential equations*, Springer-Verlag Berlin, 1971.

[3] F.X. Le Dimet, *Contribution aux methodes variationelles en meteorologie*, Universite de Clermont II, 1985.

[4] G.I. Marchuk, *Numerical solution of the problems of atmospheric and oceanic dynamics*, Leningrad, Gigrometeoizdat, 1974 (in Russian).

[5] G.I. Marchuk, *Mathematical modeling in the environmental problems*, Moscow, Nauka, 1982 (in Russian).

[6] G.I. Marchuk, *Adjoint equations and analysis of the complex systems*, Moscow, Nauka, 1992 (in Russian).

[7] G.I. Marchuk, V.V. Penenko, *Applications of perturbation theory to problems of simulation of atmospheric processes*, In: Monsoon Dynamics, Cambridge, University Press., 1981, 639–655.

[8] V.V. Penenko, *Computational aspects in simulating dynamics of atmospheric processes and estimating the influence of different factors on atmospheric dynamics*, In: Nekotorye problemy vychislitelnoy i prikladnoy matematiki, Novosibirsk, Nauka, 1971, 61–75 (in Russian).

[9] V.V. Penenko, N.N. Obraztsov, *A variational initialization method for the fields of meteorological elements*, Meteorologiya i Gidrologiya (English translation), **11**, 1976, 1–11.

[10] V.V. Penenko, A.E. Aloyan, *Models and methods for environmental problems*, Novosibirsk, Nauka, 1985 (in Russian).

[11] V.V. Penenko,*Mathematical models for the environmental protection design*, Novosibirsk, Computing Center SOAN SSSR, Preprint No. 736, 1987 (in Russian).

[12] V.V. Penenko, *Methods of numerical modeling of the atmospheric processes*, Leningrad, Gidrometeoizdat, 1981 (in Russian).

[13] V.V. Penenko, *System organization of the mathematical models for the problems of atmospheric physics, ocean and environmental protection*, Preprint No. 69, Novosibirsk, Computing Center, 1985 (in Russian).

[14] V.V. Penenko, *Application of the adjoint equations and optimization in models of hydrodynamics of the atmosphere and ocean* , In: The problems of investigation of general circulation of the atmosphere and ocean, Leningrad, Gidrometeoizdat, 1990, 89–95 (in Russian).

[15] *Proceedings of the International Symposium on Assimilation of Observations in Meteorology and Oceanography*, Clermont-Ferrand, France, 1990.

[16] V.V. Penenko, *Numerical methods of model quality estimations and assimilation of observations*, Bull. Nov. Comp. Center, Num. Model. in Atmosph.,etc., 1(1993), 69–90.

[17] V.V. Penenko, *Numerical models and methods for the solution of the problems of ecological forecast and design*, Survey of the Applied and Industry Mathematics, **1**, No. 6, 1994, 917–941.

[18] V.V. Penenko and E.A.Tsvetova, *The adjoint problem and sensitivity algorithms for the model of atmospheric hydrodynamics in σ-coordinates* , Bull. Nov. Comp. Center, Num. Model. in Atmosph.,etc., 2(1995), 53–74.

[19] V.V. Penenko, *Numerical schemes for the advective-diffusive equations with the use of the local adjoint problems*, Novosibirsk, Computing Center, Preprint No. 984, 1993 (in Russian).

[20] V.V. Penenko, *An explicit-implicit method for the solution of the problems of dynamic adjustment of meteorological fields*, Novosibirsk, Computing Center, Preprint No. 1037, 1994 (in Russian).

[21] V.V. Penenko, *Methodology of inverse modeling for the problems of climate changes and environmental protection*, In: Advanced Mathematics: Computations and applications, NCC Publisher, 1995, 358–367.

[22] L. Schwartz, *Analise matematique*, Hermann, 1967.

[23] S.M. Yermakov, A.N. Ghiglyavskii, *Mathematical Theory of Optimal Experiment*, Moscow, Nauka, 1987 (in Russian).