Bull. Nov. Comp. Center, Num. Model. in Atmosph., etc., 1 (1993), 69–90

Numerical methods of model quality estimations and assimilation of observations

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The methods of the combined use of mathematical models and observed data for the environmental monitoring and forecasting purposes are described. The interaction between models and data are based on variational principle. It includes the reconstruction of state functions, identification of parameters and diagnostic estimation of the model quality on the observed data; consistence of information from diverse observational systems; investigation of model sensitivity to the variations of input parameters; observational experiment design. The application of these techniques to the models of atmospheric hydrodynamics and transport of pollutants are presented.

1. Introduction

The questions concerned with 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. 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 combination results in the closed formulation of the problems and to the logical in its sense 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 [1–5]. Problems of analysis and assimilation of observations using numerical models offer wide possibilities for the utilization of these methods. Detailed review of different applications of variational methods in meteorology is given in [6]. This paper is based on the results of the works described in [7–13].

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 let us take the appropriate interpolation procedure as a model of such observations. In this case interpolation must be carried out from the simulated fields to the measurements, i.e., the state function values, calculated with the models, are transferred to the set of points, where measurements are made.

2. Statement of the problem and constuction of the discrete approximations

State functions and parameters are the major definitions in the description of mathematical models. 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 be also referred either to the unknown parameters or to the state functions.

For the convenience of further description let us take advantage of the operational notations. Write the model equations in the form

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

The following notations are used here:

$\vec{\varphi}$ – state vector,

$\vec{Y}$ – parameter vector,

B – diagonal matrix, some diagonal elements of which can be zero,

$G(\vec{\varphi}, \vec{Y})$ – non-linear matrix operator, depending on the state function and parameters,

$\vec{f}$ – function of sources,

$D_t = D \times [0, \bar{t}]$,

D – domain of the spacial variables $\vec{x}$,

$[0, \bar{t}]$ – time interval,

$Q(D_t)$ – space of state functions satisfying the boundary conditions,

$R(D_t)$ – range of admissible parameter values.

For the considered class of problems operator $G(\vec{\varphi}, \vec{Y})$ is defined by the hydrothermodynamic equations of the "atmosphere-ocean-earth" system and by the relations at the interface boundaries. It includes all the terms of equations except the time derivatives. With respect to the state function components $\vec{\varphi}$ this is a non-linear matrix operator with partial derivatives. In the stationary case B–matrix is zero.

The mathematical model (1) implicitly defines the transformation, in which the set of parameter values $\vec{Y}$ and the initial state $\vec{\varphi}^0$ correspond to the set of the state function values.

The computational algorithm for the solution of problem (1) fulfils the constructive realization of transformation

$$\vec{\varphi} = \vec{\varphi}(\vec{x}, t, \vec{Y}, \vec{\varphi}^0), \quad (\vec{x}, t) \in D_t, \quad \vec{Y} \in R(D_t) \tag{2}$$

determining the state vector as a function of independent variables, the model input parameters and initial data.

The generalized representation in the form of the integral identity

$$I(\vec{\varphi},\vec{Y},\vec{\varphi}^*) = \left(B\frac{\partial\vec{\varphi}}{\partial t} + G(\vec{\varphi},\vec{Y}) - \vec{f},\vec{\varphi}^*\right) = 0,$$
$$\vec{\varphi} \in Q(D_t), \quad \vec{\varphi}^* \in Q^*(D_t), \quad \vec{Y} \in R(D_t) \tag{3}$$

is used for the construction of discrete analog of the model (1). 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 (3) is formed so that all the equations of the model (1), initial and boundary conditions, conditions at the interface boundaries and external sources were included in it simultaneously. Main requirements for the choice of the functional identity are as follows:

- model descriptions for sufficiently smooth functions in the forms (1) and (3) must be equivalent;
- equations for the balance energy, mass, moments, substance amount, etc. can be obtained from the identity (3) by definite specification of trial function $\vec{\varphi}^*$ without additional differentiation and integration.

These requirements determine the structure and the type of boundary conditions of functions $\vec{\varphi}^*$. Examples of the integral identity construction for the considered class of models are given in Sections 7, 8 and in [10, 12].

One thing should be mentioned. If the energetic functional is introduced for the "atmosphere-ocean-earth" system and an identity of the type (3) is built on it, then the conditions for the fluxes at the atmosphere-ocean, atmosphere-soil, ocean-continent interface appear to be natural for the variational functional. Due to this the solution of questions, associated with the approximation of boundary conditions and the concordance of the process scales is made easier.

Depending on the aims of investigation, specification of the domain D_t, and the functions $\vec{\varphi}$, $\vec{\varphi}^*$ definition the identity is obtained for the entire "atmosphere-ocean-earth" system or for every subsystem. Domain decomposition is obtained by the specification of trial functions $\vec{\varphi}^*$.

Procedures of data assimilation require high degree of concordance between different elements of numerical model and computational algorithms. Such agreement is provided with the help of the integral identity (3) and its discrete analogs.

Let us briefly describe the method of the discrete approximation construction. To be concrete, the finite-difference approximation is considered. Discrete analogs will be denoted by the superscript h. A grid D_t^h will be introduced into the domains D and the discrete analogs $Q^h(D_t^h)$,

$Q^{*h}(D_t^h)$, $R^h(D_t^h)$ of the corresponding functional spaces will be defined on it. Then the integral identity (3) will be approximated. In the general case it includes 4-multiple integrals in time and spatial coordinates. Let us replace the integrals by cubic formulas, and the derivatives – by finite differences. Fractional steps will be introduced in time, and the space will be decomposed into subdomains when required. Then the method of weak approximation will be used, and separate terms of the identity will be approximated at different fractional steps. The properties of energetic balance, inherent in the identity (3) must be conserved. As a result the summation analog of the identity (3) will be obtained

$$I^h(\vec{\varphi},\vec{Y},\vec{\varphi}^*) = 0, \quad \vec{\varphi} \in Q^h(D_t^h), \quad \vec{\varphi}^* \in Q^{*h}(D_t^h), \quad \vec{Y} \in R^h(D_t^h). \quad (4)$$

Numerical schemes for the model (1) will be 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 $\vec{\varphi} \in Q(D_t)$ and $\vec{\varphi}^* \in Q^*(D_t)$ in the grid nodes D_t^h [10].

Constructively these conditions are realized by the operations

$$\frac{\partial}{\partial\vec{\varphi}^*} I^h(\vec{\varphi},\vec{Y},\vec{\varphi}^*) = 0, \quad \vec{\varphi}^* \in Q^*(D_t). \quad (5)$$

Differentiation is realized with respect to the function grid components at every grid point. Thus, (5) gives the set of basic equations approximating the system (1) with the boundary conditions in the grid nodes. In this case approximation is understood as weak. Its accuracy depends on deviation between functionals $I(\vec{\varphi}, \vec{Y}, \vec{\varphi}^*)$ and $I^h(\vec{\varphi}, \vec{Y}, \vec{\varphi}^*)$ in the corresponding functional spaces. If the smoothness of the functions $\vec{\varphi}$ and $\vec{\varphi}^*$ is sufficient, the obtained approximation has accuracy in a usual sense, i.e., locally at every grid point D_t^h .

The set of equations adjoint to the equation (5) is obtained similarly

$$\frac{\partial}{\partial\vec{\varphi}} I^h(\vec{\varphi},\vec{Y},\vec{\varphi}^*) + \vec{\eta}(\vec{x},t) = 0, \quad \vec{\varphi} \in Q^h(D_t^h). \quad (6)$$

Here $\vec{\eta}(\vec{x},t)$ is some given function. Its form is defined at specific utilizations of the adjoint problem. This will be considered later.

Boundary conditions in problems (5) and (6) are taken into account by coefficients and parameters of discrete equations. This is a consequence of the summation functional.

In the construction of identity (4) equations (5) and (6) there represent splitting-up schemes due to the utilization of fractional steps in time and decomposition into subdomains.

If the original model (1) is non-linear, then identities (3) and (4) are linear relative to functions $\vec{\varphi}^*$ and non-linear relative to state functions $\vec{\varphi}$. That is why linearization of the summation functional relative to some specified value of the state vector is presented in the operations (6). The notation for it will be $\vec{\varphi}_a$, and for the state vector variation in the neighbourhood $\vec{\varphi}_a$ it will be $\delta\vec{\varphi}$. If the state vector $\vec{\varphi}$ is represented in the form

$$\vec{\varphi} = \vec{\varphi}_a + \xi\delta\vec{\varphi}, \quad \vec{\varphi}_a + \xi\delta\vec{\varphi} \in Q^h(D_t^h), \tag{7}$$

where ξ is the real parameter, the algorithm for the construction of adjoint equations (6) will be rewritten as follows:

$$\frac{\partial}{\partial\delta\vec{\varphi}}\left\{\left[\frac{\partial}{\partial\xi}I^h(\vec{\varphi}_a + \xi\delta\vec{\varphi}, \vec{Y}, \vec{\varphi}^*)\right]\Big|_{\xi=0}\right\} + \vec{\eta}(\vec{x}, t) = 0. \tag{8}$$

Differentiation is made relative to all the vector components $\delta\vec{\varphi}(\vec{x}, t)$, in all the grid nodes $(\vec{x}, t) \in D_t^h$. 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 space. Description of specific approximations and methods for the realization of splitting-up schemes is given in [3, 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 identity (3). The numerical model is constructed using this property. The set of adjoint equations is a consequence of approximations of the basic model.

3. Model sensitivity functions to variations of input parameters

Before passing on to the description of algorithms for the observation assimilation let us consider the supplementary algorithm in the calculation of the model sensitivity function.

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 the studying of 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.

As a measure of the model sensitivity it is convenient to take some set of the model generalized characteristics. They are specified on the sets of the state functions $\vec{\varphi} \in Q^h(D_t^h)$ and parameters $\vec{Y} \in R^h(D_t^h)$. Functionals of the form

$$\Phi_k(\vec{\varphi}) = \int\limits_{D_t} \chi_k(\vec{x},t) F_k(\vec{\varphi}(\vec{x},t)) dDdt, \quad k = \overline{1,K} \tag{9}$$

will refer to this type of characteristics. Here $F_k(\vec{\varphi})$ are some functions of $\vec{\varphi}$ and $\chi_k(\vec{x},t)$ are non-negative weight functions, satisfying the conditions of normalization

$$\int\limits_{D_t} \chi_k(\vec{x},t) dDdt, \quad k = \overline{1,K}. \tag{10}$$

In particular, functions $\chi_k(\vec{x},t)$ can have finite support in D_t. A limiting case is when one point is a support. Then the Dirac delta-function is the weight function c $\chi_k(\vec{x},t)$. In finite dimensional case this is the Kronecker delta-function. Discrete analogs of the functionals (9) are determined by the replacement of integrals by cubage formulas. As for the functionals (9), let us assume that they are continuous, limited and differentiable on the set of functions $\vec{\varphi} \in Q(D_t)$, and their discrete analogs – on the set of functions $\vec{\varphi} \in Q^h(D_t^h)$.

It follows that the functions

$$\begin{aligned} &\vec{\eta}_k(\vec{x},t) = \mathrm{grad}_{\vec{\varphi}} \Phi_k^h(\vec{\varphi}) \equiv \frac{\partial \Phi_k(\vec{\varphi})}{\partial \vec{\varphi}}, \\ &k = \overline{1,K}, \quad (\vec{x},t) \in D_t^h, \end{aligned} \tag{11}$$

defined on the set of state function values in the grid nodes of D_t^h must exist.

In this case we obtain the algorithm

$$\delta\Phi_k(\vec{\varphi}) = (\mathrm{grad}_{\vec{Y}} \Phi_k, \delta\vec{Y}) = \frac{\partial}{\partial \xi} I^h(\vec{\varphi}, \vec{Y}_o + \xi\delta\vec{Y}, \vec{\varphi}_k^*)\big|_{\xi=0}, \tag{12}$$

$$\mathrm{grad}_{\vec{Y}} \Phi_k = \frac{\partial}{\partial \delta\vec{Y}} \left\{ \frac{\partial}{\partial \xi} I^h(\vec{\varphi}, \vec{Y}_0 + \xi\delta\vec{Y}, \vec{\varphi}_k^*)\big|_{\xi=0} \right\}, \quad k = \overline{1,K} \tag{13}$$

for the calculation of the variations $\delta\Phi_k(\vec{\varphi})$ of the functionals $\Phi_k(\vec{\varphi})$ (9) and the sensitivity functions $\mathrm{grad}_{\vec{Y}} \Phi_k$. Here ξ is the real parameter, $\delta\vec{Y}$

is the vector of parameter variations, $\vec{Y}_0$ is the vector of non-perturbed parameter values, $\vec{\varphi}$ is the solution of the basic problem (6) at $\vec{Y} = \vec{Y}_0$, $\vec{\varphi}_k^*$ is the solution of the adjoint problem (8) at the condition $\vec{\varphi}_k^*\big|_{t=\bar{t}} = 0$ and with the source function $\vec{\eta}_k(\vec{x}, t)$, calculated by (11).

The basic problem is solved once, and the adjoint problem is solved so many times as there are functionals (9). Integration of equations for the basic problems is fulfilled in the forward time direction, and for the adjoint problem – in the inverse direction.

4. Algorithm for assimilation of observations and the diagnosis of the model quality

Let us assume that there is a set of points D_t^m in the domain D_t in which the measurements for the specified characteristics of the state functions are obtained. The set of observed values will be denoted by $\vec{\Psi}_m(\vec{x}, t)$, and by $\vec{\Psi} = \vec{H}(\vec{\varphi})$ the set of values calculated with the help of the measurement models with simulated state function. The deviation between measured and calculated characteristics of the investigated processes is estimated by the difference

$$\vec{\Psi}_m - \vec{\Psi} \equiv \vec{\Psi}_m - \vec{H}(\vec{\varphi}).$$

Functions $\vec{\Psi}_m$ and $\vec{\Psi}$ are obtained on the set D_t^m and the function $\vec{\varphi}$ is obtained on the set D_t^h. Thus, the model of measurements gives some aproximation of the measured quantity in D_t^m and this approximation originates from the state functions calculated in D_t^h by the model of the processes.

So far we have considered the model for the investigated phenomena, defined by expression (1) in the ideal situation. In real conditions, however, mathematical models of the processes and measurements, the measurements themselves and initial fields have errors. These errors can be both random and determined.

So the model with errors will be taken instead of the model (1)

$$B\frac{\partial \vec{\varphi}}{\partial t} + G^h(\vec{\varphi}, \vec{Y}) = \vec{f}(\vec{x}, t) + \vec{\xi}(\vec{x}, t), \tag{14}$$

$$\vec{\Psi} = \vec{H}(\vec{\varphi}) + \vec{\chi}(\vec{x}, t), \tag{15}$$

$$\vec{\varphi}(0) = \vec{\varphi}^0 + \vec{\xi}_0(\vec{x}), \tag{16}$$

$$\vec{Y} = \vec{Y}_a + \vec{\zeta}(\vec{x}, t). \tag{17}$$

Here $G^h(\vec{\varphi}, \vec{Y})$ is the matrix discrete analog of the model operator (1), $\vec{H}(\vec{\varphi})$ is the set of the measurement models, $\vec{\varphi}^o$ and $\vec{Y}_a$ are given estimates of the initial fields $\vec{\varphi}(0)$ and parameter vector $\vec{Y}$; $\vec{\xi}(\vec{x},t)$, $\vec{\chi}(\vec{x},t)$, $\vec{\xi}_0(\vec{x})$, $\vec{\zeta}(\vec{x},t)$ are errors of the basic and model, the measurement models and estimates for the initial state and parameters. All the models are discretized in space and time. However, the expression for the derivative of the state function in time was formally left in the equation (14) for the convenience of presentation.

Let us formulate the quality criterion for the assimilation model in the form of the functional

$$J(\vec{\varphi})=\left(\left(B\frac{\partial\vec{\varphi}}{\partial t}+G^h(\vec{\varphi},\vec{Y})-\vec{f}\right)^T R\left(B\frac{\partial\vec{\varphi}}{\partial t}+G^h(\vec{\varphi},\vec{Y})-\vec{f}\right)\right)_{D_t^h}$$
$$+\left(\left(\vec{\Psi}_m-\vec{H}(\vec{\varphi})\right)^T S\left(\vec{\Psi}_m-\vec{H}(\vec{\varphi})\right)\right)_{D_t^m}$$
$$+\left(\left(\vec{\varphi}(0)-\vec{\varphi}^o\right)^T P_o^{-1}\left(\vec{\varphi}(0)-\vec{\varphi}^o\right)\right)_{D^h} \tag{18}$$
$$+\left(\left(\vec{Y}-\vec{Y}_a\right)^T L^{-1}\left(\vec{Y}-\vec{Y}_a\right)\right)_{R^h(D_t^h)},$$

where the index T denotes the operation of transposition. The vectors are arranged in columns. Floating time interval $[t_0,t_f]\subset[0,\bar{t}]$ is taken in the domain D_t^m in which observational data are accumulated for one assimilation cycle. In particular, both intervals $[t_0,t_f]$ and $[0,\bar{t}]$ can coincide.

All the four terms in the quality functional (18) have the form of scalar products with positively-defined weight matrices R, S, P_0^{-1}, L^{-1}. They are defined in the domain D_t^h, D_t^m, D^h, $R^h(D_t^h)$ respectively and are responsible for the minimality of model errors, deviations between the measured and calculated characteristics of the investigated fields, the errors of the initial state and the errors of the model parameters. Weight matrices R, S, P_0^{-1}, L^{-1} are the parameters of the assimilation model. Their choice depends on the researcher. If given information about the errors of the corresponding terms exists, it is desirable to take this information into account in the specification of these matrices.

The choice of the quality criterion itself and of the weight matrices in it is a complex problem for non-linear models. Special research is necessary in this direction.

In the solution of practical problems application of the criterion in the form (11) gives quite acceptable results. This is provided first of all by the minimization principle for the vector norms of the corresponding deviations that is the basis of this criterion. The second favourable factor is the presence of good given estimates for the unknown quantities.

Now let us pass on to the description of the basic algorithm for the solution of the problem of data assimilation.

The source function $\vec{f}(\vec{x},t)$ in model (14) will be included in the set of parameters $\vec{Y}$. The error function $\vec{\xi}(\vec{x},t)$ will be considered as an auxiliary variable. It will be denoted by

$$\vec{\xi}(\vec{x},t) = \vec{F}(\vec{x},t) \equiv B\frac{\partial\vec{\varphi}}{\partial t} + G^h(\vec{\varphi},\vec{Y}) - \vec{f}(\vec{x},t) \tag{19}$$

and (18) will be rewritten in the form

$$\begin{aligned} J(\vec{\varphi},\vec{F}) = & \left(\vec{F}^T R\vec{F}\right)_{D_t^h} + \left(\left(\vec{\Psi}_m - \vec{H}(\vec{\varphi})\right)^T S\left(\vec{\Psi}_m - \vec{H}(\vec{\varphi})\right)\right)_{D_t^m} \\ & + \left(\left(\vec{\varphi}(0) - \vec{\varphi}^0\right)^T P_O^{-1}\left(\vec{\varphi}(0) - \vec{\varphi}^0\right)\right)_{D^h} \\ & + \left(\left(\vec{Y} - \vec{Y}_a\right)^T L^{-1}\left(\vec{Y} - \vec{Y}_a\right)\right)_{R^h(D_t^h)}. \end{aligned} \tag{20}$$

The vector of initial data $\vec{\varphi}(0)$ and the vector of the model parameters $\vec{Y}$ are unknown quantities. In this case $\vec{Y}_a$ and $\vec{Y}$ are supposed to belong to the range of admissible values $R^h(D_t^h)$.

In this case the estimation problems of the state function and the quality of the model can be considered as a minimization problem for the quality functional (20) on the set of functions $\{\vec{\varphi}(0),\ \vec{F}(\vec{x},t),\ \vec{Y}\}$.

This problem must be solved under condition that the state function satisfies the set of equations for the basic model

$$B\frac{\partial\vec{\varphi}}{\partial t} + G^h(\vec{\varphi},\vec{Y}) - \vec{f} = \vec{F} \tag{21}$$

with free initial conditions, i.e., the vector $\vec{\varphi}(0)$ is not specified and only its preliminary estimate $\vec{\varphi}^0$ is known. The parameter vector $\vec{Y}$ at qiven estimate $\vec{Y}_a$ is also to be defined more exactly.

Algorithms based on the employment of the Lagrange multipliers and the maximum principle can be applied in this formulation for the solution of optimization problem. Applying the method of the Lagrange multipliers the equivalent formulation of the model with the functional

$$J_0(\vec{\varphi},\vec{F}) = J(\vec{\varphi},\vec{F}) + I^h(\vec{\varphi},\vec{Y},\vec{\varphi}^*) \tag{22}$$

is obtained. The second term in (22) is constructed in the same way as the functional of the basic identity (3) and its discrete analogs (4). In this case the function $\vec{f}$ from (1) is replaced by the sum $\vec{F}_e = \vec{f} + \vec{F}$, i.e.,

$$I^h(\vec{\varphi}, \vec{Y}, \vec{\varphi}^*) = \left(B\frac{\partial \vec{\varphi}}{\partial t} + G(\vec{\varphi}, \vec{Y}) - \vec{F}_e, \vec{\varphi}^* \right)^h . \tag{23}$$

The vector $\vec{\varphi}^*$ in expressions (22) and (23) is the vector of the Lagrange multipliers. In the construction of (3) and (4) it was assumed that $\vec{\varphi}^*$ is an arbitrary sufficiently smooth function. That is why the functionals in (4) and (23) coincide in their form but differ in their meaning. The difference is in the concrete definition of the function as the solution for the corresponding adjoint problem such as (6), (8).

Stationarity conditions of the functional (22) leads to the set of equations

$$B\frac{\partial \vec{\varphi}}{\partial t} + G^h(\vec{\varphi}, \vec{Y}) - \vec{f} = \vec{F}, \tag{24}$$

$$-B\frac{\partial \vec{\varphi}^*}{\partial t} + A^T(\vec{\varphi}, \vec{Y})\vec{\varphi}^* = \frac{\partial \vec{H}^T(\vec{\varphi})}{\partial \vec{\varphi}} \left\{ S\left(\vec{\Psi}_m - \vec{H}(\vec{\varphi})\right) \right\}_m , \tag{25}$$

$$\vec{\varphi}^*(\vec{x})\big|_{t=\bar{t}} = 0, \tag{26}$$

$$\vec{\varphi}(0) = \vec{\varphi}^0 + P_0^{-1} B\vec{\varphi}^*(0), \qquad t = 0, \tag{27}$$

$$\vec{F}(\vec{x}, t) = R^{-1}(\vec{x}, t)\vec{\varphi}^*(\vec{x}, t), \tag{28}$$

$$\vec{Y} = \vec{Y}_a - L^{-1}\frac{\partial}{\partial \vec{Y}} I^h(\vec{\varphi}, \vec{Y}, \vec{\varphi}^*), \tag{29}$$

$$A(\vec{\varphi}, \vec{Y})\vec{\varphi}' = \frac{\partial}{\partial \xi}\left[G^h(\vec{\varphi} + \xi\vec{\varphi}', \vec{Y}) \right]\Big|_{\xi=0} . \tag{30}$$

The expression in the right-hand side of equations (25) $\{S(\vec{\Psi}_m - \vec{H}(\vec{\varphi}))\}_m$ is calculated at the points $(\vec{x}, t) \in D_t^m$, all the other operations of the system (24)–(30) – at grid points D_t^h and D^h. An interesting feature of the direct and adjoint operators $\vec{H}(\vec{\varphi})$ in the models of observations manifests itself here. The "direct" operator $\vec{H}(\vec{\varphi})$ transfers information from the grid D_t^h, on which the basic model is working, to the measurements grid D_t^m. The adjoint operator $\partial \vec{H}^T(\vec{\varphi})/\partial \vec{\varphi}$ acts in the opposite way, it transfers information from the grid D_t^m to D_t^h.

Linearization of the operator $G^h(\vec{\varphi}, \vec{Y})$ from the basic model determined by the relation (30), is a consequence of linearization in (8). In (27)–(29) there are inverse and weight matrices from the quality functional. This fact must be taken into account in the choice of weight matrices as these matrices have very large dimension in practical problems.

Solution for the discrete analogs of the system (24)–(30) is found with the help of iterative procedures of the gradient type. The preliminary estimates for the initial state $[\vec{\varphi}(0)]^{(0)} = \vec{\varphi}^0$, model errors $[\vec{F}]^{(0)} = \vec{F}^{(0)}$ and parameters $[\vec{Y}]^{(0)} = \vec{Y}_a$ are specified as initial data for iterations. If qiven information for the calculation of initial error estimate by the formula (19) is absent, then it is assumed that $[\vec{F}]^{(0)} = 0$. Functions of sensitivity to the parameter variations are calculated under the condition that these variations are small. In order to.guarantee the validity of this assumption the condition for the iterated vectors $\Delta\vec{Y}^n = \vec{Y}^{n+1} - \vec{Y}^n$ of the form

$$(W\Delta\vec{Y}, \delta\vec{Y})_{R^h(D_t^h)} \leq \epsilon^2$$

will be introduced. Here ϵ is the given small quantity, n is an iteration index and W is the positive weight matrix. For calculation it is convinient to take W as a diagonal matrix which satisfies the normalization condition $(W\vec{Y}, \vec{Y})_{R^h(D_t^h)} = 1$. Here $\vec{Y}$ is the vector of the parameter scales. Although the introduced limitations make the computational algorithm somewhat more complex, it allows to control the parameter behaviour during iterations. The function of the model errors $\vec{F}(\vec{x}, t)$, calculated by formula (28), plays an important role in the diagnostic estimate of the model. It shows the ability of the model to describe specific situations, characterized by the assimilated information $\vec{\Psi}_m$. If after iterations for the solution of the system (24)–(30) the function value $\vec{F}(\vec{x}, t)$ exceeds some term in the left-hand side of the system (24), this means that the model cannot satisfactorily describe this situation. In this case it is necessary to analyze the results of observations additionally and make corrections in the model itself when required. We consider the problem of the observation assimilation in the general formulation. But it is necessary to remember that the effectiveness of algorithms for its solution depends on the number of degrees of freedom in the model. That is why, it is reasonable to consider several variants with a smaller number of the unknown functions.

1. The model is assumed to be exact and all parameters are defined, i.e., $\vec{F} = 0$, $\vec{Y} = \vec{Y}_a$. Only the vector of initial state is unknown. Solution procedure for the equations (28) and (29) is excluded from the algorithm.
2. It is assumed that the model is exact, $\vec{F} = 0$. Parameters must be defined more precisely, $\vec{\varphi}(0)$ and $\vec{Y}$ are sought. Equation (28) is excluded from the algorithm.
3. The parameters $\vec{Y} = \vec{Y}_a$ are supposed to be known. The vector estimates $\vec{F}$ and $\vec{\varphi}(0)$ are sought. Equations (29) are excluded.

Other variants are also possible, depending on the aims of investigation. The first variant with the unknown vector of initial state is the most economical. In all the cases it is desirable that the functions of sensitivity to the model parameters were calculated by (13). They give additional information about the model quality and the tendencies of some factors' influence.

In problem (24)–(28) the formal duplication of the dimension was obtained due to the introduction of a new function $\vec{\varphi}^*$. Apart from the state function $\vec{\varphi}$ solution of the adjoint problem (25) is found. However, this is completely compensated by the realization simplicity of the assimilation scheme with the iterative methods of the gradient type. Moreover, calculation of sensitivity functions using adjoint equations gives us a new quality of the modeling process.

5. An alternative realization scheme for the assimilation of observations

For the convenience of presentation it will be assumed that the models of processes and observations are linear and that B is a non-singular matrix.

For the nonlinear models linearization of the type (30) in the neighbourhood of the given state vector can be used instead of $G^h(\vec{\varphi}, \vec{Y})$ and $\vec{H}(\vec{\varphi})$. Linear versions of the model operators will be redenoted in the following way

$$G^h(\vec{\varphi}, \vec{Y}) \longrightarrow A\vec{\varphi}, \qquad \vec{H}(\vec{\varphi}) \longrightarrow C\vec{\varphi}, \tag{31}$$

where A and C are some linear matrix operators defined on the set of functions $\vec{\varphi} \in Q^h(D_t^h)$.

Time interval $[t_0, t_f]$, in which measurement data are taken into account is a generalized parameter of the measurement assimilation procedure. In order to show the dependence of functions $\vec{\varphi}$, $\vec{\varphi}^*$, $\vec{F}$, $\vec{Y}$ on the data in this interval, let us introduce the following notations $A = A(\vec{x}, t, t_f)$. The parameter can take any value in the time interval $[0, \bar{t}]$, in which the model is considered. Then let us introduce the transformation

$$\vec{\varphi}(\vec{x}, t, t_f) = \vec{q}(\vec{x}, t) - P(\vec{x}, t)\vec{\varphi}(\vec{x}, t, t_f), \tag{32}$$

where $q(\vec{x}, t)$ is the vector of the same structure and dimensionality as the state vector $\vec{\varphi}$ and $P(\vec{x}, t)$ is the square matrix. In order to find q and P let us substitute (32) into (24)–(29) taking into account renotation (31). After the transformation we obtain

$$\begin{aligned} B\frac{\partial \vec{q}}{\partial t} + A\vec{q} &= -BPB^{-1}C^T S(\vec{\Psi}_m - C\vec{q}) + \vec{f} \\ &- \left(B\frac{\partial P}{\partial t} + BPB^{-1}A^T + AP + R^{-1} + BPB^{-1}C^T SCP\right)\vec{\varphi}^*. \end{aligned} \tag{33}$$

Let the matrix P and vector $\vec{q}$ be chosen so that the coefficient at $\vec{\varphi}^*$ in (33) vanished and that conditions (26) and (27) were satisfied.

The result is the set of equations

$$B\frac{\partial \vec{q}}{\partial t} + A\vec{q} = \vec{f} - BPB^{-1}C^T S(\vec{\Psi}_m - C\vec{q}), \tag{34}$$

$$B\frac{\partial P}{\partial t} + BPB^{-1}A^T + AP + R^{-1} + BPB^{-1}C^T SCP = 0, \tag{35}$$

$$\vec{q}(0) = \vec{\varphi}^0, \qquad P(\vec{x},0) = P_0.$$

It follows from condition (26) and equation (32) that

$$\vec{\varphi}(\vec{x}, t_f, t_f) = \vec{q}(\vec{x}, t_f). \tag{36}$$

Any current time moment $t \in [0, \bar{t}]$ can be chosen as t_f. Taking this into account the set of equations is obtained from (34)–(36) for the estimation of state at any time moment

$$B\frac{\partial \vec{\varphi}}{\partial t} + A\vec{\varphi} = \vec{f} - BPB^{-1}C^T S(\vec{\Psi}_m - C\vec{\varphi}), \tag{37}$$

$$\vec{\varphi} \equiv \vec{\varphi}(\vec{x}, t), \qquad \varphi(\vec{x}, t_0) = \vec{\varphi}^0(\vec{x}). \tag{38}$$

The matrix $P = P(\vec{x}, t)$ is found from the solution of the equation (35).

With the $B = E$ set of equations (37), (38) equation (35) coincides with the scheme of the Kalman filter for problem (14)–(16) in the linear case [2, 14].

In the non-linear case it is impossible to construct a completely equivalent realization scheme such as the Kalman filter for the assimilation problem. Here we can speak only about approximate schemes of the filter type. For example, at $B \equiv E$ the scheme of the first order of accuracy

$$\begin{aligned} &\frac{\partial \vec{\varphi}}{\partial t} + G^h(\vec{\varphi}, \vec{Y}) = \vec{f} - P\Big[\frac{\partial \vec{H}(\vec{\varphi})}{\partial \vec{\varphi}}\Big]^T S(\vec{\Psi} - \vec{H}(\vec{\varphi})), \\ &\vec{\varphi}(\vec{x}, 0) = \vec{\varphi}^0(\vec{x}) \end{aligned} \tag{39}$$

is obtained [2]. Here the matrix $P \equiv P(\vec{x}, t)$ is found from the approximate equation similar to (35)

$$\begin{aligned} &\frac{\partial P}{\partial t} + PA^T + AP + R^{-1}(\vec{x}, t) = P\frac{\partial \vec{H}^T}{\partial \vec{\varphi}} S \frac{\partial \vec{H}}{\partial \vec{\varphi}} P, \\ &P(\vec{x}, 0) = P_0(\vec{x}). \end{aligned} \tag{40}$$

Thus, excluding the adjoint function and the algorithm for its determination from the set of equations we obtain the realization scheme of the observational assimilation procedure of the Kalman filtering type.

In the current models of the given class the degrees of freedom in the dimension of the state vector are in the range $10^3 - 10^7$. It will be denoted by n. Then the weight matrix has n^2 dimensions. It is known that the construction and realization of the computationally stable solution algorithm for the matrix equations such as (35), (40) is a very complex problem. The analysis of these equations shows that the matrix $P(\vec{x}, t)$ is completely defined by the matrices R, P_0, S of the quality functional and by the operators of the models for the processes and observations.

The choice of realization scheme naturally depends on the researcher. In this case the scheme with adjoint equations is clearly preferable.

The construction of the quality functional can be chosen, so that it allows to include all information available from different observational systems. Then all measurement data are taken into account by the source terms in the adjoint problem (6)–(25). Interrelation between the mathematical models and observations is carried out through the solutions of the adjoint problem. Similarly, observations and parameters are related through the sensitivity functions. Three principal points of the observational assimilation models are: large dimensionality, computational stability, inter-coordination of algorithms at all the stages of computation. We are solving those problems with the help of the variational principle, splitting-up method and the appropriate iterative procedures.

6. Experiment design

State function $\vec{\varphi}$ plays an important role in the understanding of physical processes in the climatic system. But it is difficult to estimate the observed system's 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 in virtue of sensitivity relations (12) and functions (13). From (12) it follows that sensitivity functions really are influence functions of corresponding parameter variations with respect to the functional variations. As a consequence these functions and sensitivity relations (12) may be used to provide optimal desigh of observational experiments in order to estimate the functionals (9). In sach a case using the influence functions for specific areas can be calculated and optimal plans for observations can be constructed. Calculation of the influence functions is especially useful in the solution of problems on the limited territory. In this case estimates for the areas of influence for the considered territory help to understand how to treat boundary conditions on the lateral boundaries and how to realize interaction between models of different scales.

Estimates for the areas of influence and distribution of observational devices depend on the type of the functional being estimated and on the criterion of optimality. As an example let us consider the functional

$$\Phi(\vec{\varphi}, t) = \int_D \vec{\varphi}(\vec{x}, t)\vec{\chi}(\vec{x}, t)dD, \tag{41}$$

depending continuously on time in the interval $[t_0, t_f]$. Suppose that the state function values $\vec{\varphi}(\vec{x}, 0)$ are given at the initial time moment $t = t_0$, and the weight function values $\vec{\chi}(\vec{x}, t)$ are given at the time moment $t = t_f$. The weight $\vec{\chi}(\vec{x}, t)$ function can be interpreted as distribution function of observational devices. Let us formulate the observational experiment to estimate the functional $\Phi(\vec{\varphi},)$. Construction of a plan for the experiment in this case can consist in the determination of the weight function $\vec{\chi}(\vec{x}, t)$, such that at $t = t_f$ it is equal to $\vec{\chi}(\vec{x}, t_f)$ and so that the functional value $\Phi(\vec{\varphi}, t_f)$ at the moment of the experiment's end $t = t_f$ does not depend on the variations of the state function, i.e., $\delta\Phi(\vec{\varphi}, t_f) = 0$.

Solution of this problem for the linear model is given by the solution of the adjoint problem (6) with the conditions $\vec{\varphi}^*(\vec{x}, t_f) = \vec{\chi}(\vec{x}, t_f)$ and $\vec{\eta}(\vec{x}, t) = 0$. If functional being estimated is given in more general form (9), we take adjoint problem in form (6)–(11).

7. Model of atmospheric hydrodynamics

To illustrate application of the above approaches, let us discuss two formulations of conorete problems of mathematical similation of atmospheric hydrothermodynamics and transport of atmospheric pollution.

More details of the models and methods of their practical realization are described in [7, 9, 10, 12].

As the first example, we consider a model of atmospheric hydrothermodynamics in diabatic approximation on a sphere in isobaric coordinates. Variational formulation (3)–(8) of the problem is most convenient for constructing descrete approximations and computational algorithms. Therefore we do not represent the model as a system of differential equations. Let us define it as integral identity [10]:

$$
\begin{aligned}
I\left(\vec{\varphi},\vec{Y},\vec{\varphi}^*\right) \equiv & \int_{D_t}\Big\{(\Lambda u,u^*)+(\Lambda v,v^*)+\sigma(\Lambda T,T^*)\\
&+\left(l+\frac{ctg\theta}{a}\right)(vu^*-v^*u)+(\vec{u}^*\mathrm{grad}H-\vec{u}\mathrm{grad}H^*)\\
&+\frac{R}{p}\left(T\tau^*-\frac{(\gamma_a-\gamma)\bar{T}}{g}\tau T^*\right)-\sigma\epsilon T^*\Big\}dDdt \qquad (42)\\
&+\int_{S_t}\bar{\rho}\left(\frac{\partial H}{\partial t}H^*-\frac{\partial H^*}{\partial t}H\right)\Big|_{p=p_a}dSdt+I_D(\vec{\varphi},\vec{\varphi}^*)\\
&+\frac{1}{2}\left[\int_D(uu^*+vv^*+\sigma TT^*)dD+\int_S\bar{\rho}HH^*\big|_{p=p_a}\right]\Big|_o^{\bar{t}}dS=0,
\end{aligned}
$$

where

$$
\begin{aligned}
I_D(\vec{\varphi},\vec{\varphi}^*) = & \int_{D_t}\Big\{\mu_1\left[D_T(\vec{u}_s)D_T(\vec{u}_s^*)+D_s(\vec{u}_s)D_s(\vec{u}_s^*)\right]\\
&+\chi_1\left(\frac{\partial u}{\partial p}\frac{\partial u^*}{\partial p}+\frac{\partial v}{\partial p}\frac{\partial v^*}{\partial p}\right) \qquad (43)\\
&+\sigma\left[\mu_2\left(\frac{1}{a^2sin^2\theta}\frac{\partial T}{\partial\psi}\frac{\partial T^*}{\partial\psi}+\frac{1}{a^2}\frac{\partial T}{\partial\theta}\frac{\partial T^*}{\partial\theta}\right)+\chi_2\frac{\partial T}{\partial p}\frac{\partial T^*}{\partial p}\right]\Big\}dDdt\\
&+\int_{S_t}(u^*\tau_\psi+v^*\tau_\theta+\sigma T^*q_s)\big|_{p=p_a}dSdt,
\end{aligned}
$$

$$
\begin{aligned}
D_T(\vec{u}_s) &= \frac{1}{a\quad sin\theta}\left(\frac{\partial u}{\partial\psi}+\frac{\partial(v\quad sin\theta)}{\partial\theta}\right),\\
D_s(\vec{u}_s) &= \frac{1}{a\quad sin\theta}\left(\frac{\partial v}{\partial\psi}-\frac{\partial(u\quad sin\theta)}{\partial\theta}\right), \qquad (44)\\
(\Lambda\varphi,\varphi^*) &= \frac{1}{2}\left[\left(\frac{\partial\varphi}{\partial t}\varphi^*-\frac{\partial\varphi}{\partial t}\varphi^*\right)+(\varphi^*\vec{u}\mathrm{grad}\quad\varphi-\varphi\vec{u}\quad\mathrm{grad}\varphi^*)\right],
\end{aligned}
$$

$$
\begin{aligned}
&\vec{\varphi}=(u,v,T,H,\tau), && \vec{\varphi}^*=(u^*,v^*,T^*,H^*,\tau^*),\\
&\vec{u}_s=(u,v), && \vec{u}_s^*=(u^*,v^*),\\
&D_t=D\times[o,\bar{t}], && S_t=S\times[0,\bar{t}], \qquad (45)\\
&D=\{(S\times[p_T,p_a])\}, && S=\{0\le\psi\le2\pi,0\le\theta\le\pi\},\\
&dD=dSdp. && dS=asin\theta d\theta d\Psi,
\end{aligned}
$$

The system of notations is as follows:

u, v, τ – components of the velocity vector in the direction of cordinates ψ, θ, p, respectively;

t – time;

ψ, θ – longitude and supplement to latitude;

p ($p_T \le p \le p_a$), p_T, p_a – pressure and it's upper and lower boundaries;

T, H – deviation of temperature and geopotential from their standard values $\bar{T}$ and $\bar{H}$, repectively;

$\vec{\rho}$ – standard density;

a – Earth's radius;

l – Coriolis parameter;

μ_1, χ_i ($i = 1, 2$) – turbulence coefficients in horisontal and vertical directions respectively;

ϵ – heat flux per unit volume;

γ_a – adiadbatic temperature gradient;

$\gamma - \frac{\partial \bar{T}}{\partial z}$ – standard temperature gradient;

τ_ψ, τ_θ – functions defining dynamic interaction of the atmosphere and the Earth's surface;

q_s – function of the heat flux on the Earth's surface;

σ – scale factor.

Components of vector function $\vec{\varphi}^*$ are arbitrary, sufficiently smooth functions. The input parameter vector can be defined by

$$\vec{Y} = \left(\vec{\varphi}^o, \mu_1, \mu_2, \chi_1, \chi_2, \epsilon, \tau_\psi, \tau_\theta, q_s, \bar{\rho}, \bar{T}, \frac{(\gamma_a - \gamma)}{q}, a, l \right), \tag{46}$$

where $\vec{\varphi}^0$ is the initial value of vector $\vec{\varphi}$ at $t = 0$. The integral identity (43) defines a generalized solution of the problem. It takes into consideration differential equations, boundary and initial conditions. Periodicity conditions of functions on a sphere are involved in the definition of a class of functions to which the generalized solution belongs.

Identity (43) is discretized as follows. At first we introduce in the domain D_t the grid domain D_t^h, then approximate integrals and integrands by quadrature and finite difference formulas, respectively. The fractional step approach is used for time approximation. Expressions of the same type in (43) must be approximated in the seme manner. This ensures the energy balance of discrete approximations obtained from stationary conditions of the summation functional (5) and (6).

Principles of construction numerical methods for atmosphere and ocean dynamics problems are following the idea of splitting described in [3, 10].

Here we will discuss only the structure of the basic relation (29) for realization of the feed-back between variations of functionals and parameters.

We assume that some of the parameters get perturbations

$$\delta\vec{Y} = (\delta\vec{\varphi}^{o}, \delta\mu, \delta\mu_2, \delta\chi_1, \delta\chi_2, \delta\epsilon, \delta\tau_{\psi}, \delta\tau_{\theta}, \delta q_s) \tag{47}$$

and sensitivity of the model is estimated by variations of a functional $\Phi(\vec{\varphi})$. Write down the formula (12) to compute variations of the functional by variations of the parameter vector. Let $\vec{\varphi} = (u, v, T, H, \tau)$ be solution of problem (5) for unpertured values of the parameters and $\vec{\varphi}^* = (u^*, v^*, T^*, H^*, \tau^*)$ be solution of the adjoint problem (8) provided that $\vec{\varphi}^* = 0$ at $t = \bar{t}$ and the source is equal to

$$\vec{\eta}(\vec{x}, t) = \mathrm{grad}_{\vec{\varphi}}\Phi = \frac{\partial}{\partial\delta\vec{\varphi}}\frac{\partial}{\partial\xi}\Phi^h(\vec{\varphi} + \xi\delta\vec{\varphi})\big|_{\xi=0}, \tag{48}$$

where the supercript h denotes discrete approximation of functional $\Phi(\vec{\varphi})$, ξ is a real parameter, $\delta\vec{\varphi}$ is variation of the state vector in the vicinity of the unperturbed value $\vec{\varphi}$. With the above notations expression (13) is as follows

$$\begin{aligned}
\delta\Phi(\vec{\varphi}) = & \int_{D_t}\Big\{\sigma T^*\delta\epsilon + \delta\mu_1(D_T(\vec{u}_s)D_T(\vec{u}_s^*) + D_s(\vec{u}_s)D_s(\vec{u}_s^*)) \\
& + \delta\chi_1\left(\frac{\partial u}{\partial p}\frac{\partial u^*}{\partial p} + \frac{\partial v}{\partial p}\frac{\partial v^*}{\partial p}\right) \\
& + \sigma\Big[\delta\mu_2\Big(\frac{1}{a^2 sin^2\theta}\frac{\partial T}{\partial\psi}\frac{\partial T^*}{\partial\psi} + \frac{1}{a^2}\frac{\partial T}{\partial\theta}\frac{\partial T^*}{\partial\theta}\Big) + \delta\chi_2\frac{\partial T}{\partial p}\frac{\partial T^*}{\partial p}\Big]\Big\}dDdt \\
& + \int_{S_t}(u^*\delta\tau_{\psi} + v^*\delta\tau_{\theta} + \sigma T^*\partial\delta_s)\big|_{p=p_a}dSdt \\
& + \frac{1}{2}\Big[\int_D(u^*\delta u^o + v^*\delta v^o + \sigma T^*\delta T^o)dD + \int_s\bar{\rho}H^*\delta H^o\big|_{p=p_a}dS\Big].
\end{aligned} \tag{49}$$

Comparing expressions (12) and (49) we obtain formulas for computation of components of the vector $\mathrm{grad}_{\vec{Y}}\Phi$, for example,

$$\begin{aligned}
\frac{\partial\Phi}{\delta\mu_1} &= (D_T(\vec{u}_s)D_T(\vec{u}_s^*) + D_s(\vec{u}_s)D_s(\vec{u}_s^*)) \\
\frac{\partial\Phi}{\partial\chi_1} &= \left(\frac{\partial u}{\partial p}\frac{\partial u^*}{\partial p} + \frac{\partial v}{\partial p}\frac{\partial v^*}{\partial p}\right), \\
\frac{\partial\Phi}{\partial\tau_{\psi}} &= u^*\big|_{p=p_a}, \quad \frac{\partial\Phi}{\partial u^o} = u^*\big|_{t=o}, \quad \text{etc.}
\end{aligned} \tag{50}$$

Substituting expressions for the components of vector $\text{grad}_{\vec{Y}}\Phi$ into the right-hand side of (29), we arrive at the system of equations for finding the model's parameters with respect to variations of the functional $\Phi(\vec{\varphi})$.

8. Model of the pollution transport

Simulation of the atmosphere and ocean dynamics is only a part of the environmental problems. Of great importance in the study of human impact on the environment is the problem of simulation of pollution transport. Mathematically this problem is formulated as follows [12, 13]. Let us find solution of the pollution transport equation in $D_t^o \in D_t$

$$\frac{\partial\varphi}{\partial t} + \vec{u}\text{grad}\varphi + C(\varphi) - \frac{\partial}{\partial z}\nu\frac{\partial\varphi}{\partial z} - div_s\mu\text{grad}_s\varphi = f(\vec{x}, t) \qquad (51)$$

under the conditions

$$\begin{aligned} \alpha\frac{\partial\varphi}{\partial z} + \beta\varphi + f_s = 0 \quad & \text{at } z = z_s(\vec{x}), \\ \nu\frac{\partial\varphi}{\partial z} = 0 \qquad\qquad & \text{at } z = z_H, \end{aligned} \qquad (52)$$

where the following notations are used:

$\varphi = \{\varphi_i,\ i = \overline{1,n}\}$ – function of pollutants concentrations;

$\vec{u}$ – velocity vector of air particles;

ν, μ – turbulent exchange coefficients;

$f(\vec{x}, t)$ – distribution of pollution sources;

α, β – functions defining conditions of interaction of pollution with the Earth's surface;

f_s – distribution of surface sources;

$z_s(\vec{x})$ – Earth's surface relief;

z_H – upper boundary of air mass;

$C(\varphi)$ – operator of pollutants transformation.

Operations of differentions in (51), (52) are carried out with respect to components $\varphi_i(\vec{x}, t)$, $i = \overline{1,n}$ of function $\varphi(\vec{x}, t)$. Generaly the operator $C(\varphi)$ is nonlinear and it describes the transformations of pollutants due to chemical and photochemical reactions. Atmosphere pollutants are multy-component. A number of components is the input parameter of the model. We consider the chemical transformation in the regions with a high antropogenic load which is specific for large industrial areas.

Index s denotes the operators in horizontal directions. Initial conditions for problem (51) are determined from measured concentrations of pollution in D_t^0. The structure of this domain is similar to D_t in the atmosphere dynamics model. Therefore we will use the notation of (45) adding superscript 0. Information about the state of the atmosphere is input for the pollution transport model. The deposition velocity of pollutants is included in the vertical component of vector $\vec{u}$.

To construct a numerical model, let us write a variational formulation of problem (51)–(52)

$$\begin{aligned} I(\varphi,\varphi^*) = & \int_{D_t^o} \Big[(\Lambda\varphi,\varphi^*) + (C\varphi,\varphi^*) + \nu \frac{\partial\varphi}{\partial z}\frac{\partial\varphi^*}{\partial z} \\ & + \mu \mathrm{grad}_s\varphi\ \mathrm{grad}_s\varphi^* - f\varphi^* \Big] dDdt \qquad (53) \\ & + \int_{S_t^o} \frac{\nu}{\alpha}(\beta\varphi\varphi^* + f_s\varphi^*)\big|_{z=z_s} dSdt + \frac{1}{2}\int_{D^o} \varphi\varphi^*\big|_o^{\bar{t}} dD = 0, \end{aligned}$$

where φ^* is an arbitrary, sufficiently smooth function, and $(\Lambda\varphi,\varphi^*)$ is defined by expression (45). If D_t^0 does not coincide with D_t, in (53) there appears integral of the lateral boundary of D^0. Function φ in its physical sense is non-negative. Therefore, in discretization of the model, besides ordinary requirements of approximation and stability, we must make sure that the condition of non-negativity unknown function is met.

9. Conclusion

Thus, application of adjoint problems to mathematical modelling extends the model capabilities in their interaction with the observational information. In the first place this is the construction of quantitative methods for the sensitivity analysis and the realization of direct relations and feedbacks between the models and observations. There is no doubt that the first-level models, i.e., the models of the processes and measurements, must be sufficiently complete in their physical content. Their imperfection manifests itself in the diagnostic estimation of the quality in the process of observational assimilation.

Application of variational principles and optimization methods makes internal functional relations between different elements of the models more close. This is especially useful when the model interacts with the data. Sufficiently complete utilization of all the available information by means of optimization methods leads to the decrease of influence of different uncertainties and opens possibilities for formulations of new problems. Adjoint problems are widely used in the combined models for the dynamics of atmosphere, ocean and environment. It is necessary to introduce the control of sources of anthropogenic influence into such models using some criteria and restrictions together with the traditional procedure of the field reconstruction.

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