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The adjoint problem and sensitivity algorithms for the model of atmospheric hydrodynamics in σ-coordinates*

V.V. Penenko and E.A. Tsvetova

Variational statement of the hydrodynamical atmospheric problem in σ-coordinates is considered. The system of the adjoint equations and algorithms for the sensitivity investigation of the numerical model to the variations of input parameters are constructed. The example of the system organization of the direct and adjoint problems and the schemes of their realization for the typical combination of time approximations are given.

1. Introduction

The paper is devoted to the development of the inverse methodology of modelling for the aims of monitoring, forecast and ecological design. The constructive aspects of the realization of this methodology are considered. They are connected with derivation of the direct and adjoint systems of equations and the sensitivity methods for the models. The adjoint equations are used in various applications to the modelling of natural processes [1–3, 6]. They are actively introduced in monitoring and data assimilation procedures [8].

Here we consider the hydrodynamical model in σ-coordinates. It is the model that is the most popular in the investigations of the climatic changes, general circulation of the atmosphere and the weather forecasting. As we know, the adjoint equations have not been constructed yet for them, may be due to the complexity of the such kind of models. It seems for us that the application of inverse methodology to these models is very important from the practical point of view.

The algorithmic construction are provided in the frames of general approach described in [3–5, 7]. But the σ-model posesses the specific characters which make the construction of its variational form and the ajoint equations not so simple.

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China) and Computing Center of the Siberian Division of Russia Academy of Sciences (Novosibirsk). One of the aims of this cooperation is to construct the adjoint problems and algorithms for the sensitivity investigations and data assimilation applied to the Beijing University Model (BUM) [9].

2. Statement of the problem

2.1. Governing system of basic model. Let us write governing system of equations of atmospheric hydrodynamics: the equations of motion

$$\frac{\partial \pi u}{\partial t} + M(\pi u) - f\pi v + m\pi\Big[\frac{\partial \Phi}{\partial x} + \frac{RT}{\pi + p_T/\sigma}\,\frac{\partial \pi}{\partial x}\Big] - D(u) = 0, \tag{1}$$

$$\frac{\partial \pi v}{\partial t} + M(\pi v) + f\pi u + m\pi\Big[\frac{\partial \Phi}{\partial y} + \frac{RT}{\pi + p_T/\sigma}\,\frac{\partial \pi}{\partial y}\Big] - D(v) = 0, \tag{2}$$

the thermodynamic equation

$$\frac{\partial \pi T}{\partial t} + M(\pi T) - D(T) - Q_T - \frac{RT}{c_p(\sigma + p_T/\pi)}\Big[\pi\dot{\sigma} + \sigma\Big(\frac{\partial \pi}{\partial t} + m\Big(u\frac{\partial \pi}{\partial x} + v\frac{\partial \pi}{\partial y}\Big)\Big)\Big] = 0, \tag{3}$$

the water vapour continuity equation

$$\frac{\partial \pi q}{\partial t} + M(\pi q) - D(q) - Q_q = 0, \tag{4}$$

the continuity equation

$$\frac{\partial \pi}{\partial t} + m^2\Big[\frac{\partial}{\partial x}\Big(\frac{\pi u}{m}\Big) + \frac{\partial}{\partial y}\Big(\frac{\pi v}{m}\Big)\Big] + \frac{\partial \pi\dot{\sigma}}{\partial \sigma} = 0, \tag{5}$$

the hydrostatic equation

$$\frac{\partial \Phi}{\partial \sigma} + \frac{RT}{\sigma + p_T/\pi} = 0, \tag{6}$$

the equation for the surface pressure variations

$$\frac{\partial \pi}{\partial t} + m^2 \int_0^1 \Big(\frac{\partial}{\partial x}\Big(\frac{\pi u}{m}\Big) + \frac{\partial}{\partial y}\Big(\frac{\pi v}{m}\Big)\Big)d\sigma = 0. \tag{7}$$

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

$$\pi\dot{\sigma} + \int_0^\sigma \left(\frac{\partial\pi}{\partial t} + m^2\Big(\frac{\partial}{\partial x}\Big(\frac{\pi u}{m}\Big) + \frac{\partial}{\partial y}\Big(\frac{\pi v}{m}\Big)\Big)\right) d\sigma' = 0. \tag{8}$$

The formula

$$\Phi(\sigma) = \Phi_s + \int_0^1 \frac{RT}{\sigma' + p_T/\pi} d\sigma' \tag{9}$$

is used to calculate Φ, where Φ_s is the surface geopotential. The operators $D(\varphi)$ (4), 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,

$$M(\varphi) = m^2\Big(\frac{\partial}{\partial x}\Big(\frac{u\varphi}{m}\Big) + \frac{\partial}{\partial y}\Big(\frac{v\varphi}{m}\Big)\Big) + \frac{\partial}{\partial\sigma}(\varphi\dot{\sigma}), \tag{10}$$

where $\varphi = \pi u, \pi v, \pi T, \pi q$; $\sigma = (p - p_T)/\pi$, $\pi = p_s - p_T$, 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.

2.2. The structure of the state function and trial functions. Let us define the state function vector for the system (1)–(10) and introduce some auxilary notations which we shall need later on

$$\begin{aligned}
&\vec{\varphi} = \{\varphi_i,\ i = \overline{1,8}\} \equiv \{u, v, T, q, \dot{\sigma}, \chi, \Phi, \pi\} \in Q(D_t),\\
&\vec{\varphi}^* = \{\varphi_i^*,\ i = \overline{1,8}\} \equiv \{u^*, v^*, T^*, q^*, \dot{\sigma}^*, \chi^*, \Phi^*, \pi^*\} \in Q^*(D_t),\\
&\vec{\psi} = \{\psi_i,\ i = \overline{1,8}\} \equiv \{U, V, \tilde{T}, \tilde{q}, \dot{\Sigma}, \chi, \Phi, \pi/m\} \in Q(D_t),\\
&\vec{\psi}^* = \{\psi_i^*,\ i = \overline{1,8}\} \equiv \{U^*, V^*, \tilde{T}^*, \tilde{q}^*, \dot{\Sigma}^*, \chi^*, \Phi^*, \pi^*\} \in Q^*(D_t),\\
&\delta\vec{\varphi} = \{\delta\varphi_i,\ i = \overline{1,8}\}, \quad \delta\vec{\psi} = \{\delta\psi_i,\ i = \overline{1,8}\},\\
&\{\psi_i, \psi_i^*\} \equiv \{\pi\varphi_i/m, \pi\varphi_i^*/m\}, \quad i = \overline{1,5},\\
&\delta\psi_i = (\pi\delta\varphi_i + \varphi_i\delta\pi)/m, \quad \delta\varphi_i = (m\delta\psi_i - \varphi_i\delta\pi)/\pi, \quad i = \overline{1,5},\\
&\vec{c} = \{c_i, (i = \overline{1,8})\} \equiv \{1, 1, c_p, c_q, 1, 1, 1, 1\}.
\end{aligned} \tag{11}$$

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

$$\begin{aligned} &\vec{Y} = \{Y_i,\ i = \overline{1,N}\} \in R(D_t), \\ &\delta\vec{Y} = \{\delta Y_i,\ i = \overline{1,N}\}, \quad \vec{Y} + \zeta\delta\vec{Y} \in R(D_t), \end{aligned} \tag{12}$$

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 a some redundancy in the system (1)–(8). First, as the continuity equation (5) as the two its consiquences (7), (8) 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 (11) and include auxiliary components in them.

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

$$\dot{\sigma} = 0 \quad \text{at} \quad \sigma = 0, 1. \tag{13}$$

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 interection 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 the variational formulation of the model.

3. Formulation of integral identity

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

$$(\vec{\varphi}_1, \vec{\varphi}_2) = \int_{D_t} \sum_{i=1}^{7} c_i(\varphi_{1i}\varphi_{2i})\, dD\, dt + c_8 \int_{S_t} \pi_1 \pi_2\, dS\, dt, \tag{14}$$

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

Let $G_i \equiv G_i(\vec{\varphi})$, $i = \overline{1,8}$, are the left-hand sides of the equations (1)–(4), (6), (8), (5), (7), accordingly, except the time derivatives. Then, using the operator notations, let us rewrite the system (1)–(8) in the operator form

$$B\frac{\partial \vec{\psi}}{\partial t} + \vec{G}(\vec{\psi}) = 0, \tag{15}$$

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 (1)–(4), (6), (8), (5), (7) are scalar multiplied by the arbitrary sufficiently smooth functions $\vec{\varphi}^* \in Q(D_t)$ in the accordance with (14)

$$I(\vec{\varphi}, \vec{\varphi}^*) \equiv \left(B\frac{\partial \vec{\psi}}{\partial t} + G(\vec{\psi}), \vec{\varphi}^*\right) = \int_{D_t} \left\{ \sum_{i=1}^{4} c_i \left(\frac{\partial \psi_i}{\partial t} + G_i(\vec{\psi})\right)\varphi_i^* + \right.$$
$$\left. c_5 G_5 \dot{\sigma}^* + c_6 G_6 \chi^* + c_7 \left(\frac{\partial \pi/m}{\partial t} + G_7\right)\Phi^* \right\} dD\, dt +$$
$$\int_{S_t} c_8 \left(\frac{\partial \pi/m}{\partial t} + G_8\right)\pi^* m\, dS\, dt = 0. \tag{16}$$

After substitution the expressions for G_i and c_i ($i = \overline{1,8}$) into (16), 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.

$$I(\varphi, \varphi^*) = \int_{D_t} \left\{ \sum_{i=1}^{4} c_i \left(\frac{\partial \psi_i}{\partial t} + M(\psi_i) + D(\psi_i)\right)\varphi_i^* + \right.$$
$$f(Uv^* - Vu^*) - (C_p \pi Q_T T^* + \pi C_q Q_q q^*)/m +$$
$$\frac{R\tilde{T}m}{\pi(\pi + p_T/\sigma)}\tau^* + \left(\Phi^* - \Phi\frac{\partial \sigma T^*}{\partial \sigma}\right)\frac{\partial}{\partial t}(\pi/m) +$$

$$\Big[\dot\Sigma + \int_0^\sigma N(\sigma')d\sigma' - \sigma\int_0^1 N(\sigma')d\sigma'\Big]\chi^* +$$
$$\Big[m\Big(U^*\frac{\partial\Phi}{\partial x} + V^*\frac{\partial\Phi}{\partial y}\Big) + \dot\Sigma^*\frac{\partial\Phi}{\partial\sigma}\Big] -$$
$$\Big[m\Big(U\frac{\partial\Phi^*}{\partial x} + V\frac{\partial\Phi^*}{\partial y}\Big) + \dot\Sigma\frac{\partial\Phi^*}{\partial\sigma}\Big]\Big\} m dD dt +$$
$$\int_{S_t}\Big\{\Big(\frac{\partial}{\partial t}(\pi/m) + \int_0^1 N(\sigma')d\sigma'\Big)\Big\}\pi^* m\, dS\, dt +$$
$$\int_{\Omega_t} U_n\Phi^* m\, d\Omega\, dt + \int_{S_t}\Phi_s T^*\frac{\partial}{\partial t}(\pi/m) m\, dS\, dt = 0, \qquad (17)$$

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 $\vec U_s = (U, V)$, $d\Omega = \{dx\, d\sigma/m;\ dy\, d\sigma/m\}$.

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 (8), (9) 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 (17).

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

$$\int_{D_t}\Big(\frac{\partial\psi_i}{\partial t} + M(\psi_i)\Big)\varphi_i^* m\, dDdt = -\int_{D_t}\Big(\frac{\partial\psi_i^*}{\partial t} + M(\psi_i^*)\Big)\varphi_i m\, dDdt + A(\psi_i, \varphi_i^*), \qquad (18)$$

$$\int_{D_t}\Big(\frac{\partial\psi_i}{\partial t} + M(\psi_i)\Big)\varphi_i m\, dD\, dt = 0.5A(\psi_i, \varphi_i), \qquad (19)$$

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

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,

$$D(\psi_i) = m\, \mathrm{div}_s\, \mu_i\, \mathrm{grad}_s\, \psi_i + \frac{\partial}{\partial \sigma} \nu_i \frac{\partial \psi_i}{\partial \sigma}, \tag{20}$$

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

$$k_i \frac{\partial \psi_i}{\partial n} = r_i, \quad (\vec{x}, t) \in \Omega_t, \tag{21}$$

$$\nu_i \frac{\partial \psi_i}{\partial \sigma} = 0 \text{ at } \sigma = 0; \qquad \nu_i \frac{\partial \psi_i}{\partial \sigma} = \tau_i \text{ at } \sigma = 1. \tag{22}$$

The functions r_i in (21) are defined from the real conditions of the approach of the corresponding fields to their background values. τ_i in (22) 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 (17), it turns to the energy balance equation

$$\begin{aligned} I(\vec{\varphi}, \vec{\varphi}_a) = {} & \left[\frac{1}{2} \int_D \pi (u^2 + v^2 + 2c_p T + c_q q^2) dD + \int_S \Phi_s \pi dS \right] \Big|_0^{\bar{t}} + \\ & \frac{1}{2} \int_{\Omega_t} \pi u_n (u^2 + v^2 + 2c_p T + c_q q^2 + 2\Phi) d\Omega\, dt = 0. \end{aligned} \tag{23}$$

The same property of energy balance should posess both the discrete analoque of (17) and the numerical model constructed on its basis.

4. The technique of the discrete approximations

Being based on the integral identity (17), we shall obtain now the discrete appoximations of the model with the help of variational principle. The following successive steps are done:

1. The grid domain D_t^h is introduced in the domain $D_t = D \times [0, \bar{t}]$. Here and further index h denotes a discrete analog. To simplify the algorithmic constructions, let us take the regular grids, which are obtained by means of the Cartesian product of the one-dimensional grids in each space direction:

$$D_t^h = w_x^h \times w_y^h \times w_\sigma^n \times w_t^h. \tag{24}$$

Here $w_s^h(s = x, y, \sigma, t)$ is one-dimensional grid, for example,

$$w_x^h = \{x_i = x_{i-1} + \Delta x_i, \ \ i = \overline{1, I}, \ x_0 = a, \ x_I = b\}. \tag{25}$$

The other grids are defined in the same way.

2. The finite-dimensional analogs of functional spaces are defined on the grid D_t^h

$$Q(D_t) \Longrightarrow Q^h(D_t^h), \qquad Q^*(D_t) \Longrightarrow Q^{*h}(D_t^h). \tag{26}$$

Then, the finite-dimensional analogs of the functions are

$$\begin{aligned} &\vec{\varphi}^h \in Q^h(D_t^h), \quad \vec{\varphi}^{*h} \in Q^{*h}(D_t^h), \\ &\vec{\varphi}^{(*)h} = \{\varphi_{imk}^{(*)j} = \varphi^{(*)}(x_i, y_m, \sigma_k, t_j)\}, \end{aligned} \tag{27}$$

where $\varphi^{(*)}(x, y, \sigma, t)$ is any component of the functions $\vec{\varphi}$ or $\vec{\varphi}^*$.

In physical sense, the structure of the pair $\vec{\varphi}^h$ and $\vec{\varphi}^{*h}$ is the same as that of the pair $\vec{\varphi} \in Q(D_t)$ and $\vec{\varphi}^* \in Q^*(D_t)$. In its turn, each component of the state vector is the vector which consists of the values of functions defined at the points of the D_t^h.

3. The integrals are approximated by quadratures defined on the grids D_t^h and S_t^h. For simplicity, we shall choose those quadratures from the variety of them, which are obtained by the successive application of one-dimensional quadrature formulas.

It should be mentioned that

- uniform calculation formulas can be obtained only, when the quadrature has got one and the same weight coefficients in each grid point;
- the error of quadrature is global for the model as a whole, i.e., it cannot be unproved by the use of more precise appoximations of the integrands.

4. The integrands are appoximated by finite differences or finite elements techniques or their combination. It is desirable to choose those ones from the admissible set, that their accuracy could not decrease the accuracy of the quadratures. There are some simple rules which are necessary to follow.

4.1. Symmeterized forms corresponding to the turbulent operators have to be appoximated by symmetrical finite-difference forms.

Antisymmetrical, with respect to ψ and φ^*, expressions which correspond to the transport operators should be appoximated by the antisymmetric finite-difference forms taking (18), (19) into account. Antisymmetric addends which are responsible for the concordence of the energy exchanges in the system should be approximated by antisymmetric discrete relations.

Discrete analogs of operators div and grad have to be in a mutual agreement in the sense of the scalar product (14) and integral identity (17).

It is worth to note that for the problems of environmental forecasting and design it is nessessary to use the schemes which are as divergent and energy-balanced as monotonic and transportive. To construct such schemes we use the techique of the appoximation of the operators $M(\psi_i) - D(\psi_i)$ proposed in [6]. It is based on the variational methods with finite elements obtained from the solution of the local adjoint problems for these operators.

4.2. Quadratures for the integrals

$$\int_0^1 \varphi d\sigma, \quad \int_\sigma^1 \varphi d\sigma', \quad \int_0^\sigma \varphi d\sigma' \tag{28}$$

must be in a mutual accordance at $0 \le \sigma \le 1$. The integral operators

$$\int_0^\sigma \varphi d\sigma', \quad \int_\sigma^1 \varphi d\sigma', \quad 0 \le \sigma \le 1, \tag{29}$$

are mutually adjoint with respect to scalar product

$$\int_0^1 \Big(\varphi(\sigma) \int_0^\sigma \psi(\sigma') d\sigma'\Big) d\sigma = \int_0^1 \Big(\psi(\sigma') \int_{\sigma'}^1 \varphi(\sigma) d\sigma\Big) d\sigma'. \tag{30}$$

This property has to be conserved in the discrete analogs.

4.3. For the approximation in time, we use the splitting schemes or the combinations of exlicit-implicit and explicit schemes. It depends on the problem under consideration.

4.4. Making the above mentioned successive steps, we obtain the discrete analog of (17).

Let us denote it as

$$I^h(\vec{\varphi}, \vec{\varphi}^*) = 0, \qquad \vec{\varphi} \in Q^h(D_t^h), \quad \vec{\varphi}^* \in Q^{*h}(D_t^h). \tag{31}$$

By analogy with (16) we can present (31) as

$$I^h(\vec{\varphi}, \vec{\varphi}^*) = (B\Lambda_t \vec{\psi} + A(\vec{\psi}), \vec{\varphi}^*) = 0, \tag{32}$$

$$A(\varphi) \equiv G^h(\vec{\psi}), \quad \Lambda_t \psi \equiv \Big(\frac{\partial \psi}{\partial t}\Big)^h. \tag{33}$$

Sum functional $I^h(\vec{\varphi}, \vec{\varphi}^*)$ is the function of the grid components of the functions $\vec{\psi}^h$ or $\vec{\varphi}^h$ and $\vec{\varphi}^{*h}$.

The discrete analog of balance energy equation (23) is obtained if to substitute the vector $\vec{\varphi}^{*h} = \vec{\varphi}_a^h$ into (31)

$$I^h(\vec{\varphi}, \vec{\varphi}_a) = 0. \tag{34}$$

It is important to keep in mind that functional $I^h(\vec{\varphi}, \vec{\varphi}^*)$ is linear dependent on the grid components of the vector $\vec{\varphi}^{*h}$, and it is non-linear with respect to the components of the vector $\vec{\varphi}^h$.

The algorithms of the construction of the sum analog of the integral identity are described in more detailes in [3].

Using the variational calculus techniques we obtain the discrete appoximations of the basic system of equations (1)–(8) from the stationarity conditions for the sum functional with respect to the arbitrary and independent variations of grid components of the function $\vec{\psi}^{*h}$.

These conditions are written as the system of equations

$$\frac{\partial I^h(\vec{\varphi}, \vec{\varphi}^*)}{\partial \varphi^{*j}_{imk}} = 0, \tag{35}$$

where $\varphi^* = \varphi^*_\alpha$, $\alpha = \overline{1,8}$. The set of indexes (i, m, k, j) runs successively the whole variaty of the grid domain point numbers, including those parts of the boundary where the values of state functions are not qiven.

Thus, the family of energy-balanced discrete models is obtained.

5. The algorithm of the construction of adjoint operators and sensitivity functions

Hereby we briefly describe the algorithm of the construction of adjoint equations.

Adjoint system in differential form is qenerated from the functional $I(\varphi, \vec{\varphi}^*)$ with the help of the stationarity conditions with respect to independent and arbitrary variations of the components of the state function $\vec{\psi}$. The similar procedure for the discrete form of (17) will give us the discrete analog of the adjoint equations.

There is one essential difference between the construction of the direct and adjoint problems. It is due to non-linearity of the functionals $I(\vec{\varphi}, \vec{\varphi}^*)$ and $I^h(\vec{\varphi}, \vec{\varphi}^*)$ with respect to the components of the state function $\vec{\varphi}$. Therefore it is necessary, first, to linearize these functionals. After that all operations are fulfilled by analogy with the construction of the direct problem.

5.1. The scheme of the algoritm for the construction of the adjoint operators.

1. First we construct the integral and sum functionals of the forms

$$I(\vec{\varphi}, \vec{\varphi}^*), \qquad I^h(\vec{\varphi}, \vec{\varphi}^*).$$

2. Then we introduce the vector of perturbed values of the state function as

$$\vec{\psi}_p \equiv \vec{\psi} + \xi\delta\vec{\psi} \in Q(D_t), \tag{36}$$

where $\vec{\psi}$ is the known state function, $\delta\vec{\psi}$ is the vector of variations, ξ is a real parameter. In the discrete case, the components of all these vectors $\vec{\psi}_p$, $\vec{\psi}$, $\delta\vec{\psi}$, are given in the grid points of the domain D_t^h. The connection between these vectors and $\vec{\varphi}$, $\delta\vec{\varphi}$ is given in (11). The unperturbed state function $\vec{\psi}$ in (36) is the solution of the direct problem with the prescribed values of the parameters (12). Similarly (36), the vector of perturbed values of parameters can be defined as

$$\vec{Y}_p = \vec{Y} + \xi\delta\vec{Y}, \tag{37}$$

where $\vec{Y}$ is given and $\delta\vec{Y}$ is the vector of variations (12). It is supposed that $\vec{Y}, \vec{Y}_p \in \{R(D_t), R^h(D_t^h)\}$.

3. Now we shall describe the basic operations of the algorithm.

3.1. First we substitute $\vec{\varphi}_p$ instead of $\vec{\varphi}$ in the expressions of functionals.

3.2. Then we linearize the functionals in the vicinity of $\vec{\varphi}$ and extract the terms with the components of $\vec{\delta\psi}$ by means of the operations

$$\frac{\partial}{\partial\xi} I(\vec{\varphi} + \xi\delta\vec{\varphi}, \vec{\varphi}^*)_{\xi=0} \equiv C(\vec{\varphi}, \delta\vec{\psi}, \vec{\varphi}^*), \tag{38}$$

$$\frac{\partial}{\partial\xi} I^h(\vec{\varphi} + \xi\delta\vec{\varphi}, \vec{\varphi}^*)_{\xi=0} \equiv C^h(\vec{\varphi}, \delta\vec{\psi}, \vec{\varphi}^*). \tag{39}$$

3.3. Now we put together the expressions including the variations of the components of the state function $\vec{\varphi}$, as it is prescribed by the definition of the inner product (14)

$$\begin{aligned} C(\vec{\varphi}, \delta\vec{\psi}, \vec{\varphi}^*) &= \Big(\tilde{B}\frac{\partial\vec{\varphi}^*}{\partial t} + A_L^*(\vec{\varphi})\vec{\varphi}^*, \delta\vec{\psi}\Big), \\ C^h(\vec{\varphi}, \delta\vec{\psi}, \vec{\varphi}^*) &= \big((\tilde{B}\Lambda_t^* + A_L^*(\vec{\varphi}))\vec{\varphi}^*, \delta\vec{\psi}\big)^h \end{aligned} \tag{40}$$

where Λ_t^* is the adjoint operator to Λ_t. The last is the operator of the discrete approximation of the time derivatives; $A_L^*(\vec{\varphi})$ is the operator of the adjoint problem with respect to the space variables; $A_L^{*h}(\vec{\varphi})$ is its discrete analog; $\tilde{B}\frac{\partial\vec{\varphi}^*}{\partial t} + A_L^*(\vec{\varphi})\vec{\varphi}^*$ is the operator of the adjoint problem, $\tilde{B}$ is the weight matrix. In the discrete case, the operator of the adjoint problem is obtained from the algorithm

$$\frac{\partial}{\partial\delta\psi_{imk}^j} C^h(\vec{\varphi}, \delta\vec{\psi}, \vec{\varphi}^*) \equiv \tilde{B}\Lambda_t^*\varphi^* + A_L^{*h}(\vec{\varphi})\vec{\varphi}^*, \quad \varphi^* \in Q^{*h}(D_t^h). \tag{41}$$

Here all indexes i, m, k, j run the whole set of the point numbers of the grid domain D_t^h. The concrete structure of the operators Λ_t and Λ_t^* for the three-time-level numerical schemes will be described later on.

3.4. Finaly, the adjoint problem is formulated in the following way

$$\tilde{B}\Lambda_t^* \varphi^* + A_L^{*h}(\vec{\varphi})\vec{\varphi}^* = \vec{\eta}, \qquad \vec{\varphi}^*|_{t=\bar{t}} = 0, \tag{42}$$

where $\vec{\eta}$ is some given vector. Usually it is generated by the quality functional of the model.

3.5. The construction of the main sensitivity relation is made according to the algorithm

$$\delta I^h(\vec{\varphi}, \vec{\varphi}^*) = \frac{\partial}{\partial \xi} I^h(\vec{\varphi}, \vec{\varphi}^*, \vec{Y} + \xi \delta \vec{Y})_{\xi=0} \equiv R^h(\vec{\varphi}, \vec{\varphi}^*, \delta \vec{Y}), \tag{43}$$

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

3.6. The calculation of the sensitivity function is made by the formula

$$\frac{\partial I^h}{\partial Y_i} = \frac{\partial}{\partial \delta Y_i} R^h(\vec{\varphi}, \vec{\varphi}^*, \delta \vec{Y}), \qquad i = \overline{1, N}. \tag{44}$$

6. 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 (17) 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 (17)

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

has got the rather complicated dependence on its arguments. That is why, for the 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 $\delta\vec{\psi}$ (see (39), (40)), and (2) terms with the variations $\delta\vec{Y}$ (see (43)). Finally, the first group generates the adjoint problems (41), (42), and the second one – the main sensitivity relation (43) and the sensitivity functions themselves (44).

6.1. The form with the transport operators. The following terms in (17) are of this type

$$A_1(\vec{\varphi},\vec{\varphi^*}) \equiv \int_{D_t}\Big\{\sum_{i=1}^{4} c_i\Big(\frac{\partial\psi_i}{\partial t}+M(\psi_i)\Big)\varphi_i^*\Big\} m\,dD\,dt$$
$$= \sum_{i=1}^{4} c_i\Big\{\int_{D_t}\Big(-\frac{\partial\varphi_i^*}{\partial t}+M^*(\vec{\varphi})\varphi_i^*\Big)\psi_i m\,dD\,dt +$$
$$\int_D \psi_i\varphi_i^* m\,dD\Big|_0^{\bar t} + \int_{\Omega_t} U_n\psi_i\varphi_i^*\frac{m^2}{\pi}d\Omega dt\Big\}, \qquad (45)$$

where

$$M^*(\vec{\varphi})\varphi^* = -m\Big[U\frac{m}{\pi}\frac{\partial\varphi^*}{\partial x}+\frac{Vm}{\pi}\frac{\partial\varphi^*}{\partial y}\Big] - \frac{\dot\Sigma m}{\pi}\frac{\partial\varphi^*}{\partial\sigma}$$

is the operator formally adjoint to $M(\psi_i)$. The boundary conditions $\dot\sigma = 0$ at $\sigma = 0,1$ are taken into account in (45). The variation of the functional $A_1(\vec{\varphi},\vec{\varphi})$ is in the form:

$$\delta A_1(\vec{\varphi},\vec{\varphi^*}) = \sum_{i=1}^{4} c_i\Big\{\int_{D_t}\Big(-\frac{\partial\varphi_i^*}{\partial t}+M^*(\vec{\varphi})\varphi_i^*\Big)\delta\psi_i m\,dDdt + \int_D \delta\psi_i\varphi_i^* m\,dD\Big|_0^{\bar t}\Big\} -$$
$$\int_{D_t}\Big\{\delta U\sum_{i=1}^{4} c_i\Big(\frac{m^2}{\pi}\Big)\psi_i\frac{\partial\varphi_i^*}{\partial x} + \delta V\sum_{i=1}^{4} c_i\Big(\frac{m^2}{\pi}\Big)\psi_i\frac{\partial\varphi_i^*}{\partial y} +$$
$$\delta\dot\Sigma\sum_{i=1}^{4} c_i\Big(\frac{m^2}{\pi}\Big)\psi_i\frac{\partial\varphi_i^*}{\partial\sigma}\Big\} m\,dD\,dt +$$
$$\int_{D_t}\Big\{\frac{\partial\pi}{\pi^2}\sum_{i=1}^{4}\Big[m^2 c_i\psi_i\Big(m\vec{U}_s\,\mathrm{grad}_s\,\varphi_i^* + \dot\Sigma\frac{\partial\varphi_i^*}{\partial\sigma}\Big)\Big]\Big\} m\,dD\,dt +$$
$$R_1(\vec{\varphi},\vec{\varphi_i^*},\delta\vec{Y}), \qquad (46)$$

$$R_1(\vec{\varphi},\vec{\varphi_i^*},\delta\vec{Y}) \equiv \int_{\Omega_t}\Big\{\delta U_n\sum_{i=1}^{4} c_i\psi_i\varphi_i^*\frac{m^2}{\pi} + \sum_{i=1}^{4} c_i U_n\delta\psi_i\varphi_i^*\frac{m^2}{\pi} -$$
$$\frac{\delta\pi}{\pi^2}\sum_{i=1}^{4} m^2 c_i U_n\psi_i\varphi_i^*\Big\} d\Omega\,dt. \qquad (47)$$

6.2. The form with the turbulent operators.

$$A_2(\vec{\varphi},\vec{\varphi^*}) = \int_{D_t}\sum_{i=1}^{4} c_i(D(\psi_i)\varphi_i^*)m\,dD\,dt + A_i +$$
$$\sum_{i=1}^{4} c_i\Big\{\int_{\Omega_t} r_i\varphi_i^* m\,d\Omega\,dt + \int_{S_t}\tau_i\varphi_i^* m\,dS\,dt\Big\}, \qquad (48)$$

$$A_i = -\int_{D_t}\sum_{i=1}^{4} c_i\Big(mu_i\,\mathrm{grad}_s\,\psi_i\,\mathrm{grad}_s\,\varphi_i^* + \frac{\nu_i}{m}\frac{\partial\psi_i}{\partial\sigma}\frac{\partial\varphi_i^*}{\partial\sigma}\Big)m^2 dDdt$$

or

$$\int_{D_t}\sum_{i=1}^{4} c_i(D(\varphi_i^*)\psi_i)m\,dD\,dt.$$

The uniform boundary conditions agreed with (21), (22) are taken for the functions φ_i^*, $i=\overline{1,4}$,

$$\frac{\partial\varphi_i^*}{\partial n} = 0,\ \ (\vec{x},t)\in\Omega_t,\ \ \frac{\partial\varphi_i^*}{\partial\sigma} = 0 \ \text{at}\ \sigma = 0,1. \tag{49}$$

The variations of the functional $A_2(\vec{\varphi},\vec{\varphi}^*)$ are

$$\delta A_2(\vec{\varphi},\vec{\varphi}^*) = \int_{D_t}\sum_{i=1}^{4} c_i(D(\psi_i^*)\delta\psi_i)m\,dD\,dt + R_2(\vec{\varphi},\vec{\varphi}_i^*,\delta\vec{Y}), \tag{50}$$

where

$$R_2(\vec{\varphi},\vec{\varphi}_i^*,\delta\vec{Y}) \equiv \sum_{i=1}^{4} c_i\Big\{\int_{D_t}\Big[\delta\mu_i\,\mathrm{grad}_s\,\psi_i\,\mathrm{grad}_i\,\varphi_i^* + \frac{\delta\nu_i}{m}\frac{\partial\psi_i^*}{\partial\sigma}\frac{\partial\varphi_i^*}{\partial\sigma}\Big]m^2\,dDdt + \int_{\Omega_t}\delta r_i\varphi_i^* m\,d\Omega\,dt + \int_{S_t}\delta\tau_i\varphi_i^* m\,dS\,dt\Big\}, \tag{51}$$

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

6.3. The form with the operators of the energy exchanges. The rest terms in (17) belong to the third group. They are connected with the operators of the energetic exhange, the continuity equation and the two its consequences. Inspite of their cumbersome form they can be directly variated without difficalties. That is why we do not write them here.

Getting together the results of the variations of three groups, we obtain the common expression for the variation of (17). Formally, it is the superposition of (38) and (43).

6.4. The adjoint system. In accordance with (41), (42), 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

$$-\frac{\partial u^*}{\partial t} + M^*u^* + fv^* - m\Big(\frac{\partial\Phi^*}{\partial x} + aT^*\frac{\partial\pi}{\partial x} + \frac{\partial}{\partial x}\Big(\int_\sigma^1\chi^* d\sigma' - \int_0^1\sigma'\chi^* d\sigma'\Big)\Big) - \sum_{i=1}^{4} c_i\Big(\frac{m^2}{\pi}\Big)\psi_i\frac{\partial\varphi_i^*}{\partial x} - D(u^*) + \eta_1 = 0, \tag{52}$$

$$-\frac{\partial v^*}{\partial t} + M^*v^* - lu^* - m\Big(\frac{\partial \Phi^*}{\partial y} + aT^*\frac{\partial \pi}{\partial y} + \frac{\partial}{\partial y}\Big(\int_\sigma^1 \chi^* d\sigma' - \int_0^1 \sigma'\chi^* d\sigma'\Big)\Big) -$$
$$\sum_{i=1}^{4} c_i\Big(\frac{m^2}{\pi}\Big)\psi_i\frac{\partial \varphi_i^*}{\partial y} - D(v^*) + \eta_2 = 0, \tag{53}$$

$$-\frac{\partial T^*}{\partial t} + M^*T^* + \frac{Rm}{\pi(\pi + p_1/\sigma)}\tau^* - D(T^*) + \eta_3 = 0, \tag{54}$$

$$-\frac{\partial q^*}{\partial t} + M^*q^* - D(q^*) + \eta_4 = 0, \tag{55}$$

$$m\Big(\frac{\partial U^*}{\partial x} + \frac{\partial V^*}{\partial y}\Big) + \frac{\partial \dot{\Sigma}^*}{\partial \sigma} + \frac{\partial \sigma T^*}{\partial \sigma}\frac{\partial}{\partial t}\Big(\frac{\pi}{m}\Big) - \eta_5 = 0, \tag{56}$$

$$\chi^* - \frac{a\pi T^*}{\sigma} - \frac{\partial \Phi^*}{\partial \sigma} - \sum_{i=1}^{4} c_i\psi_i\frac{\partial \varphi_i^*}{\partial \sigma} + \eta_6 = 0, \tag{57}$$

$$\Phi^* - \pi a T^* + \eta_7 = 0, \tag{58}$$

$$\frac{\partial}{\partial t}(\pi^*/m) + \frac{a(2\pi + p_T/\sigma)}{\pi(\pi + p_T/\sigma)}\tau^* + \frac{a}{\sigma}(\dot{\Sigma}^* - \dot{\Sigma}T^*) +$$
$$m\Big(\frac{\partial}{\partial x}a(U^* - UT^*) + \frac{\partial}{\partial y}a(V^* - VT^*)\Big) +$$
$$\frac{1}{\pi^2}\sum_{i=1}^{4} m^2 c_i\psi_i\Big(\vec{U}_s\,\mathrm{grad}_s\,\varphi_i^* + (\dot{\Sigma}/m)\frac{\partial \varphi_i^*}{\partial \sigma}\Big) - \eta_8 = 0, \tag{59}$$

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

The conditions

$$u^* = 0, \quad v^* = 0, \quad T^* = 0, \quad q^* = 0, \quad \pi^* = 0, \quad \text{at } t = \bar{t} \tag{60}$$

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 (56)–(58) 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 $\vec{\psi}$.

6.5. Dependence on the input parameters. If to suppose that the function $\vec{\varphi}^*$ satisfies the homogenious system (52)–(59) (i.e., at $\vec{\eta} = 0$), and the condition (60), it is obtained

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

$$= \int_{D_t}(c_3\delta Q_T T^* + c_4\delta Q_q q^*)dD\,dt + \int_D \sum_{i=1}^{4} c_i\delta\psi_i\varphi_i^*\big|_{t=0} m\,dD +$$

$$R_1(\vec{\varphi},\vec{\varphi}^*,\delta\vec{Y}) + R_2(\vec{\varphi},\vec{\varphi}^*,\delta\vec{Y}) + R_3(\vec{\varphi},\vec{\varphi}^*,\delta\vec{Y}), \qquad (61)$$

where R_1, R_2 are given by (47), (51), and

$$R_3(\vec{\varphi},\vec{\varphi}^*,\delta\vec{Y}) \equiv \int_{\Omega_t}\{\Phi^*\delta U_n + U_n^*\delta\Phi + (U_n^* - U_n T^*)\delta\pi - \pi T^*\delta U_n\} m\,d\Omega\,dt -$$

$$\int_S (T^*\delta(\Phi_s\pi) + \pi^*\delta\pi)\big|_{t=0} dS. \qquad (62)$$

6.6. The sensitivity relations. To study the model behaviour, let us introduce the set of general characterictics, which take the form of the functionals defined on the set of the values $\vec{\varphi}$

$$J_k(\vec{\varphi}) = \int_{D_t} F_k(\vec{\varphi})\omega_k(\vec{x},t) m\,dD\,dt, \quad k=\overline{1,K}, \quad k \geq r, \qquad (63)$$

where $F_k(\vec{\varphi})$ are the given functions differentiable with respect to $\vec{\varphi}$, $\omega_k(\vec{x},t)$ is non-negative functions defined in D_t.

The variations of functionals

$$\delta J_k(\vec{\varphi}) = (\mathrm{grad}_{\vec{Y}}\, J_k(\vec{\varphi}),\delta\vec{Y}), \quad k=\overline{1,K}, \qquad (64)$$

are used as the measure of the model sensitivity, where

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

is the set of the sensitivity functions of (63) 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:

1. The direct problem with the undisturbed values of the parameter vector is solved in the discrete form (35). As a result, the solution $\vec{\varphi}$ is obtained.

2. The set of the vectors are calculated

$$\vec{\eta}_k = \frac{\partial J_k^h(\vec{\varphi})}{\partial\vec{\psi}} \equiv \Big\{\eta_{ki} = \frac{\partial F_k^h(\vec{\varphi})}{\partial\vec{\psi}_i}\omega_k(\vec{x},t), \ i=\overline{1,8}\Big\}, \quad k=\overline{1,K}. \qquad (65)$$

3. The set of the adjoint problems (52)–(60) 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

$$\delta J_k^h(\vec{\varphi}) = R^h(\vec{\varphi}, \vec{\varphi}_k^*, \delta\vec{Y}), \quad k = \overline{1,K}, \tag{66}$$

where $R^h(\vec{\varphi}, \vec{\varphi}_k^*, \delta\vec{Y})$ is obtained from (61) 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 (64) and (66) are equated with each other. This action is equivalent to the calculations of

$$\operatorname{grad}_{\vec{Y}} J_k^h(\vec{\varphi}) = \left\{\frac{\partial}{\partial \delta Y_i} R^h(\vec{\varphi}, \vec{\varphi}_k^*, \delta\vec{Y}),\ i = \overline{1,N}\right\}, \quad k = \overline{1,K}. \tag{67}$$

The differentiation in (67) 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.

7. The system organization of the direct and adjoint problems

The structure of the ajoint system is uniquely defined by the structure of both the direct problem and the integral identity, and by the ways of their discretization. For the description of the direct problem it is enough to present its local structure and the time behaviour. But it is not the case for the adjoit problem and sensitivity methods. It is neccessary to describe complitely both the local and global structures of the direct and adjoint problems simultaniously. In principle, it is reached by the discretization of the integral identity. The different combinations of the approximation in time, which provide the stable computations, are used in modern models. In this sense the typical example of the time approximations is the atmospheric model of the Beijing University (BUM) [9]. We take this model as one of the basic models for the construction of the algorithms of the sensitivity theory. Now we describe the system organization of the direct and ajoint problem for this type of models. (The system organization for the models with splitting schemes was described in [3–4]). To make it as simple as possible, we leave the local space structure and physical sense of the state functions out of the present description. They are presented in (11) and (27). We concentrate on the time structure. For conviniency, the notations for the operators and the state and the trial vectors are slightly changed: the vectors are reorganized as blocks and the only shown index of the block is the time index.

7.1. The time structure of the state functions. Three kinds of time approximations are used in the BUM model realization:

a) two-step two-level Euler–Backward–Matsuno scheme (EBM);

b) three-layer leap-frog scheme, (LF);

c) smoothing procedure (S).

Lef us define the following notations: φ is the state function in the LF scheme and at the first step of EBM scheme; $\tilde{\varphi}$ is an auxiliary function at the second step of EBM scheme; φ^s the state function after smooting; β is a number of steps on EBM scheme ($\beta = 8$); α is a number of steps on LF scheme ($\alpha = 40$); K is a number of cycles of $(\alpha + \beta)$ steps in time; j is a current step number in the combined scheme {EBM; LF; S}; $K(\alpha + \beta)$ is the number of the time steps.

Computations are cyclically repeated in $(\alpha + \beta + 1)$ steps (uncluding smoothing). For the convinience, let us introduce a block structure of the state functions of the model

$$\vec{\Phi} = \{\vec{\Phi}_k,\ k = \overline{0,K}\} \equiv \left\{\varphi_\kappa,\ \kappa = \overline{0, K(2\beta + \alpha + 1)}\right\},$$

where k is an index of a vector-block. It coincides with the cycle number; κ is a current index running the whole time interval, $\kappa \in \overline{0, K(2\beta + \alpha + 1)}$. Each block $\vec{\Phi}_k$ consists of $2\beta + \alpha + 1$ vectors:

$$\vec{\Phi}_k = \left\{\varphi_{jk} \equiv \{\varphi^s_{0k}, \varphi_{1k}, \tilde{\varphi}_{1k}, \ldots, \varphi_{\beta k}, \tilde{\varphi}_{\beta k}, \varphi_{\beta+1 k}, \ldots, \varphi_{\alpha+\beta k}\}\right\},$$

where $j \in \overline{0, \alpha + \beta}$ is the current index of the state function in the k-th block.

The relation between the indexes j, k and the time step number ξ is

$$\xi = k(\beta + \alpha) + j, \quad k = \overline{0, K}, \quad j = \overline{0, \alpha + \beta}.$$

Smoothing procedure does not increase the time step number $\varphi^s_{\alpha+\beta k} \equiv \varphi^s_{0k+1}$; $\varphi^s_{00} = \varphi_0$ is the initial state function.

As for the relations between the indexes ξ, k of the block-vectors and the index κ in the current numeration, they are defined as

$$\varphi_{jk} = \varphi_\kappa, \quad \begin{cases} \kappa = kM + 2j, & j \le \beta, \\ \kappa = kM + j + \beta, & j > \beta, \end{cases}$$

$$\tilde{\varphi}_{jk} = \varphi_\kappa, \quad \kappa = kM + 2j - 1, \quad j \le \beta,$$

$$\varphi^s_{jk} = \varphi_\kappa, \quad \kappa = kM + j,$$

$$M = 2\beta + \alpha + 1.$$

7.2. Definition of the scalar product in time. Let

$$(\vec{\Phi}, \vec{\Psi}) = \sum_{k=0}^{K} \Big\{ \sum_{j=0}^{\beta-1} \Big[(\vec{\varphi}_j, \vec{\psi}_j)_k \Delta t + (\vec{\tilde{\varphi}}_j, \vec{\tilde{\psi}}_j)_k \Delta t \Big] + \sum_{j=\beta}^{\alpha+\beta} (\vec{\varphi}_j, \vec{\psi}_j)_k 2\Delta t \Big\}. \quad (68)$$

This is the discrete analog of (14). Here and further the expressions of the form $(\vec{\varphi}_j, \vec{\psi}_j)$ denote the scalar product of the corresponding vector functions with respect to the space variables in (14).

7.3. The time structure of the basic sum functional. Now we discuss the structure of the appoximations for the integrals and derivatives in time. They are included in the definition of the scalar product (14) and integral identity (17). Namely, the formula (68) is the appoximation of the integral in time in (14) and (17). In this section we do not touch the space structure at all.

The following sum identity corresponds to the basic model

$$\begin{aligned} I(\vec{\Phi}, \vec{\Phi}^*) \equiv \sum_{k=0}^{K-1} \Big\{ \sum_{j=0}^{\beta-1} \Big\{ \Big(\frac{\tilde{\varphi}_{j+1} - \varphi_j}{\Delta t} + A_j \varphi_j - f_j \Big) \tilde{\varphi}^*_{j+1} \Delta t + \\ \Big(\frac{\varphi_{j+1} - \varphi_j}{\Delta t} + \tilde{A}_j \tilde{\varphi}_{j+1} - \tilde{f}_j \Big) \varphi^*_{j+1} \Delta t \Big\} + \\ \sum_{j=\beta}^{\alpha+\beta-1} \Big[\Big(\frac{\varphi_{j+1} - \varphi_{j-1}}{2\Delta t} + A_j \varphi_j \Big) \varphi^*_{j+1} 2\Delta t \Big] + \\ \Big(\frac{\varphi^S_{\alpha+\beta} - \varphi_{\alpha+\beta}}{\Delta t} - S_{\alpha+\beta} \varphi_{\alpha+\beta} \Big) \varphi^{*S}_{\alpha+\beta} \Delta t \Big\}_k = 0, \end{aligned} \quad (69)$$

where A_{jk} is the operator of basic model (32), (33) calculated at the time moment t_{jk} with the state functions φ_{jk}; $\tilde{A}_{jk}$ is the operator of basic model calculated with the function $\tilde{\varphi}_{jk}$, i.e.,

$$\{A_{jk}; \tilde{A}_{jk}\} \equiv \{G^h(\vec{\varphi}_{jk}); G^h(\vec{\tilde{\varphi}}_{jk})\};$$

f_{jk} is a vector of right-hand sides of the discrete equations of the model at the time moment t_{jk}; $\tilde{f}_{jk}$ is a vector of right-hand sides at the time moment t_{jk} calculated on the second step of the EBM scheme. For simplicity the matrix B is formally omited here. Nevertheless, it is taken into account in the structure of the time-difference operator.

7.4. Algorithm of the direct model realization in time. The algorithm of the realization of basic model in time can be written as the following succession of items:

1. Inital data: φ_0, $k = 0$.

The beginning of the k-th cycle:

2. Scheme EBM (β time steps)

$$\Big(\frac{\tilde{\varphi}_{j+1} - \varphi_j}{\Delta t} + A_j\varphi_j - f_j = 0\Big)_k,$$
$$\Big(\frac{\varphi_{j+1} - \varphi_j}{\Delta t} + A_j\tilde{\varphi}_j - f_j = 0\Big)_k, \quad j = \overline{0, \beta - 1}.$$

3. Scheme LF (α time steps)

$$\Big(\frac{\varphi_{j+1} - \varphi_{j-1}}{2\Delta t} + A_j(\varphi_j) - f_j = 0\Big)_k, \quad j = \overline{\beta, \alpha + \beta - 1}.$$

4. Smoothing (1 step)

$$\Big(\frac{\varphi_j^s - \varphi_j}{\Delta t} - S_j\varphi_j = 0\Big)_k, \quad j = \alpha + \beta.$$

5. $k = k + 1$.
6. Repetition of the items 2–4.
7. The end of the computation at $k = K + 1$. The vector $\vec{\varphi}_K$ is the final result.

7.5. Construction of the adjoint system of equations. The adjoint system of equations is obtained from the stationary conditions of the sum functional (69) under arbitrary and independent variations of the components of the state function $\vec{\Phi}$ in the vicinity of their unperturbed values. As such values, the solution of the direct problem with the given input parameters is used.

Formally, the algorithm of the construction of the adjoint system (38)–(42) is described by the operator formula

$$\frac{\partial}{\partial \delta\varphi_x}\Big[\frac{\partial}{\partial \xi} I^h(\vec{\Phi} + \xi\delta\vec{\Phi}, \vec{\Phi})\Big]_{\xi=0} = 0, \tag{70}$$

$$\kappa = \overline{1, (K+1)M}, \quad M = 2\beta + \alpha + 1.$$

To construct the general form of the ajoint problem and algorithm for its realization, let us fulfil all essential operations on the block level without description of their inner structure.

Successively providing all operations, one obtaines the following algorithm for the solution of the adjoint problem:

1. $\varphi^{*s}_{(K+1)(\alpha+\beta)}$ is given, $J = (K+1)(\alpha+\beta)$.
2. First two steps are carried out

$$\varphi^*_J = \varphi^{*s}_J + \Delta t S^*_J \varphi^s_J, \qquad \varphi^*_{J-1} = -2\Delta t A^*_{J-1}\varphi^*_J.$$

3. The adjoint LF scheme is

$$\varphi^*_j = \varphi^*_{j-2} - 2\Delta t A^*_j \varphi^*_{j+1}, \quad j = J-2, \ldots, J-\alpha.$$

4. Transition from the adjoint LF scheme to the adjoint EBM scheme

$$j = J - \alpha, \quad \tilde{\varphi}^*_j = -\Delta t \tilde{A}^*_{j-1}\varphi^*_j, \tag{71}$$

$$\varphi^*_{j-1} = \tilde{\varphi}^*_j + \varphi^*_j + \varphi^*_{j+1} - \Delta t A^*_{j-1}\tilde{\varphi}^*_j. \tag{72}$$

5. The adjont EBM scheme

$$\tilde{\varphi}^*_{j+1} = -\Delta t \tilde{A}^*_j \varphi^*_{j+1}, \quad \varphi^*_j = \tilde{\varphi}^*_{j+1} + \varphi^*_{j+1} - \Delta t A^*_j \tilde{\varphi}^*_{j+1},$$
$$j = J - \alpha - 2, \ldots, J - (\alpha+\beta).$$

   It should be mentioned that

$$A^*_{J-(\alpha+\beta)} \equiv A^{*(s)}_{J-(\alpha+\beta)}.$$

   It means that smoothed solution of the direct problem is used at this step.

6. $J = J - (\alpha+\beta)$. If $J \neq 0$, then the calculations should be continued cyclically starting with item 2. If $J = 0$, the calculation are finished. And φ^*_0 is the solution of the adjoint problem at the time moment $t = 0$.

The following definitions are accepted above: A^*, $\tilde{A}^*$, S^* are the adjoint operators with respect to the linearized operators A, $\tilde{A}$, S of the direct problem, i.e., $A^* = A^*_L(\bar{\varphi})$ from (40)–(42). Linearization is provided in the vicinity of the undisturbed state. Indexes of the operators show the current time step numbers. The operators A_j and $\tilde{A}_j$ depend on the solution of the direct problem at the moment $t = t_j$. In contrast to the direct problem, integration of the adjont problem is carried out in the opposite time direction.

8. Conclusion

The presented algorithms of the construction of the direct and adjoint equations for the numerical models are the basis for the development of the methods for the combined use of the models and measured data. The realization of the direct and feed-back relations between models and data are provided by the sensitivity methods. They take part in the optimal technique of the assimilation of observations and in the identification of the models. This is the means for the realization of the inverse methodology for studying the natural processes and for the solution of the problems of environmental protection.

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