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VARIATIONAL DATA ASSIMILATION METHODS IN GEOPHYSICAL HYDRODYNAMICS MODELS AND THEIR APPLICATION

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We consider direct and inverse problems of geophysical hydrodynamics, associated with prediction, posterior analysis, and variational assimilation of observational data. The focus is on numerical algorithms for solving problems with incomplete information (initial and boundary conditions). Along with the classical algorithms, an approach to setting and solving these problems developed in the works of G. I. Marchuk and his scientific school is presented. The approach is based on a combination of splitting methods and adjoint equations. This leads to the construction of flexible, hierarchically developed models of complex systems with a modular structure and efficient implementation. The main part of this approach is splitting a complex nonlinear system of equations for physical processes into a number of energetically balanced subsystems. Each individual subsystem can reuse splitting into subsystems of a simpler structure. The methodology is illustrated by solving the problems in hydrodynamics of the World Ocean and the Black Sea.

1. INTRODUCTION

In recent decades, the growing interest in the problems of assimilation of observational data in mathematical models of geophysical hydrodynamics is determined by significant progress in three areas of science and technology. This includes the creation of increasingly powerful computing systems, the development of new satellite and contact measurement technologies, and also new methods and computational algorithms. The ability to analyze and process large flows of information and use it in models has led to the setting of new mathematical problems of geophysical hydrodynamics. The need to synthesize measurement and simulation data has given rise to the most complex scientific and technological problems associated with the improvement of computational methods for modeling and analyzing natural phenomena.

Mathematical models are used in problems of geophysical hydrodynamics to study the general behavior of hydrodynamic flows, as well as to predict their dynamics, as, e. g., in the case of problems of meteorology and oceanography [1].

A distinctive feature of the study of hydrodynamic flows is the importance of the observational data availability. First of all, due to the non-linearity, we cannot expect global theoretical results regarding hydrodynamic flows. We can only speak about some neighborhood of a specific situation where data are available. In addition, the geophysical sciences are not strictly experimental, i. e., a particular hypothesis cannot be tested by repeating a full-scale experiment. Every moment of time (episode) is unique. Therefore, hydrodynamic flows can be explored using both observational data and a model as the source of information about a particular episode.

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The "data assimilation" methods are used to link these sources of information and then predict the state of the flow at an appropriate time. In recent decades, significant progress has been reached in the Earth sciences due to the improvement of observation systems and the understanding of the geosystem laws. The goal of data assimilation is to find the best estimate of the state of a particular physical system, using both the information obtained from observations of the system and its mathematical model. Data assimilation techniques are widely used in the Earth sciences. They have received their greatest applications in meteorology and oceanography, where observations of the atmosphere and the ocean are assimilated into atmospheric and oceanic models in order to obtain initial conditions (or other model parameters) for the further simulation and prediction. In recent years, the data assimilation techniques have also been applied to the analysis of other geosystem measurements, including the biosphere, cryosphere, and soil surface.

The description of theoretical and practical ideas of data assimilation can be found in various fields of science [2–9]. The development of this area is largely based on works by Guriy I. Marchuk. In the 1970s, G. I. Marchuk formulated a fundamental approach to solving the problems of long-term weather forecast and climate variability based on the adjoint equations of atmospheric and oceanic hydrothermodynamics. Later, the theory of adjoint equations and perturbation algorithms was developed in G. I. Marchuk's works for a study of different classes of problems in mathematical physics described by complex systems and mathematical models [3]. These approaches were the main content of the long-term research of G. I. Marchuk and his scientific school at the Institute of Numerical Mathematics of the Russian Academy of Sciences in different areas of mathematics and its applications to the problems of geophysical hydrodynamics, models of environmental protection, the theory of climate and its variations, mathematical problems of processing of information from satellites, the theory of tides, etc.

At present, significant qualitative changes in measurement systems are taking place, and the world scientific community is receiving more and more data on the different features of our geosystem. Therefore, the development of technologies for variational assimilation of observational data, which are based on modern approaches and allow for the latest achievements in this field, is a topical problem.

This paper presents approaches to solving problems of variational data assimilation developed at the Marchuk Institute of Numerical Mathematics of the Russian Academy of Sciences and based on a combination of splitting methods and adjoint equations. This methodology is illustrated by solving the problems of hydrothermodynamics of the World Ocean and the Black Sea.

2. IDEAS AND METHODS FOR DATA ASSIMILATION

Let us briefly discuss the development of ideas and methods for data assimilation in the Earth sciences [1].

The first attempt to analyze the data objectively was made by Panofski [10]. The essence of his method is two-dimensional (2D) polynomial interpolation of observational data. This approach was further developed by Gilchrist and Cressman [11], who introduced the impact area for each observation and proposed the use of the so-called "background field" — the first approximation field.

In the approach of Bergthorsson and Doos [12], the first approximation field plays a more important role: their method of assimilation is based on the analysis of the difference between the observational data and the first approximation field, but not the values of the observation function themselves. They tried to optimize the weights assigned to each observation. Later, a modification of this approach was given by Cressman [13] and consisted of several iterations of the analysis — the so-called Sequential Correction Method (SCM). Although this method has its drawbacks (by using it, we approach observational data that may contain errors), it has found application for operational use in many meteorological offices.

The approach based on the method of statistical interpolation goes back to the papers by Gauss, Kolmogorov, and Wiener and became known in the Earth sciences due to Gandin's monograph [14]. This approach is usually called the Optimal Interpolation (OI) [15]. Observations are assigned weights related to their errors. The optimal interpolation method has been used in many operational centers since the late 1970s [15]. This method was further developed in the papers by Lorenc [16], who used different approximations to solve the equations of state of the system and also proposed a “hybrid” of two methods — optimal interpolation and successive corrections.

The optimal interpolation method and its modifications are still used for operational data analysis in weather forecast [16, 17], as well as for oceanographic data assimilation [18]. The ensemble optimal interpolation method (EnOI) has become very popular [19, 20], and this technique is exploited to develop parallel algorithms for data assimilation [21].

Kalman proposed a statistical method for assimilation in 1960, which became known as the Kalman filter. The continuous analog of this method is called the Kalman–Bucy filter [22]. There are different generalizations of this method to the nonlinear case [23]. Currently, the extended Kalman filter (EKF) method [24], which uses the linearization of the model near a certain state, as well as the ensemble Kalman filter (EnKF) method [25], which uses the Monte Carlo method at each time step, are very popular. A multi-element four-dimensional analysis of hydrophysical fields based on dynamic-stochastic models was developed at the Marine Hydrophysical Institute [26]. Modifications of the Kalman algorithm based on covariance matrix approximations were used to simulate the Black Sea circulation [27].

In the next section, we will focus on another approach — variational data assimilation.

3. VARIATIONAL DATA ASSIMILATION METHODS

A significant breakthrough in solving the data assimilation problems was the use of variational methods and, in particular, optimal control methods. The idea of minimizing some functional associated with the observational data on the trajectories (solutions) of the considered model appeared to be very fruitful (see, e. g., [1]). Thus, the data assimilation problem is formulated as an optimal control problem. Theoretical foundations for the study and solution of such problems are laid in the classical papers by R. Bellman, L. S. Pontryagin, N. N. Krasovskiy, J.-L. Lions, and G. I. Marchuk.

The variational formalism was used for the first time in meteorology by Sasaki [28], and in the problems of dynamic oceanography by Provost and Salmon [29].

Three-dimensional variational data assimilation (3D-VAR) for operational analysis was first used in the National Centers for Environmental Prediction NCEP (USA) [30], and later used in the European Center for Medium-term Weather Forecast (ECMWF) and NASA Data Assimilation Office [31].

Currently, four-dimensional data assimilation (4D-VAR), in which linearized models and those adjoint to them are used to assimilate observational data over a given time interval, is of increasing interest. The 4D-VAR system was first applied in practice in the European Center for Medium-term Weather Forecast [32].

As is well known, it becomes necessary to calculate the gradient of the initial functional when minimization problems are addressed. The use of the theory of adjoint equations by G. I. Marchuk and J.-L. Lions was an important step in this direction. Since the well-known papers [33–36], the use of adjoint equations for studying and numerically solving data assimilation problems (including the functional gradient calculation) has widely been practiced by many researchers [37-44].

We now illustrate the problem of four-dimensional variational data assimilation by the example of the problem of recovery of the initial condition. Consider the problem on the $(0, T)$ interval:

$$\frac{\mathrm{d}\varphi}{\mathrm{d}t} = A(\varphi, t), \qquad t \in (0, T), \qquad \varphi|_{t=0} = \varphi_0 \tag{1}$$

and introduce the functional of its solution:

$$J(\varphi_0) = \frac{1}{2}\Big(C_1\left(\varphi_0 - \varphi_0^{\mathrm{b}}\right), \varphi_0 - \varphi_0^{b}\Big) + \frac{1}{2}\int\limits_0^T \left[C_2(\mathcal{H}\varphi - \psi^0), \mathcal{H}\varphi - \psi^0\right] \mathrm{d}t,$$

where $\mathcal{H}$ is a (linear) observation operator, ψ^0 is an observation function, φ_0^{b} is a given vector, C_1 and C_2 are weight operators, and $(\cdot, \cdot)$ is a scalar product. As a rule, C_1 and C_2 are chosen in the form of $C_1 = B^{-1}$

and $C_2 = R^{-1}$, where B and R are the covariance error operators $\xi = \varphi_0^{\rm b} - \varphi^{\rm t}\big|_{t=0}$ and $\varepsilon = \psi^0 - \mathcal{H}\varphi^{\rm t}$, respectively, where $\varphi^{\rm t}$ is an exact solution of system (1). Such weight operators (or their approximations) are often chosen in practical problems [24, 45, and 46].

Suppose that the initial condition φ_0 is unknown. Then the data assimilation problem is formulated as follows: find φ_0 and φ such that they satisfy system (1) and on the set of solutions the functional J reaches its lowest value:

$$\frac{{\rm d}\varphi}{{\rm d}t} = A(\varphi, t), \qquad t \in (0, T), \qquad \varphi|_{t=0} = \varphi_0, \qquad J(\varphi_0) = \inf_v J(v). \tag{2}$$

By definition,

$$J'(\delta\varphi_0) = \left(C_1\left(\varphi_0 - \varphi_0^{\rm b}\right), \delta\varphi_0\right) + \int_0^T \left(C_2\left(\mathcal{H}\varphi - \psi^0\right), \mathcal{H}\,\delta\varphi\right)\,{\rm d}t,$$

where $\delta\varphi$ satisfies the TLM (tangent linear model) system:

$$\frac{{\rm d}\delta\varphi}{{\rm d}t} = A'(\varphi, t)\,\delta\varphi, \qquad t \in (0, T), \qquad \delta\varphi|_{t=0} = \delta\varphi_0. \tag{3}$$

Let

$$-\frac{{\rm d}\varphi^*}{{\rm d}t} = \left[A'(\varphi, t)\right]^*\varphi^* - p, \qquad \varphi^*|_{t=T} = 0, \tag{4}$$

where $p = \mathcal{H}^* C_2(\mathcal{H}\varphi - \psi^0)$, $\mathcal{H}^*$ is the operator adjoint to $\mathcal{H}$, and φ^* is the solution of adjoint problem (4). Then from the adjoint relation

$$\int_0^T (p, \delta\varphi)\,{\rm d}t = -(\varphi^*|_{t=0}, \delta\varphi_0)$$

we obtain the gradient

$$J'(\delta\varphi_0) = \left(C_1\left(\varphi_0 - \varphi_0^{\rm b}\right), \delta\varphi_0\right) + \int_0^T (p, \delta\varphi)\,{\rm d}t = \left(C_1\left(\varphi_0 - \varphi_0^{\rm b}\right) - \varphi^*|_{t=0}, \delta\varphi_0\right).$$

The necessary optimality condition [2] reduces the problem to a system of equations for three unknowns, namely, φ_0, φ, and φ^*:

$$\frac{{\rm d}\varphi}{{\rm d}t} = A(\varphi, t), \qquad t \in (0, T), \qquad \varphi|_{t=0} = \varphi_0; \tag{5}$$

$$-\frac{{\rm d}\varphi^*}{{\rm d}t} = [A'(\varphi, t)]^*\varphi^* - \mathcal{H}^* C_2(\mathcal{H}\varphi - \psi^0), \qquad \varphi^*|_{t=T} = 0; \tag{6}$$

$$C_1(\varphi_0 - \varphi_0^{\rm b}) - \varphi^*|_{t=0} = 0, \tag{7}$$

where $[A'(\varphi, t)]^*$ is the operator adjoint to the derivative of the model operator A. System (5)–(7) is called the "optimality system" and plays an important role for studying and numerically solving the data assimilation problems.

This system can also be obtained from the Pontryagin maximum principle formulated for the original minimization problem [39], or by the Lagrange multiplier method [47].

The solvability of nonlinear data assimilation problems and rigorous substantiation of numerical methods for their solution is not an easy problem. Sufficiently complete results concerning the solvability of linear optimal control problems of forms (2) and (5)–(7) were obtained by J. L. Lions, using the HUM (Hilbert Uniqueness Method), a general approach he developed. The further development of this approach, as well as other methods for studying optimal control problems, were considered in the papers by K. Bardos, D. Russel, A. I. Egorov, A. V. Fursikov, E. Zuazua, V. I. Agoshkov, and others. Some results on the solvability of weakly nonlinear data assimilation problems were obtained in [38, 43]. Further generalizations and new applications were proposed in subsequent years [44, 48, 49].

Well-known minimization methods can be used, or the optimality system can be solved, to develop a numerical algorithm for solving the data assimilation problem. When solving the problem numerically, it is often necessary to calculate the gradient of the initial functional J. This can be done by using an appropriately selected adjoint problem. In this example, the gradient of the functional is calculated as follows: for a given v we find sequentially solutions to the direct and adjoint problems:

$$\frac{\mathrm{d}\varphi}{\mathrm{d}t} = A(\varphi, t), \qquad t \in (0, T), \qquad \varphi|_{t=0} = v; \tag{8}$$

$$-\frac{\mathrm{d}\varphi^*}{\mathrm{d}t} = \left[A'(\varphi, t)\right]^* \varphi^* - \mathcal{H}^* C_2(\mathcal{H}\varphi - \psi^0), \qquad \varphi^*|_{t=T} = 0 \tag{9}$$

and assume

$$J'(v) = C_1(v - \varphi_0^{\mathrm{b}}) - \varphi^*|_{t=0}\,. \tag{10}$$

In the papers by many authors, much attention is paid to the numerical construction of the adjoint model (9), which can be obtained both by discretizing the continuous problem [50, 51] and by direct transposing of the code of a discrete linearized problem [44, 52]. In the latter case, automatic differentiation methods are often used [47]. A comparison of these two approaches to the construction of a discrete adjoint problem is performed in, e. g., [50].

To date, algorithms for four-dimensional data assimilation [1, 6, 7, and 9] seem to be the most effective. Many papers comparing the Kalman ensemble method and variational data assimilation have appeared in recent years [53, 54]; in addition, the so-called hybrid approach was developed, combining the ensemble method and variational data assimilation [55, 56], as well as the 4D-VAR ensemble method [57, 58].

Note that the 4D-VAR method requires storing a fairly large amount of data, since when solving an adjoint problem, it is necessary to have the data obtained during the solution of a direct problem. Also, the 4D-VAR method requires additional computational effort in solving direct and adjoint problems when the data are assimilated and the results of assimilation are used in the model. These drawbacks can be reduced to some extent by using the splitting method and applying parallel algorithms for the problem solution.

4. 4D-VAR METHODS IN THE OCEAN DYNAMICS MODEL

The application of the methodology of variational data assimilation is illustrated by solving the problem of ocean surface temperature assimilation in a model of large-scale circulation of the World Ocean. Let the problem be considered in the range $D = \{(x, y, z) : (x, y, R) \in \Omega,\ 0 < z < H(x, y)\}$. We represent the boundary of the $\Gamma \equiv \partial D$ range as a combination of four non-intersecting parts, namely, Γ_S, $\Gamma_{w,\mathrm{op}}$, $\Gamma_{w,c}$, and Γ_H, where $\Gamma_S \equiv \Omega$ is the "undisturbed surface," $\Gamma_{w,\mathrm{op}}$ is the liquid (open) part of the vertical lateral boundary, $\Gamma_{w,c}$ is the solid part of the vertical lateral boundary, and Γ_H is the ocean (sea) floor. The characteristic functions of the boundary parts Γ_S, $\Gamma_{w,\mathrm{op}}$, $\Gamma_{w,c}$, and Γ_H will be denoted m_S, m_{op}, m_c, and m_H, respectively.

Consider the system of equations of hydrothermodynamics in the Boussinesq approximation and hydrostatics in the form [1]

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} + \begin{bmatrix} 0 & -f \\ f & 0 \end{bmatrix} \mathbf{u} - g\nabla\,\xi + A_u\mathbf{u} + (A_k)^2\mathbf{u} = \mathbf{f} - \frac{1}{\rho_0}\nabla\,P_a - \frac{g}{\rho_0}\nabla\int_0^z \rho_1(T, S)\,\mathrm{d}z',$$

$$\frac{\partial\xi}{\partial t} - m\frac{\partial}{\partial x}\left[\int_0^H \Theta(z)u_1\,\mathrm{d}z\right] - m\frac{\partial}{\partial y}\left[\int_0^H \Theta(z)\frac{n}{m}u_2\,\mathrm{d}z\right] = f_3,$$
$$\frac{\mathrm{d}T}{\mathrm{d}t} + A_T T = f_T, \qquad \frac{\mathrm{d}S}{\mathrm{d}t} + A_S S = f_S. \tag{11}$$

Here, $\mathbf{u} = (u, v)$ is the velocity vector, ξ is the level function, T is the temperature, S is the salinity, $\rho_1(T,S) = \rho_0\beta_T(T - T^{(0)}) + \rho_0\beta_S(S - S^{(0)}) + \gamma\rho_0\beta_{TS}(T,S) + f_P$, $\mathbf{f} = (f_1, f_2)$, f_T, f_S, and f_P are given functions of the "internal" sources, $g = \mathrm{const} > 0$, ρ_0, $T^{(0)}$, and $S^{(0)}$ are the "unperturbed" values of water density, temperature, and salinity, respectively, β_T and β_S are the coefficients, $\beta_{TS}(T,S)$, P_a, and $f_3 \equiv f_3(x,y,\xi,t) \equiv f_3(x,y,t)$ are given functions, and γ is a numerical parameter. Hereafter, the following weight function is used: $\Theta(z) \equiv r(z)/R$, R is the Earth's radius, $n = 1/r$, $m = 1/(r\cos y)$, and H is the ocean (sea) depth. Then we introduce the differential operator $A_\varphi\varphi \equiv -\mathrm{div}(\nu_\varphi\nabla\varphi)$, where φ can take the values u, v, T, and S, and $(A_k)^2$ is a fourth-order operator for $A_\varphi = A_k$, which is determined by the $\hat{k} = \mathrm{diag}\{k_{ii}\}$ matrix with non-negative diagonal k_{ii} elements that are viscosity indices in respective directions.

The boundary conditions on the ocean surface will be determined as follows:

$$\left(\int_0^H \Theta\mathbf{u}\,\mathrm{d}z\right)\mathbf{n} + \beta_0 m_{\mathrm{op}}\sqrt{gH}\,\xi = m_{\mathrm{op}}\sqrt{gH}\,d_s \text{ at the boundary } \partial\Omega;$$
$$U_n^{(-)}u - \nu\frac{\partial u}{\partial z} - k_{33}\frac{\partial}{\partial z}A_k u = \tau_x^{(a)}/\rho_0 \qquad U_n^{(-)}v - \nu\frac{\partial v}{\partial z} - k_{33}\frac{\partial}{\partial z}A_k v = \tau_y^{(a)}/\rho_0;$$
$$A_k u = 0, \qquad A_k v = 0;$$
$$U_n^{(-)}T - \nu_T\frac{\partial T}{\partial z} + \gamma_T(T - T_\mathrm{a}) = Q_T + U_n^{(-)}d_T;$$
$$U_n^{(-)}S - \nu_S\frac{\partial S}{\partial z} + \gamma_S(S - S_\mathrm{a}) = Q_S + U_n^{(-)}d_S.$$

Here, $\mathbf{U} = (u, v, w) \equiv (\mathbf{u}, w)$, $U_n = (\mathbf{UN}) = u_1N_1 + u_2N_2 + wN_3$, $\mathbf{N}$ is the unit vector of the external normal to the boundary, $U_n^{(-)} = (|U_n| - U_n)/2$, τ_x, and τ_y are the components of the vectors of shear stresses in the wind along the coordinate axes, γ_T and γ_S are the coefficients of relaxation to specified values of temperature and salinity, respectively, k_{33} is the vertical viscosity index, ν is the turbulent exchange ratio, and Q_T and Q_S are the surface heat and salinity fluxes, respectively. The remaining boundary and initial conditions are specified according to [41, 44].

The problem of large-scale ocean dynamics in terms of the u, v, ξ, T, and S functions is formulated as follows: find u, v, ξ, T, and S, satisfying Eqs. (11) under appropriate boundary and initial conditions.

One of the features of solving this problem is the use of the splitting method. We present a splitting model used to approximate the original mathematical model of ocean dynamics and find a complete solution to the problem $\phi = (u, v, \xi, T, S)$.

To approximate the resulting problem, we apply one of the models of the total approximation method, which consists of making the following steps. The problem for temperature is solved in the first step of this method:

$$T_t + (\mathbf{U},\nabla)T - \mathrm{div}(\nu_T\cdot\nabla T) = f_T \text{ in } D\times(t_{j-1},t_j);$$
$$T = T_{j-1} \text{ at } t = t_{j-1} \text{ in the range } D;$$
$$U_n^{(-)}T - \nu_T\frac{\partial T}{\partial z} + \gamma_T(T - T_a) = Q_T + U_n^{(-)}d_T \text{ at the boundary } \Gamma_S\times(t_{j-1},t_j);$$
$$\frac{\partial T}{\partial\mathbf{N}} = 0 \text{ at the boundary } \Gamma_{w,c}\times(t_{j-1},t_j);$$

$$U_n^{(-)}T + \frac{\partial T}{\partial \mathbf{N}} = U_n^{(-)} d_T + Q_T \text{ at the boundary } \Gamma_{w,\text{op}} \times (t_{j-1}, t_j);$$
$$\frac{\partial T}{\partial \mathbf{N}} = 0 \text{ at the boundary} \, \Gamma_H \times (t_{j-1}, t_j). \tag{12}$$

The problem for salinity is solved in the second step of the splitting method:

$$S_t + (\mathbf{U}, \nabla)S - \operatorname{div}(\nu_S \cdot \nabla S) = f_S \text{ in the range } D \times (t_{j-1}, t_j);$$
$$S = S_{j-1} \text{ at } \; t = t_{j-1} \text{ in } \; D;$$
$$\mathbf{U}_n^{(-)} S - \nu_S \frac{\partial S}{\partial z} + \gamma_S (S - S_a) = Q_S + U_n^{(-)} d_S \text{ at the boundary } \Gamma_S \times (t_{j-1}, t_j);$$
$$\frac{\partial S}{\partial \mathbf{N}} = 0 \text{ at the boundary } \Gamma_{w,c} \times (t_{j-1}, t_j);$$
$$U_n^{(-)} S + \frac{\partial S}{\partial \mathbf{N}} = U_n^{(-)} d_S + Q_S \text{ at the boundary } \Gamma_{w,\text{op}} \times (t_{j-1}, t_j);$$
$$\frac{\partial S}{\partial \mathbf{N}} = 0 \text{ at the boundary } \Gamma_H \times (t_{j-1}, t_j). \tag{13}$$

The third step of the splitting scheme is to solve the subproblem for determining u, v, and ξ:

$$\frac{d\mathbf{u}}{dt} + \begin{pmatrix} 0 & -f \\ f & 0 \end{pmatrix} \mathbf{u} - g \, \nabla \xi + A_u \mathbf{u} + (A_k)^2 \mathbf{u}$$
$$= \mathbf{f} - \frac{1}{\rho_0} \nabla \left[P_\text{a} + g \int_0^z \rho_1(\bar{T}, \bar{S}) \, \mathrm{d}z' \right] \quad \text{in the range } \; D \times (t_{j-1}, t_j);$$
$$\xi_t - \operatorname{div} \left(\int_0^H \Theta \mathbf{u} \, \mathrm{d}z \right) = f_3 \text{ in the range } \; \Omega \times (t_{j-1}, t_j);$$
$$\mathbf{u} = \mathbf{u}_{j-1}, \qquad \xi = \xi_{j-1} \text{ for } t = t_{j-1};$$
$$\left(\int_0^H \Theta \mathbf{u} \, \mathrm{d}z, \mathbf{N} \right) n + \beta_0 m_\text{op} \sqrt{gH} \, \xi = m_\text{op} \sqrt{gH} \, d_s \text{ at the boundary } \; \partial\Omega \times (t_{j-1}, t_j). \tag{14}$$

Thus, when making steps 1 to 3, after the first step, we get an approximation to T, after the second, to S, and after the third, to $\mathbf{u} = (u, v)$ and ξ, i. e., the subproblems in these steps are independent of each other and can be solved in parallel. It is possible to further use appropriate splitting methods for the implementation of this algorithm. For example, splitting along three spatial coordinates was performed in this paper when obtaining a complete numerical model and in the numerical experiments given below.

Note that splitting in the development of numerical algorithms leads to the appearance of additional terms in the difference scheme, which causes a deterioration in the approximation features of the numerical algorithm. The calculations should take into account the possible loss of stability at the intermediate steps of the splitting scheme due to the possible loss of the positive definiteness property for the constituent operators.

We now formulate the problem of variational assimilation of the ocean surface temperature data. Consider the equation for the temperature unit in the form

$$T_t + (\mathbf{U}, \nabla)T - \mathbf{div}(\nu_T \cdot \nabla T) = f_T \text{ in the range } \; D \times (t_{j-1}, t_j);$$
$$T = T_{j-1} \text{ at } t = t_{j-1} \text{ in the range } \; D, \quad -\nu_T \frac{\partial T}{\partial z} = Q \quad \text{at the boundary } \; \Gamma_S \times (t_{j-1}, t_j),$$

$$\frac{\partial T}{\partial \mathbf{N}} = 0 \text{ on the boundary } \Gamma_{w,c}\times(t_{j-1},t_j);\ \ U_n^{(-)}T + \frac{\partial T}{\partial \mathbf{N}} = U_n^{(-)}d_T + Q_T \text{ at the boundary } \Gamma_{w,\mathrm{op}}\times(t_{j-1},t_j);$$
$$\frac{\partial T}{\partial \mathbf{N}} = 0 \text{ at the boundary } \Gamma_H \times (t_{j-1},t_j);\quad T_j \equiv T \text{ in the range } \ D\times(t_{j-1},t_j).$$

Let the additional unknown (control) be the function of the total flux Q. We now introduce a cost functional of the form

$$J_\alpha \equiv J_\alpha(Q,\phi) = \frac{1}{2}\int\limits_0^{\bar{t}}\int\limits_\Omega \alpha\,|Q - Q^{(0)}|^2\,\mathrm{d}\Omega\,\mathrm{d}t + J_0(\phi);$$
$$J_0(\phi) = \frac{1}{2}\int\limits_0^{\bar{t}}\int\limits_\Omega m_0|T - T_{\mathrm{obs}}|^2\,\mathrm{d}\Omega\,\mathrm{d}t.$$

Here, the function $\alpha \equiv \alpha(\lambda,\theta,t)$ plays the role of a regularizer (the case where $\alpha(\lambda,\theta,t) = \mathrm{const} \geq 0$ is possible) and can be a dimensional quantity, and $Q^{(0)} \equiv Q^{(0)}(\lambda,\theta,t)$ is a given function.

The variational assimilation problem is formulated as follows: it is needed to find the problem solution ϕ and the function Q, such that the functional takes the lowest value on them.

This problem is known to have an equivalent representation in terms of the optimality system. We now introduce the adjoint problem. Then the optimality system for T will take the classical form

$$T_t + \frac{1}{2}\left[w_1\frac{\partial T}{\partial z} + \frac{1}{r^2}\frac{\partial(r^2 w_1 T)}{\partial z}\right] - \frac{1}{r^2}\frac{\partial}{\partial z}r^2\nu_T\frac{\partial T}{\partial z} = f_T, \qquad T = T_1(t_j);$$
$$-\nu_T\frac{\partial T}{\partial z}\Big|_{z=0} = Q, \qquad \nu_T\frac{\partial T}{\partial z}\Big|_{z=H} = 0,$$
$$T_t^* - \frac{1}{2}\left[w_1\frac{\partial T^*}{\partial z} + \frac{1}{r^2}\frac{\partial(r^2 w_1 T^*)}{\partial z}\right] - \frac{1}{r^2}\frac{\partial}{\partial z}\left(r^2\nu_T\frac{\partial T^*}{\partial z}\right) = 0;$$
$$\nu_T\frac{\partial T^*}{\partial z}\Big|_{z=H} = 0, \qquad \left(-w_1T^* - \nu_T\frac{\partial T^*}{\partial z}\right)\Big|_{z=0} = m_0(T - T_{\mathrm{obs}});$$
$$\alpha(Q - Q^{(0)}) + T^* = 0.$$

As follows from the theory of inverse problems and the theory of adjoint equations, the solution of this system provides a minimum to the previously introduced functional. With the regularization parameter $\alpha > 0$, the obtained optimal estimate for Q will be stable with respect to the observation errors.

To solve the formulated problem, the following iterative algorithm was used in this paper: if $Q^{(k)}$ is an already constructed approximation to Q, we solve the direct problem $Q \equiv Q^{(k)}$, then the adjoint problem, and after that determine the next approximation $Q^{(k+1)}$ using the formulas

$$Q^{(k+1)} = Q^{(k)} - \gamma_k[\alpha(Q^{(k)} - Q^{(0)}) + T_2^*] \quad \text{on the surface } \ \Omega.$$

Here, the γ_k parameter is chosen in such a way that the considered iterative process converges. After determining $Q^{(k+1)}$ the solution of the problems is repeated with a new approximation $Q^{(k+1)}$, and then $Q^{(k+2)}$ is calculated, etc. Iterations are repeated until an appropriate convergence criterion of the process is met. So, in the numerical experiments presented below, the iterative process was completed once the relative error between iterations reached 10^{-3}.

Note that the convergence rate may vary depending on the choice of the iterative parameter. The case where the process converges very slowly or does not converge at all is possible. However, in theory there are cases where the parameter can be selected in such a way that the process will converge over 5–10 iterations. In the experiment under consideration, the parameter was calculated based on the features of the system itself, and the algorithm converged to machine precision over 3–5 iterations.

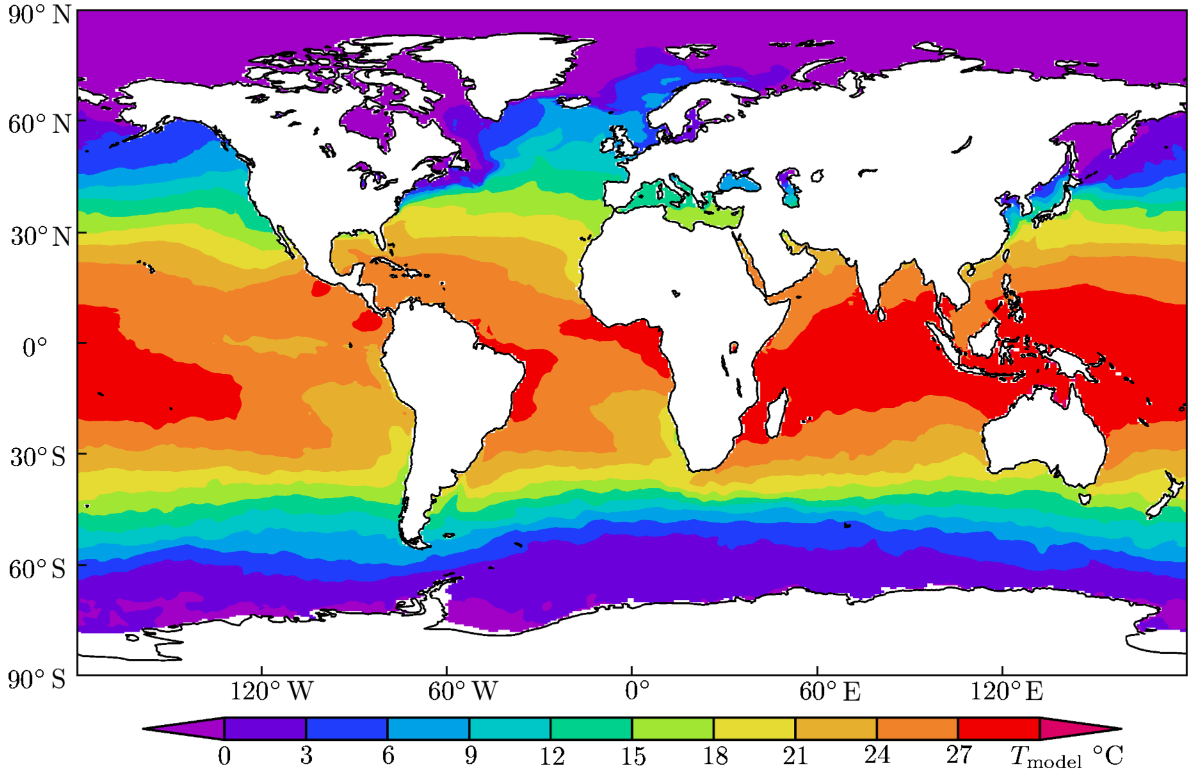

Fig. 1. Calculation without the assimilation unit, January 2004.

5. CALCULATION RESULTS. HYDRODYNAMIC MODEL OF THE WORLD OCEAN

The three-dimensional model of ocean hydrothermodynamics developed for experiments at the INM RAS [1] was supplemented with the above-described procedure of ocean surface temperature T_{obs} assimilation in order to retrieve heat fluxes [41].

The water area of the World Ocean was considered as the object of modeling. The parameters of the considered area and its geographical coordinates can be described as follows: "σ-grid" [1], the number of points is $360 \times 337 \times 40$ (in latitude, longitude, and depth, respectively). The first point of the "C grid" [1] is a point with coordinates 22.5° east longitude and 78.25° south latitude. The grid steps for λ and θ are constant and equal to 1.0° and 0.5°, respectively. The time step is $\Delta t = 1$ h.

The ocean surface temperatures [59] presented by S. A. Lebedev (Geophysical Center of the Russian Academy of Sciences) on the model grid for January 2004 at every moment of time (i. e., every hour) were used as T_{obs}. The average climatic flux for January 2004 obtained from the NCEP (National Centers for Environmental Prediction) reanalysis was used as $Q^{(0)}$. The calculations included the T_{obs} assimilation; a time period of up to 30 days (January 2004) was calculated.

The numerical experiment, the results of which are given below, is aimed at checking the possibility of assimilation of incomplete information about the ocean surface temperature to obtain all hydrothermodynamic parameters. The model which serves as the interpolant is used to construct consistent fields of the entire system.

The results of the numerical experiment are shown in Figs. 1–4. For example, Fig. 1 shows the results of calculating the ocean surface temperature in terms of the model without using the T_{model} assimilation unit. Figure 2 shows the calculation of the ocean surface temperature, which was performed with the assimilation unit according to the procedure described in the previous section (T_{assim}). The difference between the ocean surface temperature values obtained by calculating with and without the assimilation unit is shown in Fig. 3. Figure 4 shows the difference between the observational data averaged over 20 h and the calculation using

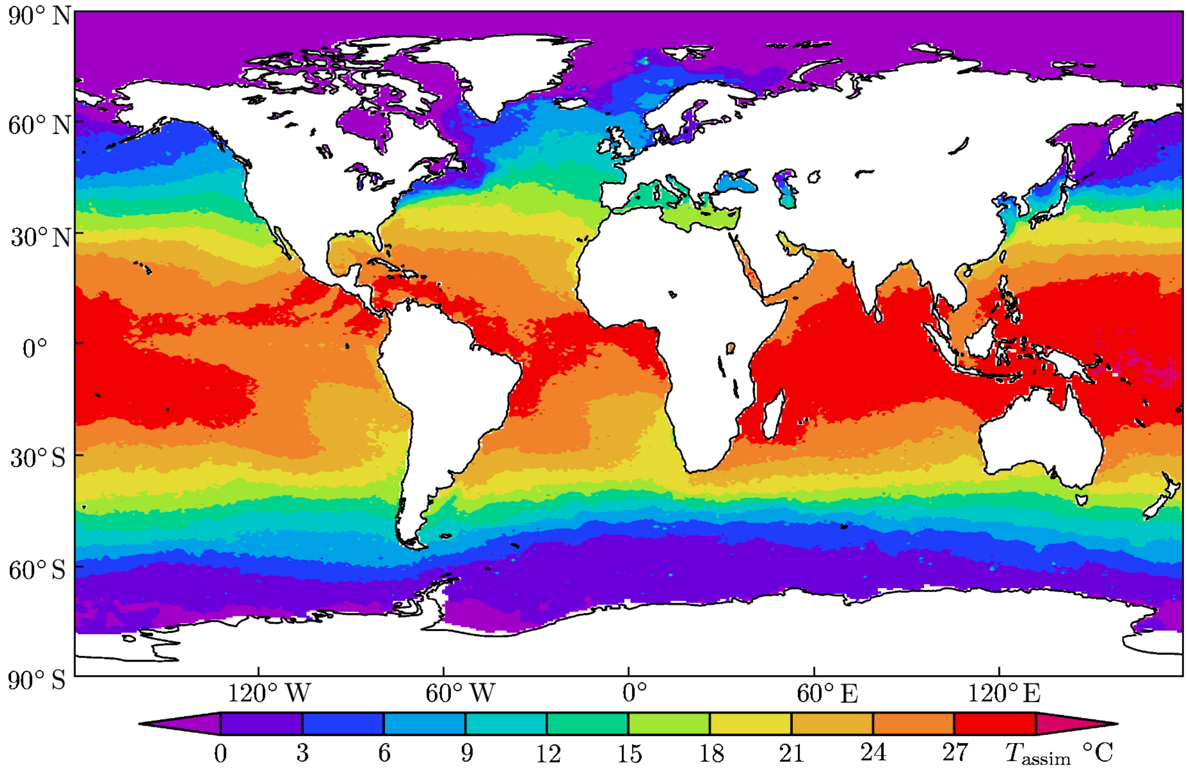

Fig. 2. Calculation with the assimilation unit, January 2004.

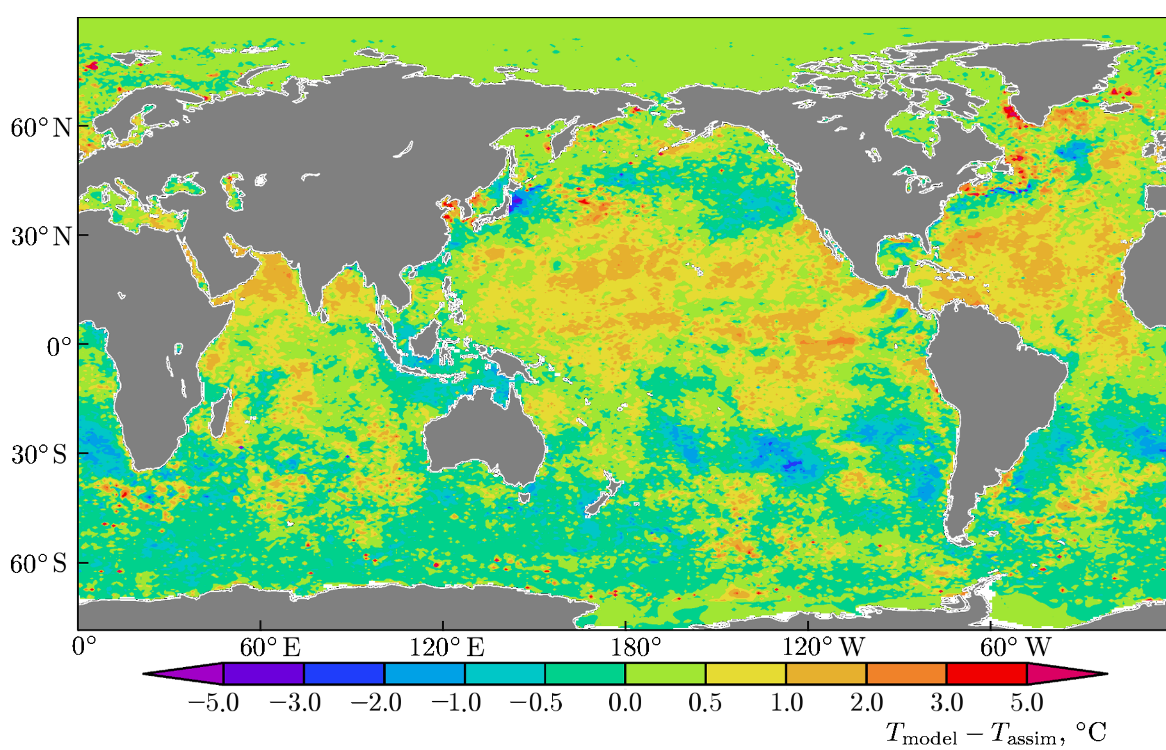

Fig. 3. Difference in the ocean surface temperatures calculated using the model with and without the assimilation unit, January 2004.

the model with a data assimilation unit for the same time period. Note that the data are known only from the trajectory of the satellite flying over the water area, that is why there are gaps in them, marked in white in the figure.

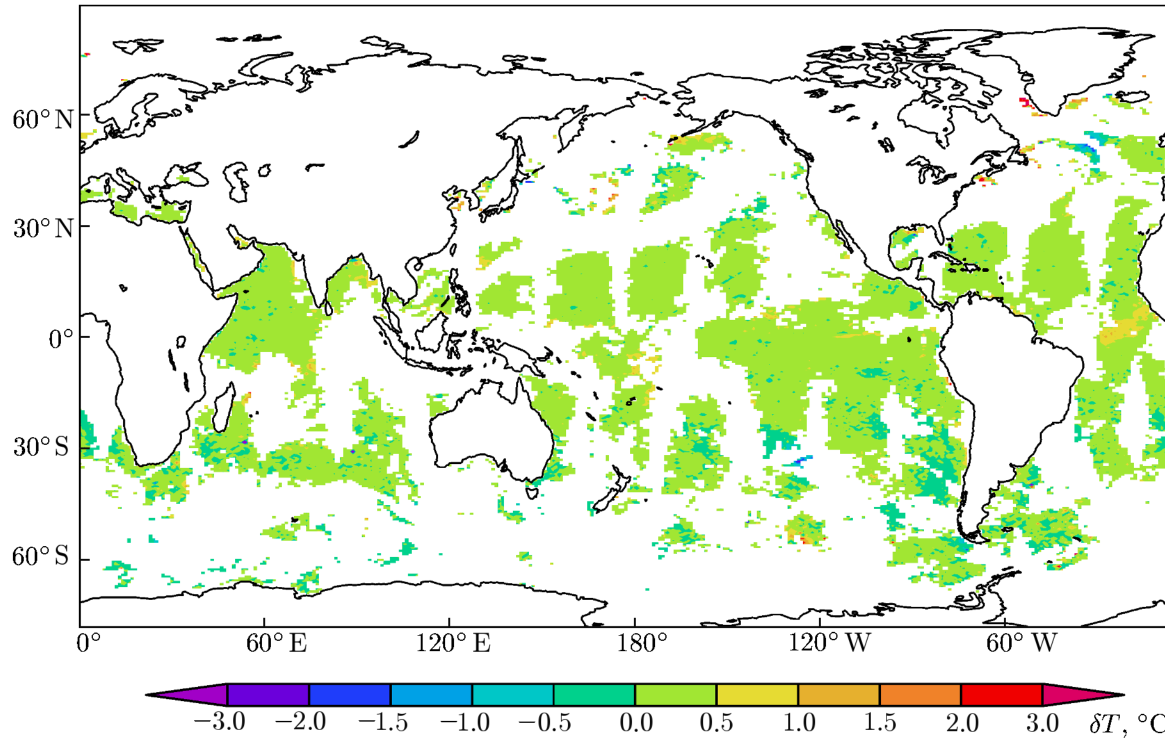

Fig. 4. Deviation of the temperature δT calculated with the assimilation unit from the observational data (averaging over 20 h), January 2004.

In general, the model with the assimilation algorithm shows a good reproduction of the ocean surface temperature. Based on the results of the numerical experiments, we can conclude that the ocean surface temperature becomes closer to the actually observed temperature in the equatorial region, especially in the Atlantic Ocean and the Bay of Bengal. The ocean surface temperature became closer to the observed data on average by 0.5°C. In some parts of the World Ocean, the difference between calculations with and without the data assimilation was 2°C. We also note that the fields of all hydrothermodynamic parameters of the ocean remain consistent. However, the assimilation of the ocean surface temperature affects only slightly the remaining hydrodynamic features of the World Ocean. Other types of data, such as temperature and salinity profiles in the considered water area and calculations over a longer period of time are required for a greater impact.

6. HYDRODYNAMIC MODEL OF THE SEA WITH VARIATIONAL ASSIMILATION OF TEMPERATURE AND SALINITY

To date, the Marchuk Institute of Numerical Mathematics of the Russian Academy of Sciences has developed several models of hydrodynamics of the seas and oceans. This is the above model of the World Ocean, the model of the Black Sea (including the waters of the Sea of Azov), the Baltic Sea, etc. [60–62]. The numerous experiments have shown the computational efficiency of the models and the adequacy of their reproduction of real circulations. Note the important resources for the further improvement of models, including the upgrade of numerical algorithms and methods for observational data assimilation. Consider the problem of modeling the dynamics of the Black Sea and the Sea of Azov with variational assimilation of observational data as the example. The model of marine dynamics is based on a system of primitive equations written in a spherical coordinate system in the hydrostatics and Boussinesq approximations [1]. These are equations of the form (11) in the σ-coordinate system, where $\sigma = (z-\zeta)\big/(H-\zeta)$, z is the ordinary vertical coordinate, H is the sea depth, and ζ is the deviation of the sea level from the unperturbed state. The equations are solved using the splitting method.

We now describe the subsystem of four-dimensional variational assimilation of the temperature and salinity fields. The transport/diffusion equations of temperature and salinity are used as direct equations. For simplicity, we assume that the flow field, that is, all components of the velocity vector, are known. A significant problem that arises in the marine forecast modeling is the setting of the initial condition for all predictive functions at a certain time. There are no such observational data for the whole Black Sea area. The problem of constructing the initial fields based on a combination of measurements and model calculations arises. As observations, we use the average monthly climate estimates of the temperature and salinity fields. The four-dimensional variational assimilation procedure is defined for the temperature and salinity transport/diffusion subsystem linearized on the calculated model trajectory.

We will use the following notation in the further description of the system: $\lambda \equiv x$, $\theta \equiv y$. Let the transport/diffusion equations be written in the σ coordinate system, and the velocity vector components $u(x, y, \sigma, t)$, $u_2(x, y, \sigma, t)$, and $\omega(x, y, \sigma, t)$ and the turbulent exchange coefficients μ_T, μ_S, and ν be known functions. Let also $\Omega(x, y, z)$ and $\mathrm{mes}(\Omega)$ be the three-dimensional area and volume of the Black Sea, respectively, $\Omega_0(x, y) = \Omega(x, y, 0)$ and $\mathrm{mes}(\Omega_0)$, the two-dimensional surface of the sea and its square, respectively, $(0, \bar{t})$, the assimilation interval, $T(x, y, z, t)$ and $S(x, y, z, t)$, the potential temperature and salinity, $\rho_{\text{pot}} = \rho_{\text{pot}}(T, S)$, the potential density, $Q_T(x, y, t)$ and $Q_S(x, y, t)$, the heat and salt fluxes on the sea surface, $\hat{T}\text{and}\hat{S}$, the observational data, and $T^0\text{and}S^0$, the values of the corresponding functions at the initial time $t = 0$. Assume that there is no complete information about the initial temperature and salinity fields, but some current estimate of $\hat{T}^0\text{and}\hat{S}^0$ is known. We now formulate the following variational problem. Find the minimum of the functional

$$J = \frac{1}{2\mathrm{mes}(\Omega)\bar{t}} \int_{\Omega} \int_{0}^{\bar{t}} \left[\alpha_T (T - \hat{T})^2 + \alpha_S (S - \hat{S})^2\right] \mathrm{d}t\,\mathrm{d}\Omega + \frac{1}{2\mathrm{mes}(\Omega)} \int_{\Omega} \left[\alpha_T^0 (T^0 - \hat{T}^0)^2 + \alpha_S^0 (S^0 - \hat{S}^0)^2\right] \mathrm{d}\Omega + \frac{1}{2\mathrm{mes}(\Omega_0)\bar{t}} \int_{\Omega_0} \int_{0}^{\bar{t}} \left[\beta_T (Q_T - \hat{Q}_T)^2 + \beta_S (Q_S - \hat{Q}_S)^2\right] \mathrm{d}\,t\,\mathrm{d}\Omega_0 \quad (15)$$

on the set of solutions of the following system of equations:

$$\rho - \rho_{\text{pot}}(T, S) = 0; \quad (16)$$

$$0 < \sigma < 1 : \nu - \nu\left(\frac{\partial \rho_{\text{pot}}}{\partial \sigma}\right) = 0; \quad (17)$$

$$H\frac{\partial T}{\partial t} + \frac{1}{2}\left[\frac{\partial}{\partial \sigma}(\omega T) + \omega \frac{\partial T}{\partial \sigma}\right] + N_{x,y} T = \frac{1}{H}\frac{\partial}{\partial \sigma}\nu \frac{\partial T}{\partial \sigma} + \Lambda_{x,y,\sigma} T; \quad (18)$$

$$H\frac{\partial S}{\partial t} + \frac{1}{2}\left[\frac{\partial}{\partial \sigma}(\omega S) + \omega \frac{\partial S}{\partial \sigma}\right] + N_{x,y} S = \frac{1}{H}\frac{\partial}{\partial \sigma}\nu \frac{\partial S}{\partial \sigma} + \Lambda_{x,y,\sigma} S; \quad (19)$$

$$\sigma = 0 : \frac{\nu}{H}\frac{\partial T}{\partial \sigma} = -Q_T^0, \qquad \frac{\nu}{H}\frac{\partial S}{\partial \sigma} = -Q_S^0; \quad (20)$$

$$\frac{\mu_T}{r_x r_x}(Z_x T_\sigma - Z_\sigma T_x) Z_x + \frac{\mu_T}{r_y r_y}(Z_y T_\sigma - Z_\sigma T_y) Z_y + \nu \frac{\partial T}{\partial \sigma} = 0;$$

$$\sigma = 1 : \frac{\mu_S}{r_x r_x}(Z_x S_\sigma - Z_\sigma S_x) Z_x + \frac{\mu_S}{r_y r_y}(Z_y S_\sigma - Z_\sigma S_y) Z_y + \nu \frac{\partial S}{\partial \sigma} = 0. \quad (21)$$

Here,

$$N_{x,y} a = \frac{1}{2}\left[\frac{1}{r_y r_x}\frac{\partial}{\partial x}(H u_1 r_y a) + \frac{H u_1}{r_x}\frac{\partial a}{\partial x} + \frac{1}{r_x r_y}\frac{\partial}{\partial y}(H u_2 r_x a) + \frac{H u_2}{r_y}\frac{\partial a}{\partial y}\right],$$

$$\Lambda_{x,y,\sigma} = \Lambda_{x,x} + \Lambda_{y,y} + \Lambda_{x,\sigma} + \Lambda_{y,\sigma},$$

$N_{x,y}$ and $\Lambda_{x,y,\sigma}$ are the operators describing horizontal advection and lateral turbulent exchange, α_T, α_S, α_T^0, α_S^0, β_T, andβ_S are given weight functions, $\nu_T = \nu_S = \nu$, and H is the sea depth.

Solving the variational assimilation problem is reduced to solving the optimality system constructed from the necessary condition of the functional extremum (15). The optimality system includes the direct model equations (16)–(21) and the system of adjoint equations. The system of adjoint equations and boundary conditions has the form

$$-H\frac{\partial S^*}{\partial t} - \frac{1}{2}\left[\frac{\partial}{\partial\sigma}(\omega S^*) + \omega\frac{\partial S^*}{\partial\sigma}\right] + \alpha_S(S - \hat{S}) - N_{x,y}S^* = \frac{1}{H}\frac{\partial}{\partial\sigma}\nu\frac{\partial S^*}{\partial\sigma} + \Lambda_{x,y,\sigma}S^* + \frac{\partial\rho}{\partial S}\rho^*; \tag{22}$$

$$-H\frac{\partial T^*}{\partial t} - \frac{1}{2}\left[\frac{\partial}{\partial\sigma}(\omega T^*) + \omega\frac{\partial T^*}{\partial\sigma}\right] + \alpha_T(T - \hat{T}) - N_{x,y}T^* = \frac{1}{H}\frac{\partial}{\partial\sigma}\nu\frac{\partial T^*}{\partial\sigma} + \Lambda_{x,y,\sigma}T^* + \frac{\partial\rho}{\partial T}\rho^*; \tag{23}$$

$$\nu^* - \frac{1}{H}\left(\frac{\partial T}{\partial\sigma}\frac{\partial T^*}{\partial\sigma} + \frac{\partial S}{\partial\sigma}\frac{\partial S^*}{\partial\sigma}\right) = 0; \tag{24}$$

$$\rho^* - \frac{\partial}{\partial\sigma}(\nu'\nu^*) = 0; \tag{25}$$

$$\sigma = 0 : \nu\frac{\partial T^*}{\partial\sigma} = 0, \qquad -T^* + \beta_T(Q_T - \hat{Q}_T) = 0;$$

$$\sigma = 0 : \nu\frac{\partial S^*}{\partial\sigma} = 0, \qquad -S^* + \beta_S(Q_S - \hat{Q}_S) = 0; \tag{26}$$

$$\frac{\mu_T}{r_x r_x}(Z_x T^*_\sigma - Z_\sigma T^*_x)Z_x + \frac{\mu_T}{r_y r_y}(Z_y T^*_\sigma - Z_\sigma T^*_y)Z_y + \nu\frac{\partial T^*}{\partial\sigma} = 0;$$

$$\sigma = 1 : \frac{\mu_S}{r_x r_x}(Z_x S^*_\sigma - Z_\sigma S^*_x)Z_x + \frac{\mu_S}{r_y r_y}(Z_y S^*_\sigma - Z_\sigma S^*_y)Z_y + \nu\frac{\partial S^*}{\partial\sigma} = 0. \tag{27}$$

Here, $\nu' \equiv \mathrm{d}\nu(\eta)/\mathrm{d}\eta$ is the derivative with respect to the argument $\eta = \partial\rho_{\text{pot}}/\partial\sigma$, $r_x = R\sin y$, $r_y = R$, $r_z = 1$, $Z = (H - \zeta)\sigma + \zeta$, $Z_x \equiv \partial Z/\partial x \approx \sigma\partial H/\partial x$, $Z_y \equiv \partial Z/\partial y \approx \sigma\partial H/\partial y$, and $Z_\sigma \equiv \partial Z/\partial\sigma \approx H$.

The time boundary conditions for Eqs. (16)–(27) have the form

$$\text{at } t = \bar{t} : T^* = S^* = 0;$$

$$\text{for } t = 0 : -HT^* + \alpha_T^0(T^0 - \hat{T}^0) = 0, \qquad -HS^* + \alpha_S^0(S^0 - \hat{S}^0) = 0. \tag{28}$$

Thus, solving the variational assimilation problem consists in finding such T, S, T^0, S^0, $Q_T, andQ_S$ at which the optimality equations (16)–(28) are fulfilled and the functional minimum (15) is achieved.

The formulated differential problem is approximated by a finite-difference scheme with respect to three spatial coordinates x, y, and σ and implicitly with respect to the time t. The obtained system of discrete equations can be solved by an iterative method, e.g., using one of the well-known standard procedures such as gradient descent.

7. CALCULATION RESULTS. HYDRODYNAMIC MODEL OF THE BLACK SEA

Note some well-known hydrological features of the Black Sea. This sea is characterized by a high average water temperature (8.9°C). The greatest changes occur in the shallow north–western region in winter, where the temperature can vary widely (from 1°C to 7°C). In summer, there is a good heating of the surface layer of water on average up to 25–26°C. The temperature rises from the north–west to the south–east, and this process is more gradual in summer than in winter. The average salinity of the Black Sea waters is quite high (an average of 18 PSU), but it is almost two times less than the average salinity of the World Ocean waters. The salinity distribution over the water area is characterized by a slight increase from the north–west to the south–east. Desalination near the Kerch Strait and the eastern coast of Crimea is caused by the flow of less salty waters of the Sea of Azov (having an average salinity of 11 PSU) into this region. The scheme of currents of the Black Sea highlights a cyclonic current which encircles the entire water area near the shores. There are two cyclonic gyres inside the water area, named after Knipovich (the hydrologist who first described these currents). This motion is mainly caused by the Coriolis force, but the direction and force of the wind in the water area play a significant role and lead to a change in the overall current, making it unstable.

From a physical point of view, the peculiar dynamics of the Black Sea is connected with its great depth and relatively small horizontal size. The depth of the open part of the Black Sea is about 2 km, and the horizontal size is about 1000 km. The Rossby radius, which is responsible for the characteristic scale of vortices, is quite large in the Black Sea, being about 20–30 km. This makes it possible to describe the vortex variability of dynamics using the considered numerical model. The calculated area includes the waters of the Black Sea and the Sea of Azov with a grid step of 4 km in longitude and latitude. Forty levels are set vertically with a thickening at the surface, with a time step of 5 min. The ERA-Interim data are used to specify the atmospheric impact [63]. A detailed description of the numerical model, the algorithm for four-dimensional variational assimilation of observational data, and information about the results of numerical calculations are given in [62]. The main feature of the numerical algorithm for solving the optimality system is that it is based on an implicit scheme of splitting along three geometric coordinates.

The goal of the numerical experiments presented below in the waters of the Black Sea and the Sea of Azov was to determine the initial conditions for the numerical prediction of the state of the considered water area, as well as to study the influence of physical factors on the formation of the features of the Black Sea circulation.

The Black Sea dynamics was calculated in the "variational initialization — prediction" mode for a period of 1–2 years according to the following algorithm.

At the time $t = t_0$ (at the beginning of each month), the initial conditions are specified: $u_1(t_0, x, y, \sigma)$, $u_2(t_0, x, y, \sigma)$, $\zeta(t_0, x, y)$, $T(t_0, x, y, \sigma)$, and $S(t_0, x, y, \sigma)$.

On the time interval $t_0 \le t \le t_1$, a complete system of equations such as (11) is solved with the initial conditions $u_1(t_0, x, y, \sigma)$, $u_2(t_0, x, y, \sigma)$, $\zeta(t_0, x, y)$, $T(t_0, x, y, \sigma)$, and $S(t_0, x, y, \sigma)$; the velocity vector components $u_1(t, x, y, \sigma)$, $u_2(t, x, y, \sigma)$, and $\omega(t, x, y, \sigma)$, as well as the vertical turbulent exchange coefficients $\nu(x, y, \sigma, t)$, are calculated.

The problem of variational minimization of the functional J (15), described by the optimality system (16)–(28), is solved on the assimilation interval $t_0 \le t \le t_1$. As a result, the optimal initial conditions $T_{\text{opt}}(t_0, x, y, \sigma)$ and $S_{\text{opt}}(t_0, x, y, \sigma)$ are found.

The calculated optimum initial conditions for temperature and salinity replace the initial conditions $T(t_0, x, y, \sigma)$ and $S(t_0, x, y, \sigma)$. The complete model system of equations (11) is calculated with new initial conditions at $t = t_0$, namely, $u_1(t_0, x, y, \sigma)$, $u_2(t_0, x, y, \sigma)$, $\zeta(t_0, x, y)$, $T_{\text{opt}}(t_0, x, y, \sigma)$, and $S_{\text{opt}}(t_0, x, y, \sigma)$ for a month in the prediction mode.

The main goal of the computational experiments described below was to study the influence of physical factors on the formation of the features of the Black Sea circulation, in particular, the influence of global and local thermohaline effects on the formation of large-scale circulation, the role of salinity in mesoscale variability, and the effects of temperature and salinity assimilation in the sea level reproduction. The structure of the simulations is the following. The preliminary simulation (runup) of the model was conducted without any assimilation of the observational data for a period of one year from January 1, 2007 to December 31, 2007. Later, several simulations were performed for a year from June 1, 2008 to December 31, 2008 with different observational data. The first was the reference version without assimilation of observations — the continuation of the preliminary simulation, and the rest were carried out in the "variational initialization — prediction" mode. The monthly average temperature and salinity fields for the entire water area, only the salinity field for the entire water area, and the temperature and salinity fields for the south–eastern subregion of the sea were used as assimilated data. We highlight several interesting features of the obtained results.

The "initialization–prediction" mode is characterized by a higher level of kinetic energy compared to

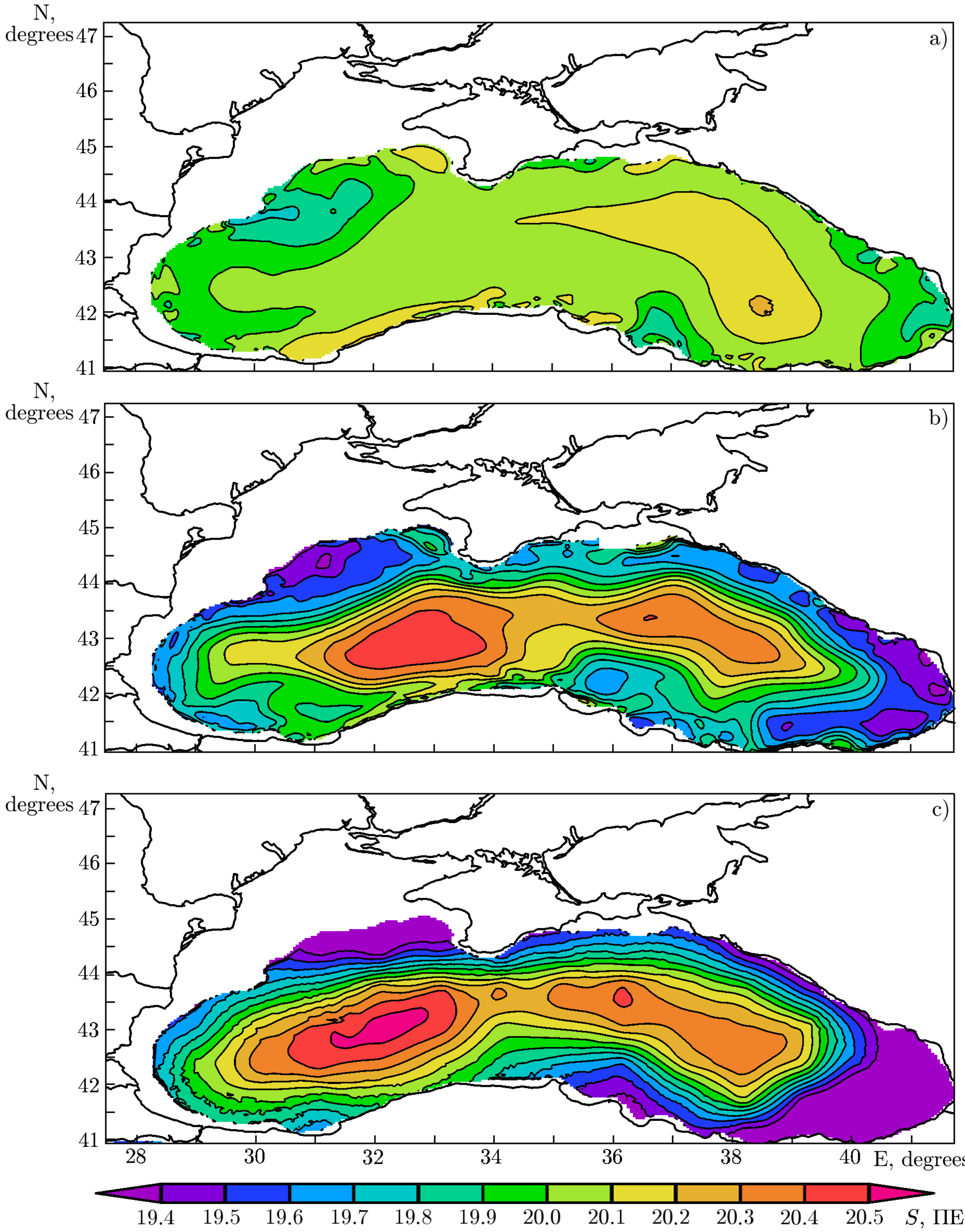

Fig. 5. Monthly average salinity at a depth of 100 m for July 2008: calculation without assimilation (*a*), calculation with assimilation of T and S (*b*), and observational data (*c*).

the usual simulation without data assimilation. In the experiment with the assimilation of T and S, the calm summer period from June to September is notably distinguished. It is connected with the observed natural weakening of the intensity of atmospheric impact over the Black Sea region at this time. The climate signal is distinctly manifested and the simulation results are much closer to the observational data in the model

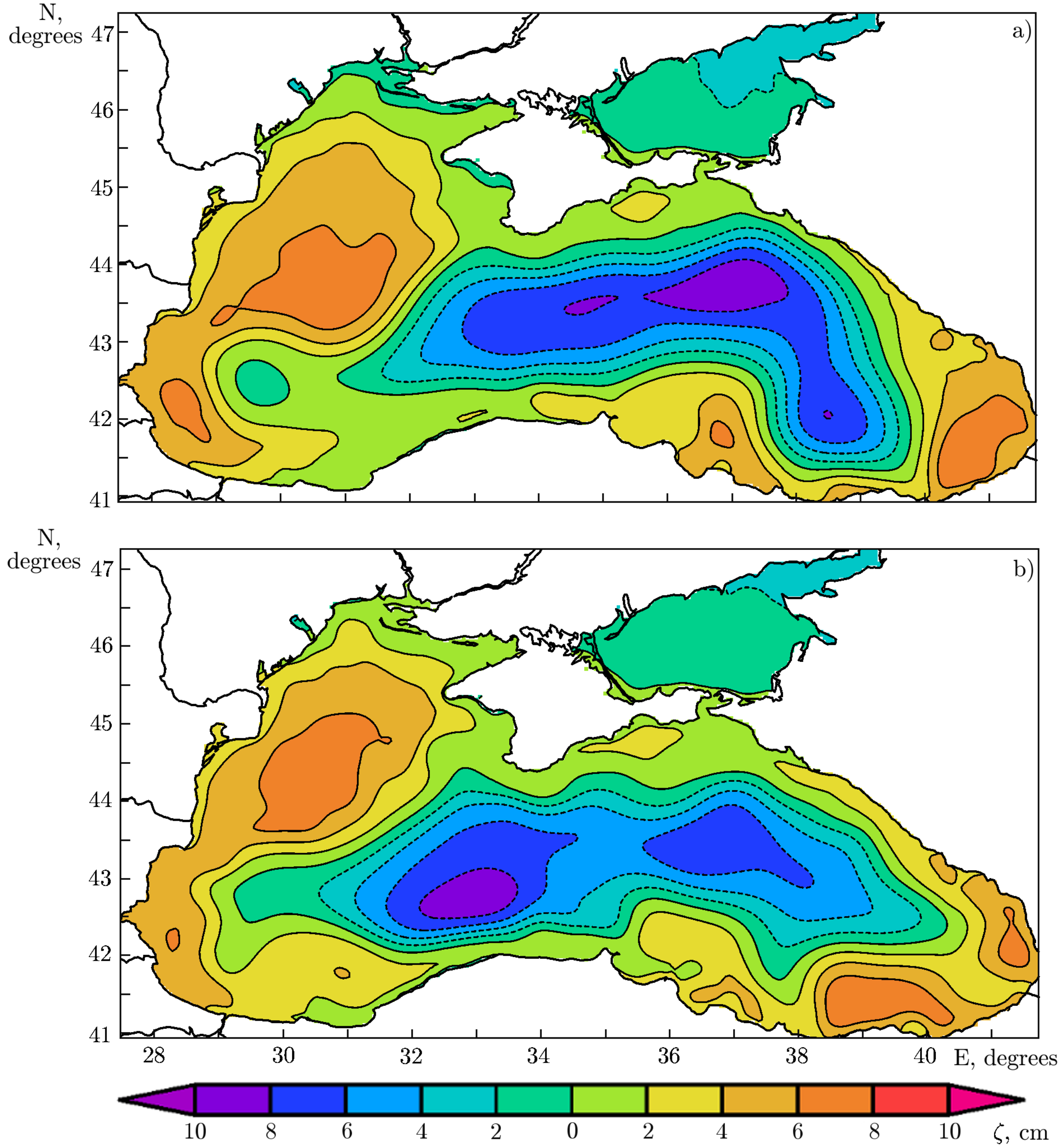

Fig. 6. Monthly average sea level deviation for July 2008: calculation without assimilation (*a*) and calculation with assimilation of T and S (*b*).

with the assimilation of the average monthly temperature and salinity fields (Fig. 5). The difference in the average July temperature between simulations with and without assimilation is about 2–3 ∘C (in the middle part of the Black Sea water area and near the Russian coast). The highest temperature difference at 100 m is observed in the north–eastern part of the Black Sea near the coast of Bulgaria, where it is approximately 0.50–0.75°C. In the salinity field at depths of 10 m, the highest difference 0.5 PSU is seen in the open sea and in the northern part near the Russian coast. In general, the simulation of the model in the “variational initialization — prediction” mode shows the adequacy of reproducing large-scale fields of the Black Sea. In comparison with the calculation without assimilation, the description of the salinity vertical structure is improved (Fig. 5), and, as a result, the reproduction of the cold intermediate layer is improved as well.

All simulations demonstrate the cyclonic nature of the circulation, covering the entire central part of the sea. This is the main Black Sea current observed during the year. It is most intense in winter; in summer, its speed decreases, and in the south–eastern part of the sea, vortices occur near the Georgian and Russian coasts.

We single out three striking circumstances. The first is the enhancement of the level field gradient and an increase in vortex-free currents during the observational data assimilation (Fig. 6). The second is a relatively small difference between simulations with the assimilation of the temperature and salinity fields and the salinity field alone. This means that salinity makes a very significant contribution to the formation of large-scale variability of the Black Sea level. The third is a distinct reproduction of vortices in the south–eastern part of the sea when observations in the summer period are assimilated. This is a subregion characterized by a significant rearrangement of the dynamics in summer, a change in the main Black Sea current, and the formation of local vortices. The experiment shows that the dynamics of this subregion is particularly sensitive to the assimilated observational data.

It should be noted that the model reproduces sufficiently the large-scale hydrodynamics of the Black Sea. The deviation of the prediction without assimilation from the observational data in the main region is slightly more than 1°C. In the north–western part the temperature gradient is realistically reproduced. Simulation with assimilation improves the prediction result by about 0.5°C.

8. CONCLUSIONS

This paper gives a review on data assimilation methods developed in recent decades. The main attention is paid to the methods of variational assimilation of observational data, which are being developed at the Marchuk Institute of Numerical Mathematics. A method for constructing a numerical implementation of the variational data assimilation algorithm is considered, and the results of the numerical experiments based on this method are reported.

The work of major scientific centers all over the world is devoted to the problems of modeling the state of the World Ocean and its water areas. Various algorithms of data assimilation are developed and introduced into the forecast systems at each center. We mention some of these systems. For example, the Forecast Ocean Assimilation Model (FOAM) in Great Britain uses the NEMO model (Nucleus for European Modeling of the Ocean) and the sea ice model with variational assimilation and use of the 3D-VAR model (three-dimensional variational assimilation). A real-time ocean forecast system using a multi-dimensional data acquisition method is implemented at the U.S. National Centers for Environmental Prediction (NCEP). The Japan Meteorological Research Institute has developed a multivariate ocean assessment system with multidimensional data acquisition based on 3D-VAR. Among the systems for modeling and forecast of the state of the marine environment in the Black Sea, we single out the system developed by a consortium of several countries (Bulgaria, France, Germany, and Turkey). It includes three-dimensional variational assimilation of observational data and is used to predict the state of the marine environment for 10 days. The Marine Hydrophysical Institute (MHI) of the Russian Academy of Sciences has a real-time forecast system for calculating the state and ecology of the Black Sea. Satellite information in this system is assimilated using the optimal interpolation method.

Thus, this study is topical, and the results obtained at the IVM RAS are comparable to the world research in the field of variational assimilation of observational data. Further, we describe the features of the data assimilation modeling that were identified in the numerical experiments.

In general, the model with an assimilation algorithm for modeling the hydrothermodynamics of the World Ocean shows a good reproduction of its surface temperature. The iterative procedures used for the four-dimensional variational assimilation of the sea surface temperature in the World Ocean showed good convergence, and no more than 10–15 iterations were required to obtain the optimal flux Q. In some experiments, the parameter of the iterative process can be calculated based on the features of the system itself, and in this case it is possible to achieve convergence of the process over 3–5 iterations.

Based on the results of numerical experiments, it can be concluded that in the equatorial region, the ocean surface temperature becomes closer to the actual observed temperature, especially in the Atlantic Ocean and the Bay of Bengal. Also note that the ranges of all hydrothermodynamic parameters of the ocean remain consistent. However, the assimilation of only the surface temperature of the World Ocean affects slightly its remaining hydrodynamic characteristics. Other types of data, such as temperature and salinity profiles in the considered water area, as well as calculations over a longer period of time, are required for a greater impact.

The paper also presents a numerical model of the hydrodynamics of the Black Sea and the Sea of Azov with a grid step of 4 km in longitude and latitude and 40 vertical levels. The model includes modules of four-dimensional variational assimilation of the temperature and salinity fields. The currents, sea level, temperature, and salinity in 2007 and 2008 were simulated for a given atmospheric impact. Simulations show that hydrodynamic characteristics of the Black Sea are adequately reproduced.

Circulations of the Black Sea and the Sea of Azov with different variants of assimilation of three-dimensional temperature and salinity fields have been simulated. When the data are assimilated, model fields approach observational data, and the reproduction of the current field, the vertical structure of salinity, and the cold intermediate layer improves. Note that the assimilation of temperature and salinity fields causes notable changes in the sea level. In particular, mesoscale vortices in the south–eastern part of the Black Sea are more distinctly reproduced in the summer period.

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