Determination of the Concentration of Contaminants at the Outlet of the Underwater Source Based on the Variation Algorithm

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Abstract. A variation algorithm for determining the concentration of the contaminating admixture at the outlet of the underwater source C_p is proposed. It is based on a minimization of the quadratic functional, which is determined by the residual values of the measured and calculated values of the pollution concentration and the solution of the corresponding problem in variations. The algorithm for determining the C_p tested in the framework of numerical three-dimensional hydrothermodynamic model of the spread of sewage in the coastal zone of the Crimean Peninsula, adjacent to the city of Sevastopol. Numerical experiments were carried out to restore the C_p for different number of measurements and different levels of random noise in the measurements. A measurement scheme was used in which a moving sensor consistently measured the vertical profile of pollution concentration at fifteen stations. It is shown that without taking into account the random noise in the initial data, the C_p parameter is restored accurately for any number and combination of stations. When random noise is taken into account, parameter C_p recovery occurs when the most informative stations are used. The proposed algorithm can be useful in the interpretation and planning of natural experiments on the study of wastewater distribution in coastal waters.

Keywords: Numerical modeling · Problem in variations · Functional minimization · Parameters identification · Data assimilation

1 Introduction

The environmental situation in coastal waters is influenced by various factors, including the release of pollutants from underwater reservoirs. Knowledge of reliable information about the situation in the area of releases is important for management decisions. The generation of such information is most often based on the use of clock and remote sensing methods of observations [1–3], as well as the use of mathematical modeling methods [4–6].

In mathematical modeling there is a problem of identification of model parameters on the available real information. The methods of parameter identification are most

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often based on the minimization of the quality functional, which characterize the deviations of the model estimates of the concentration of the mixture from the measurement data. Approaches to minimization of such functionals can be different. One of the effective ways to find the optimal parameter is the linearization method [7, 8].

The aim of this work is to build and verify an algorithm for identifying the input parameters of the pollutant transport model. As a first step for solving problems of this type, we consider a numerical hydrothermodynamic model [9], in which the identification parameter is the concentration of pollution at the outlet of the underwater source (hereinafter C_p). It should be noted that the identification of the C_p parameter is a practically important problem, since it is usually not possible to obtain accurate C_p values for a number of reasons.

2 Dynamic Model

To calculate the flow fields, admixture concentration, temperature and salt content of sea water in the area of underwater discharge, a nonlinear baroclinic model described in [9–11] is used. The model is based on the system of three-dimensional equations of ocean dynamics in the Boussinesq and hydrostatics approximation. The system uses a dimensionless vertical coordinate $\sigma = (\mathrm{z} - \eta)/D$, $D = h + \eta$ – dynamic depth, h – bottom relief, η – sea level.

The numerical algorithm for solving the system of equations is based on the division of the problem into barotropic and baroclinic modes and the use of explicit schemes for horizontal coordinates and implicit schemes for coordinates. The coefficients of horizontal turbulent diffusion is calculated with the formula Smagorinsky [12]. Vertical turbulent viscosity and diffusion coefficients are determined using the Mailor-Yamada model [9, 13]. TVD [14, 15] schemes are used for the approximation of advective operators in model equations. These schemes have the property of monotonicity, which is a necessary condition for adequate modeling of fields with large spatial gradients. A detailed description of the numerical algorithm of the model is given in [10].

The problem is solved at a time interval $[0, t_0]$ in a rectangular region $\Omega = \{0 \le x \le L; 0 \le y \le L; -1 \le \sigma \le 0\}$ with liquid lateral boundaries and a free surface (Fig. 1). At the initial time $t = 0$ the following conditions are set:

$$u = U_0, v = w = 0, \eta = 0, T = T_0(\sigma), S = S_0(\sigma), C = 0. \tag{1}$$

Here u, v, w – are the components of the flow velocity along the axes, x, y, σ respectively U_0 – he depth constant velocity of the background flow; T, S – temperature and salinity of water; $T_0(\sigma)$ – background temperature distribution; $S_0(\sigma)$ – background salinity distribution; C – concentration of the contaminant.

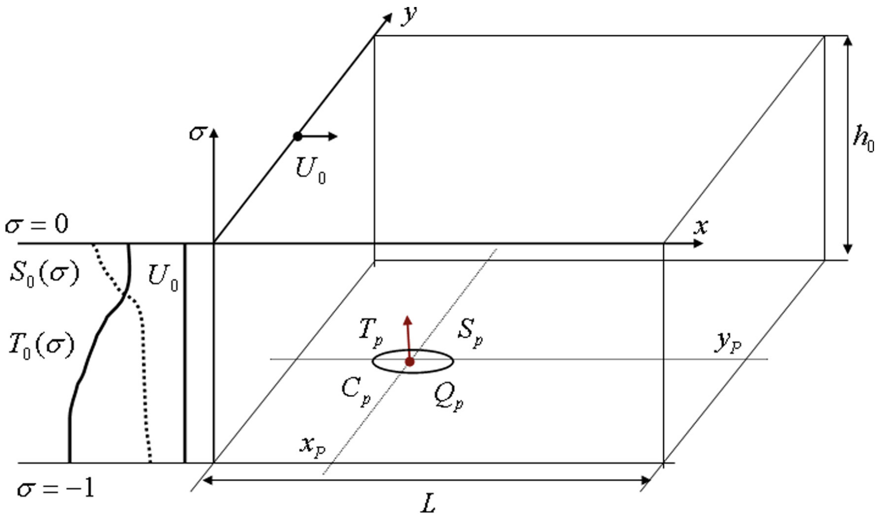

Fig. 1. Scheme of the computational domain and input model.

At $t > 0$ at the bottom of the pool $(\sigma = -1)$ in the local area Ω_p the mass source having the following parameters begins to operate in the local area: w_p – the rate of water flow from the source; T_p, S_p – the temperature and salinity of the flowing water; C_p – the concentration of the admixture at the outlet of the source.

The field of admixture concentration C in the region Ω_p is described by a three-dimensional transport-diffusion equation:

$$\frac{\partial}{\partial t}(DC) + \Lambda C = \frac{\partial}{\partial x}\left(A_C \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(A_C \frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial \sigma}\left(\frac{K_C}{D}\frac{\partial C}{\partial \sigma}\right), \tag{2}$$

where $\Lambda C = \frac{\partial}{\partial x}(DuC) + \frac{\partial}{\partial y}(DvC) + \frac{\partial}{\partial \sigma}(wC)$ – is the transfer operator; A_C and K_C – are the coefficients of horizontal and vertical turbulent diffusion coefficients.

On the free surface $(\sigma = 0)$ and out-of-source at the bottom $\left(\sigma = -1; (x, y) \notin \Omega_p\right)$ boundary conditions have the form

$$\frac{K_C}{D}\frac{\partial C}{\partial \sigma} = 0, \tag{3}$$

The boundary conditions at the bottom in the area of the source $\left(\sigma = -1; (x, y) \in \Omega_p\right)$ are written in the form [11]:

$$\frac{K_C}{D}\frac{\partial C}{\partial \sigma} = w_p\left(C - C_p\right) \tag{4}$$

3 Algorithm for Identification of Pollution Concentration in the Source

When choosing C_p as a parameter to be identified, the problem can be solved on the basis of the linearization method [7]. Let $V = \frac{\delta C}{\delta C_p}$ – the variation function C relative to the unknown parameter C_p. Following [16], we set in accordance to (2)–(4) the problem in variations:

$$\frac{\partial}{\partial t}(DV) + \Lambda V = \frac{\partial}{\partial x}\left(A_C \frac{\partial V}{\partial x}\right) + \frac{\partial}{\partial y}\left(A_C \frac{\partial V}{\partial y}\right) + \frac{\partial}{\partial \sigma}\left(\frac{K_C}{D}\frac{\partial V}{\partial \sigma}\right) \tag{5}$$

$$\frac{K_C}{D}\frac{\partial V}{\partial \sigma} = 0 \quad at \quad \sigma = 0 \tag{6}$$

$$\frac{K_C}{D}\frac{\partial V}{\partial \sigma} = 0 \quad at \quad \sigma = -1 \quad and \quad (x, y) \notin \Omega_p \tag{7}$$

$$\frac{K_C}{D}\frac{\partial V}{\partial \sigma} = w_p(V - 1) \quad at \quad \sigma = -1 \quad and \quad (x, y) \in \Omega_p \tag{8}$$

Let the problem (5)–(8) be solved on the time interval $[0, t_0]$ in the region Ω. Then, to solve the problem of C_p parameter identification, it is required to find the minimum of the following functional:

$$J = \frac{1}{2}\langle P(RC - C_{obs}), P(RC - C_{obs})\rangle \tag{9}$$

where $\langle a, b\rangle = \int_0^{t_0}\int\int\int_\Omega abd\Omega \mathrm{dt}$ – the scalar product; C_{obs} – the measured values of C at the given points of the domain Ω at given points in time; R – a projection operator in the points of observations; P – the fill operator the residuals field with zeros in the absence of measurement data.

Let's imagine a variable in the form:

$$C = \bar{C} + V\left(C_p - C_p^*\right), \tag{10}$$

where $\bar{C}$ – some assessment of the concentration of pollution, and C_p^* – its true value, to be determined. After substitution (10) in (9) we get:

$$J = \frac{1}{2}\left\langle P\left(R\left(\bar{C} + V\left(C_p - C_p^*\right)\right) - C_{obs}\right), P\left(R\left(\bar{C} + V\left(C_p - C_p^*\right)\right) - C_{obs}\right)\right\rangle \tag{11}$$

Further, for simplicity, omit the entry line $\bar{C}$. From the condition $\frac{\partial J}{\partial C_p} = 0$, finally have:

$$C_p^* = C_p + \frac{\langle P(RC - C_{obs}), PRV \rangle}{\langle PRV, PRV \rangle} \tag{12}$$

The formula (12) is also valid for the case when the measurements come, for example, only from the sea surface. The problem of constructing the quality functional (10) is solved by the appropriate choice of projection operators P and R.

Thus, the C_p parameter identification algorithm consists of the following:

– the problem (1)–(4) is solved with some initial given C_p;
– forecast residuals are calculated and the functional (9) is constructed;
– the problem in variations (5)–(8) is solved;
– evaluation is made C_p^{n+1} by the formula:

$$C_p^{n+1} = C_p^n + \frac{\langle P(RC - C_{obs}), PRV \rangle}{\langle PRV, PRV \rangle}.$$

These steps are repeated until the convergence criterion is met:

$$\left| C_p^{n+1} - C_p^n \right| < \varepsilon,$$

where ε – is the specified accuracy of the C_p parameter definition.

4 Numerical Experiments and Discussion of Results

Model calculations were carried out for the area of the Blue Bay of the Sevastopol city, where the main city wastewater is located. The estimated area had a horizontal size L is 2 km and a depth h_0 is 30 m (Fig. 1). A rectangular grid with a step d is 20 m horizontally and a discreteness of 1 m vertically was used. The integration step time was 5 s. On the western border of the computational domain ($x = 0$) was set conditions of the form (1). On other liquid boundaries, smooth continuation conditions were used for all variables: $\partial\varphi/\partial x = 0$ for $x = L$; $\partial\varphi/\partial y = 0$ for $y = 0$ and $y = L$.

The center of the source of pollution was located at the point with coordinates: $x_p = 600$ m; $y_p = 1000$ m. Horizontal size of the source along the x, y axes was equal to the step of the calculated grid d. It was assumed that the water flowing from the source is zero salinity $\left(S_p = 0\right)$, and its temperature is equal to the ambient temperature, i.e. $T_p = T_0(-1)$. As T_0 and S_0 was obtained from the sensing in the area of underwater production, performed May 20, 2016 based on data from ADCP measurements in the area of the Heraklean Peninsula [17], the value of U_0 was taken to be equal to 0.05 m/s.

At first, a “reference” calculation of dynamic characteristics and pollution concentration caused by the action of the source with a “true” value C_p^* is 0,05 kg/m^3 was carried out. The total integration time was 6 h. For the first hour of model time, the water flow at the source Q_p is linearly increased from 0 to 1.4 m^3/s and then remained unchanged. The rate of water flow from the source was estimated by the formula $w_p = Q_p/d^2$.

The spatial distribution of the field of contaminated water on a fixed level $\sigma = -0,3166\,(z = -9,5\,\text{m})$ for t = 6 h is shown in Fig. 2. There are isolines of relative concentration $c = 100\% \cdot C/C_p^*$. Dimensionless horizontal coordinates are of the form: $X = x/2d$; $Y = y/2d$. On Fig. 3. for t = 6 h the contours of the relative concentration at the section along the axis $X(Y = 25)$ are shown.

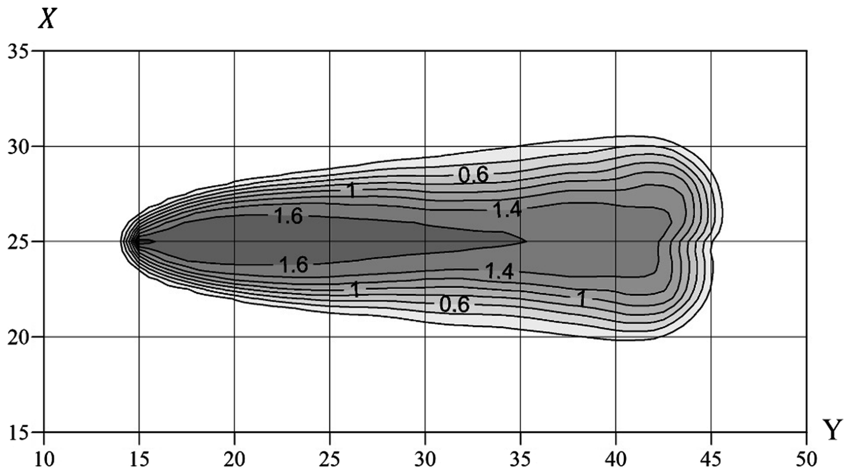

Fig. 2. Horizontal distribution of the relative concentration of the mixture C (%) in the area of the underwater source at $\sigma = -0,3166$ ($z = -9,5\,\text{m}$).

The figures show that the field of polluted water consists of a plum and a jet stretched in the direction of the background flow and concentrated in the density jump layer (8–10 m). Detailed description of the influence of density stratification of sea water and the speed of the background flow on admixture this field given in [10, 11].

In the process of "reference" to calculate the value of C was accumulated in accordance with the scheme of measurements is shown in Fig. 4 as a numbered set of points. It was assumed that a moving sensor consistently measures the vertical profile C from the free surface to a depth of $z = 25\,\text{m}$ $(\sigma_B = -0,8333)$ at stations 1–15. Measurements begin at time $t_1 = 2\,\text{h}$ at point $(X_1, Y_1) = (25,\ 20)$ and end at time $t_{15} = 5,5\,\text{h}$ at point $(X_{15}, Y_{15}) = (35, 30)$. The time resolution of measurements is 15 min. The specified measurement scheme is chosen from the considerations that in field studies the identification of contaminated waters is usually carried out by a series of vertical probes perpendicular to the direction of the jets [3].

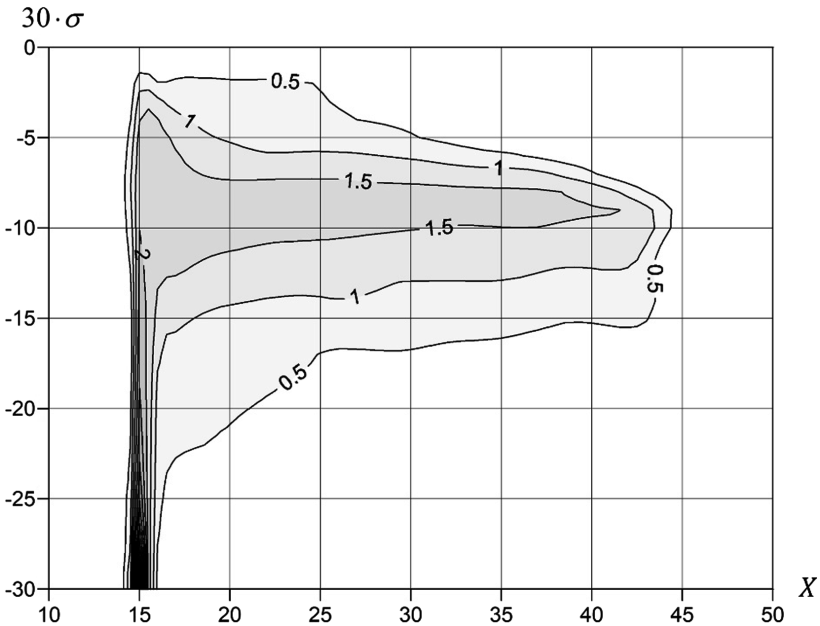

Fig. 3. Vertical structure of the field of relative concentration of C (%) in the area of the underwater source at $Y = 25$.

Functionality $I = \frac{1}{C_p^*} \int_{\sigma_B}^{0} C(\sigma) d(\sigma)$ characterizes the level of informativeness of measurements. Value I for each of the stations are given in Fig. 5. As you can see, the highest values of the I (stations 3, 8, 13) correspond to the hit of the sensor on the axis of the polluted water jet, and the lowest values of the I (stations 1, 2, 5, 6, 11, 12, 15) – cases where the sensor "slipped" the axial portion of the jet.

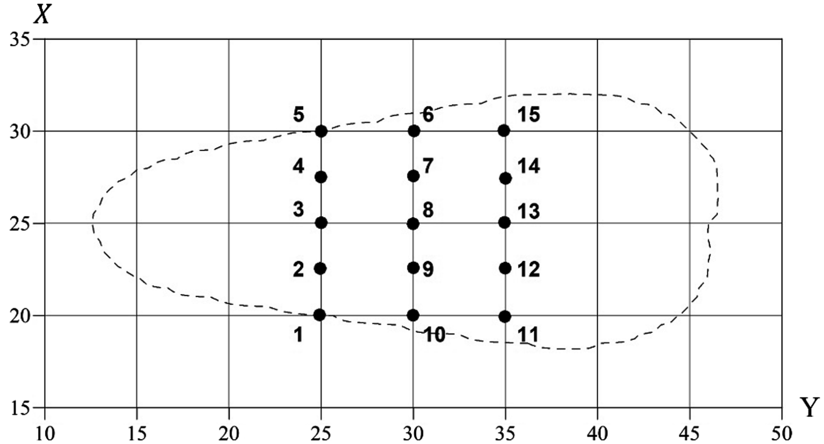

Fig. 4. Scheme of measurement of the admixture concentration field in the area of the underwater source. The position of the stations marked by points.

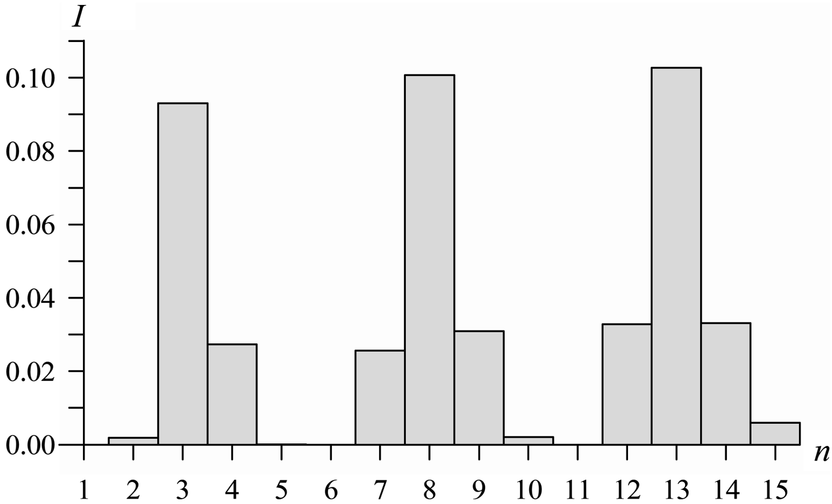

Fig. 5. Dependence of the functional I value on the station number n.

In parallel with the "reference" calculation, the problem was solved in variations (6)–(9). At its decision vertical profiles in at stations 1–15 in the moments of time $t_1 - t_{15}$ were kept. Since V is independent of the parameter C_p, the problem (6)–(9) was solved once.

Then a series of numerical experiments on testing the above algorithm of parameter C_p identification was performed. Numerical experiments were carried out with a different number of stations. In addition, the "measured" vertical profiles $C(\sigma)$ were supplemented with random noise $\xi \in [-r/2, r/2]$, where $\xi = r(\delta - 1/2)$; r – is a given noise level; $\delta \in [0, 1]$ – a normally distributed random variable. The initial approximation was set to $C_p = 0, 1\,\mathrm{kg/m^3}$. It is established that 2, 3 iterations are necessary for convergence of the iteration process. Moreover, the main decrease in the residual functional (10) occurs already at the first iteration.

The results of numerical experiments to recover the parameter C_p or different combinations of stations at $0 < r \le C_p^*/10$ are given in the table. As the comparison shows, without taking into account the random noise (experiments 1, 5 and 9), the parameter C_p is restored exactly regardless of the number and informativeness of the stations used. When random noise is taken into account, the best recovery occurs when the most informative stations 3, 8 and 13 are used.

Results of restoration of pollution concentration at the output from the underwater source C_p at different number of stations and different noise level in the input data

№	Station	r, kg/m^3	Noise level $100\% \cdot r/C_p^*$, %	Recovering C_p, kg/m^3	Error recovery $100\% \cdot C_p/C_p^*$, %
1	1–15	0,0000	0,0	0,5000	0,0
2	1–15	0,0125	2,5	0,5276	5,5
3	1–15	0,0250	5,0	0,6487	29,7
4	1–15	0,0500	10,0	0,9670	93,4
5	3, 8, 13	0,0000	0,0	0,5000	0,0
6	3, 8, 13	0,0125	2,5	0,4791	4,2
7	3, 8, 13	0,0250	5,0	0,5814	16,3
8	3, 8, 13	0,0500	10,0	0,8432	68,6
9	1, 2, 5, 6, 11, 12, 15	0,0000	0,0	0,5000	0,0
10	1, 2, 5, 6, 11, 12, 15	0,0125	2,5	0,5836	16,7
11	1, 2, 5, 6, 11, 12, 15	0,0250	5,0	0,6932	38,6
12	1, 2, 5, 6, 11, 12, 15	0,0500	10,0	1,0986	119,7

5 Conclusions

On the basis of the analysis of the numerical experiments, correct work of the linearization algorithm is shown for the identification of the selected input parameter of the problem. The algorithm has a good iterative convergence of the process, which allows to quickly assess the concentration in the source of pollution. The algorithm can be used to solve a wide range of environmental problems, as well as to interpret and plan full-scale experiments on the study of wastewater distribution in coastal waters.

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