Reconstruction of a passive tracer boundary source in an open water area

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Received 15 August 2019 | Accepted by V. Pešić: 20 September 2019 | Published online 8 November 2019.

Abstract

Marine pollution is one of the most serious environmental problems nowadays. Identification of sources of contaminants is among the main objectives of environmental researchers. In such problems pollutants are sometimes considered as passive tracers. In this paper, a problem of detecting and localization of the passive tracer boundary sources in an open water area is considered. A mathematical model of the sea surface pollution spread based on the system of linear unsteady convection-diffusion-reaction equations is used. The inverse problem of restoring the pollution sources on the domain boundary is formulated under the consideration that the pollution concentration data are given. The method based on the theory of adjoint equations and optimal control is used. The iterative algorithm for the solution of the problem is proposed. The article presents the results of the numerical experiment on application of the proposed algorithm to the problem of recovering pollution sources on the Black Sea coastline.

Key words: marine pollution, passive tracer, variational methods, open boundaries, inverse problems, adjoint equations, mathematical modeling, numerical methods, iterative algorithms.

Introduction

At present, marine pollution is one of the most actual environmental problems. Pollution caused by chemical substances that are dissolved in the sea water or drifting on its surface is a well-known global concern. Particularly, pollution of the coastal zone has increased dramatically in recent years, primarily due to agricultural activities, sewage rates increase, new oil terminals and offshore drilling rigs usage, volume of oil sea transportation increase and uncontrolled discharge of by-products of many industrial processes into the rivers (Islam & Tanaka, 2004). Consequently, pollution level monitoring has become one of the most important and actual environmental safety task. Timely assessment of the effects of anthropogenic impacts on the environment and the pollution sources localization can help to take necessary actions on time and reduce harmful effects.

After the development of satellite systems with sufficiently high spatial resolution and possibility of providing daily data for any area of observation, it has become possible to develop technologies for a marine...
environment monitoring. Operational satellite monitoring makes it possible to map the dynamic characteristics and parameters of water pollution, to determine the types and scales of pollution, to track its migration routes, to observe the mechanisms of water self-purification (Bedritskii et al., 2009). Sometimes it is possible to obtain some quantitative characteristics of pollution (e.g., the area of pollution and its change rate). Due to an integrated (multi-sensor) approach to operational satellite monitoring, including joint analysis of a variety of satellite, oceanographic and meteorological information, many of the problems associated with the correct detection of marine surface pollution can be solved (Lavrova, & Mityagina, 2013).

Identification of the sources of contaminants and investigation of the basic processes of the pollutant evolution is among the main objectives of environmental researchers. Mathematical modeling is a cost effective and practical way to conduct research, since less sophisticated equipment is needed. Also, mathematical modeling is often the only way to analyze aquatic ecosystems, phenomena and processes. The application of mathematical modeling in environmental monitoring is a relatively new and evolving field.

The closest to reality mathematical models of the considered phenomena often depend on a large number of parameters (many of them are usually unknown) and their numerical implementation is quite complex. For example, while simulating the evolution of oil spill on the sea surface, the modelers should take into account various physical processes (gravitational spreading, transport of substances by sea currents, wind drift, evaporation, dispersion, emulsification, etc.) (Aseev & Sheloput, 2016). Therefore, models become difficult and nonlinear. The study of inverse problems for such models is also sophisticated. At the same time, researchers are interested mostly in the major features of the phenomena, so different simplifications are used. For example, pollutants are often considered as passive tracers (Sarat et al., 2017).

In this paper, the mathematical model of the sea surface pollution spread based on the system of linear unsteady convection-diffusion-reaction equations is used. The model require pre-calculated velocity field that can be obtained via the simulation with a hydrodynamics model. If the marine area is open, the hydrodynamics model should account for open boundaries. The inverse problem of restoring the pollution sources on the domain boundary is formulated under the consideration that the pollution concentration data are given. The method based on the theory of adjoint equations and optimal control is used to solve the problem (Marchuk et al., 1996). The iterative algorithm for the solution of the problem is proposed. Similar methods were previously used in other problems on estimation of the pollution source parameters (Penenko, 2009), as well as in the problems of determining the concentration of passive admixtures (Dymova et al, 2018). In this paper the results of the numerical experiment on the application of the proposed algorithm for the problem of recovering pollution sources on the Black Sea coastline are presented and discussed.

Formulation of the considered problem

Let a domain $\Omega$ represent a marine area, and $\Gamma$ is the boundary of $\Omega$. Suppose that release of pollutants occurs on $\Gamma_{in}$, that is some part of $\Gamma$. The exact locations of pollution sources are a priori unknown, but they are considered to be located on $\Gamma_{in}$ (see Figure 1).

![Figure 1](image)

**Figure 1.** Possible arrangement of $\Omega$, $\Gamma$, $\Omega_{ob}$, $\Gamma_{in}$.
We assume that there are given data in domain \( \Omega_{ob} \subseteq \Omega \). These data contain an approximate estimation of pollutant concentration in \( \Omega_{ob} \). Further in the paper these data are mention to as “observational data”. Suppose that there is a pre-calculated velocity field that can be obtained via the simulation with a hydrodynamics model (for example, with a regional model (Blumberg & Mellor, 1987) or informational computational system (Agoshkov et al., 2015; Agoshkov et al., 2018)). In these assumptions we formulate a problem of reconstruction of pollutant boundary source. To describe pollution spreading process we will use the system of linear unsteady convection-diffusion-reaction equations.

**Mathematical formulation of the problem**

Consider a domain \( \Omega \) with Lipschitz piecewise continuous boundary \( \Gamma \) from \( \mathbb{R}^2 \) space of variables \((x, y)\). Let \( \Omega \) be a domain contained in or matching \( \Omega_{ob} \), and also let \( \Gamma_{in} \) be a curve contained in or matching \( \Gamma \). By \( \varphi \) we denote the pollutant concentration \((\varphi \geq 0)\), and by \( \varphi_{ob} \) we denote the data of observations in the domain \( \Omega_{ob} \).

Now, let us present the problem of finding functions \( \varphi, v \) with the required smoothness, that satisfy the following system of partial differential equations:

\[
\begin{align*}
\frac{\partial \varphi}{\partial t} &- \text{div}(\mu \text{ grad } \varphi) + \text{div}(U \varphi) + b \varphi = f, \quad (x, y, t) \in \Omega \times (0, T), \\
U_n^{(-)} &+ \mu \frac{\partial \varphi}{\partial n} = G, \quad (x, y, t) \in \Gamma_\times (0, T), \\
\varphi &= \varphi_0, \quad (x, y) \in \Omega, \quad t = 0,
\end{align*}
\]

and meet additional (closure) condition

\[
\varphi = \varphi_{ob}, \quad (x, y, t) \in \Omega_{ob} \times (0, T),
\]

where \( \mu, b = \text{ const} > 0 \), \( U \) – velocity vector, \( U = (u_1, u_2) \in \left(C^{1,0}(\Omega \times (0, T))\right)^2 \) and \( \text{div}(U) = 0 \),

\[
U_n^{(\pm)} = \left[\left(U, n\right) \pm \left(U, n\right)\right]/2,
\]

\[
G = \begin{cases} 
\varphi_0, & (x, y, t) \in \Gamma_{in} \times (0, T), \\
\varphi_{ob}, & (x, y, t) \in \Gamma \setminus \Gamma_{in} \times (0, T),
\end{cases}
\]

\( f, g, \varphi_0, \varphi_{ob} \) – given functions. By \( \vec{n} \) we denote the unit vector of the outer normal to \( \Gamma \).

We formulate the class of optimal control problems (Marchuk et al., 1996), where condition (2) is considered in a least squares sense: find functions minimizing the functional:

\[
J_\alpha(\varphi, u) = \arg \inf_u J_\alpha(\varphi, u),
\]

\[
J_\alpha(\varphi, u) = \frac{\alpha}{2} \left\| \varphi_{ob} - \varphi \right\|_{L_2(\Omega_{ob} \times (0, T))}^2 + \frac{1}{2} \left\| \varphi \right\|_{L_2(\Omega \times (0, T))}^2 
\]

where \( \alpha \geq 0 \). If we formulate the problem (1)-(2) in operator form (Marchuk et al., 1996), the necessary condition for the minimum of the functional will take the form of an equation in terms of Tikhonov regularization method (Tikhonov & Arsenin, 1977) where \( \alpha \) – regularization parameter, therefore, we will further call \( \alpha \) the regularization parameter.
Algorithm for solving the optimal control problem

We use gradient descent method to solve the minimization problem (3). Gradient of the functional $J_\alpha$ could be obtained from solution of adjoint problem (Marchuk et al., 1996). Ultimately, gradient descent method could be written in the following form:

- **Step 1. Computing the solution of the straight problem**

$$
\frac{\partial \varphi^k}{\partial t} - \text{div}(\mu \text{grad} \varphi^k) + \text{div}(U \varphi^k) + b \varphi^k = f, \quad (x, y, t) \in \Omega \times (0, T),
$$

$$
U_n^{(-)} \varphi^k + \mu \frac{\partial \varphi^k}{\partial n} = G^k_\alpha, \quad (x, y, t) \in \Gamma \times (0, T),
$$

$$
\varphi^k = \varphi_0, \quad (x, y) \in \Omega, t = 0,
$$

$$
G^k_\alpha = \begin{cases}
\varphi^k, (x, y, t) \in \Gamma_{in} \times (0, T), \\
g, (x, y, t) \in \Gamma \setminus \Gamma_{in} \times (0, T).
\end{cases}
$$

- **Step 2. Computing the solution of the adjoint problem:**

$$
- \frac{\partial \varphi^*_k}{\partial t} - \text{div}(\mu \text{grad} \varphi^*_k) - (U, \text{grad} \varphi^*_k) + b \varphi^*_k = m_{ob}(\varphi^k - \varphi_{ob}), \quad (x, y, t) \in \Omega \times (0, T),
$$

$$
U_n^{(+)} \varphi^*_k + \mu \frac{\partial \varphi^*_k}{\partial n} = 0, \quad (x, y, t) \in \Gamma \times (0, T),
$$

$$
\varphi^*_k = 0, \quad (x, y) \in \Omega, t = T,
$$

- **Step 3. Find new approximation to $v$ by:**

$$
v^{k+1} = v^k - \lambda^k (\alpha v^k + m_{ob} \varphi^*_k),
$$

where $k = 1, 2, \ldots$ – number of iteration, $\lambda^k$ – iterative parameter. When a suitable convergence criterion is met, we accept element $v^k$ as an approximate solution to the inverse problem. The convergence criterion should be chosen depending on parameters of iteration process, size of modeling area and given accuracy. Algorithm (Step 1)-(Step 3) is guaranteed to converge when parameter $\lambda^k \equiv \lambda = \text{const} > 0$ is small enough (Marchuk et al., 1996).

**Numerical experiment**

In this section we discuss the results of the numerical experiment for a model problem. The Black Sea area was chosen as the domain $\Omega$. The numerical experiment was implemented in the following stages:

- **Stage 1.** Prior calculation of the velocity field $U$ was performed with the model of hydrothermodynamics of the Black Sea (Zalesny et al., 2012).
- **Stage 2.** Values of parameters $\mu$, $b$ were set and functions $f$, $g$, $\varphi_0$ were defined.
- **Stage 3.** Preliminary calculation for the straight problem (1) was performed with a given function $v_p$ on $\Gamma_{in}$. The results were used to set $\varphi_{ob}$ on $\Omega_{ob}$, and the value of $v_p$ became «forgotten».
- **Stage 4.** The optimal control problem (1), (3) with some small positive $\alpha$ was solved using the algorithm (5)-(7), where the solution of the straight problem (on $\Omega_{ob}$) obtained at the previous stage was taken as $\varphi_{ob}$.
To obtain the numerical solution of the systems of differential equations (Step 1, Step 2) the implicit Euler method for time discretization and the finite element method for domain discretization were used. In the gradient descent method, the iterative parameter $\lambda^k \equiv \lambda > 0$ was chosen constant. The iterative process was stopped after 50 iterations. The initial approximation $v^0$ was set zero.

Further in this section, the numerical solution of the optimal control problem (1), (3) will be denoted by $(\varphi_{ah}, v_{ah})$, and the result of the preliminary calculation (Stage 3) will be denoted by $(\varphi_p, v_p)$.

Let $(x, y)$ denote the geographical longitude and latitude. In the experiment we use

$$\Omega_{ob} = \{(x, y) \in \Omega : 31.0 \leq x \leq 37.0, y \leq 43.5\},$$

$$\Gamma_{in} = \{(x, y) \in \Gamma : 32.0 \leq x \leq 36.0, y \leq 42.5\}.$$

Such choice was made due to high advection rate in the selected region (Figure 2).

![Figure 2. Velocity field $U$, $t = 0$.](image-url)

The other parameters and functions were defined in the following way:

- **System coefficients:** $\mu = 0.1$, $b = 0.0$.
- **Given functions:** $f = g = \varphi_0 \equiv 0.0$.
- **Analytic form of $v_p$**
  
  $$v_p = \begin{cases} 
  2.0, 32.0 + i \leq x \leq 32.5 + i, i = 0, 1, 2, 3, \\
  0.0, \text{otherwise}. 
  \end{cases}$$

- **Regularization parameter** $\alpha = 10^{-3}$, iterative parameter $\lambda = 2.0 \cdot 10^{-3}$.

The iterative algorithm converged with the chosen parameter $\lambda$. The value of the functional $J_\alpha$ decreased, as well as the difference between the solution $\varphi_{ah}$ and the observations $\varphi_{ob}$ (see Figure 3). The convergence of the $L_2$-norm of the difference between the calculated function $v_{ah}$ and the exact function $v_p$ presented in Figure 4 (dash line).
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The solution of the optimal control problem $\varphi_{ab}$ is presented in Figure 6. It could be compared with the result of the preliminary calculation $\varphi_p$, presented in Figure 5. The difference between these concentration fields is shown in Figure 7. It could be noted that the difference is relatively small.

The most interesting result of the numerical experiment is that the algorithm (Step 1 – Step 3) was able to recover the locations of the boundary sources. In Figure 8 the exact function $\nu_p$ and the restored function $\nu_{ah}$ are presented. We could note that the calculated values of $\nu_{ah}$ provided satisfactory, though not perfect fit to analytical function.
Conclusion

In this paper, the problem of detecting and localization of the boundary sources of the contaminants considered as passive tracers in the open water area was numerically solved. The mathematical model of the sea surface pollution propagation based on the system of linear unsteady convection-diffusion-reaction equations was used. The inverse problem of restoring the pollution sources on the domain boundary is formulated under the consideration that the pollution concentration data are given. The iterative algorithm for the inverse problem solution was proposed. The algorithm was tested in the problem of recovering of the pollution sources on the Black Sea coastline. For this purpose the prior calculation of the velocity field with the hydrothermodynamics model of the Black Sea was performed. The twin experiment was carried out. As expected, the algorithm converged with the constant iterative parameter and the calculated concentration fitted the given data. It was shown that the algorithm is able to recover the locations of the boundary sources. Moreover, the calculated source function provided satisfactory fit to the exact one.

Note, that this paper was only the first stage of the study. To estimate the approach, its quality and the possibility of application to realistic problems, more experimental results should be provided. In this study rough approximations were used, but the general approach outlined here may be extended to more complicated cases. The algorithm requires pollution concentration data, so it is necessary to check the stability of the algorithm to observational data errors.

Acknowledgements

The work was partly supported by the Russian Science Foundation (project 19-71-20035, results of the numerical experiments) and by the project "Intelligent analysis of big data in the problems of ecology and environmental protection", carried out as part of the Competence Center Program of the National Technological Initiative "Big Data Storage and Analysis Center", supported by the Ministry of Science and Higher Education of the Russian Federation under the Contract between the Lomonosov Moscow State University and the Project Support Fund of the National Technological Initiative dated December 11, 2018 No. 13/1251/2018 (statement and study of the problem).
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