

Mathematical Modeling and Numerical Algorithms for Simulation of Oil Pollution

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Received: 6 June 2011 / Accepted: 16 August 2011 / Published online: 6 September 2011
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Abstract This paper deals with the mathematical modeling and algorithms for the problem of oil pollution. For solving this task, we derive the adjoint problem for the advection–diffusion equation describing the propagation of oil slick after an accident, which we call the main problem. We prove a fundamental equality between the solutions of the main and the adjoint problems. Based on this equality, we propose a novel method for the identification of the pollution source location and the accident time of oil emission. This approach is illustrated on an example for an accident in the offshore of the central part of the Vietnamese coast. Numerical simulations demonstrate the effectiveness of the proposed method. Besides, the method is verified for 1D model of substance propagation.

Keywords Oil transport problems · Oil spilling · Weathering · Adjoint equation approach · Pollution source identification

Mathematics Subject Classifications (2010) 62P12 · 65M06 · 65M32

1 Introduction

In this work, we study a mathematical model of oil spill processes in seas (arising from tanker or offshore accidents, liquid waste, etc.), such as advection, turbulent diffusion, surface spreading, evaporation, dissolution, and emulsification. These processes may influence the transport of oil spill. There exist a wide range of research articles focused on the surface movement of oil spills and describing the numerical simulation of oil spills in accidents occurred in some seas [28]. However, a large part of mathematical investigations of the used computational schemes is still almost open. Therefore, the first goal of this paper is the analysis of numerical schemes for simulating oil spills in order to obtain accurate predictions of the movement and the fate of the spilled oil. This forecast gives an idea of the oil spill impact and is crucial for properly designed clean-up recovery operations and the protection of ecologically sensitive zones. After completing this task, we shall obtain good numerical schemes for predicting the oil slick at any time.

Another task, which may be even more important than the prediction of the oil pollution, is the determination of the location, the time, and the total power of oil emission if an oil slick is detected. From mathematical point of view, this is an inverse problem, and it is

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more difficult than the direct problem of the prediction of oil pollution. Hence, the second goal of this work is the elaboration of methods and numerical schemes for solving the above inverse problem.

Since the oil spilling heavily depends on the velocity of the wind and surface current, the above direct and inverse problems of oil spill are posed under the assumption that the wind and the flow fields in the sea are known. These data in sea may be collected from experimental measurements or are obtained in the results of the problem of flow and wind. Having in hand the data of sea flow and wind in the Vietnamese coast and sea (from the Buro of Hydrology and Meteorology, Hanoi) we shall simulate the spreading of oil after being discharged from a source and solve the inverse problem of determining the position, the time, and the power of the pollution emitter.

2 The 2D Oil Spill Problem

In this section, we will give a brief introduction to the 2D mathematical model and follow the notation of Skiba, cf. [23, 24]. Let $r_0 = (x_0, y_0)$ denote the location of an oil tanker or oil platform. D is some two-dimensional open sea domain with boundary S . At $t = 0$, the accident happens at the site r_0 with a *rate of oil spilling* in unit time $F(t)$ and the *oil slick thickness* $\varphi(r, t)$ on the sea surface at point $r = (x, y)$ and time $t > 0$. The oil slick propagation in D and time interval $(0, T)$ is described by the 2D advection–diffusion equation

$$L\varphi \equiv \frac{\partial \varphi}{\partial t} + \operatorname{div}(\mathbf{U}\varphi) + \sigma\varphi - \nabla \cdot \mu \nabla \varphi = f(r, t), \quad r \in D, \quad t \in (0, T), \quad (1)$$

with the emission forcing function

$$f(r, t) = F(t) \delta(r - r_0), \quad (2)$$

where $\mu(r, t)$ is the diffusion coefficient, ∇ is the two-dimensional gradient, and $\delta(r - r_0)$ is the Dirac mass at the accident point r_0 . The parameter $\sigma \geq 0$ characterizes the decay of $\varphi(r, t)$ due to evaporation which is the most dominant weathering process during the first several days [17]. The velocity $\mathbf{U}(r, t) = (u(r, t), v(r, t))$ of the oil propagation is assumed to be known. This velocity field can be calculated by using the climatic (seasonal or monthly) sea surface currents and winds [8], or the real currents and winds from dynamic models.

In case the velocity field satisfies the *continuity equation*

$$\nabla \cdot \mathbf{U} = \frac{u}{x} + \frac{v}{y} = 0, \quad (3)$$

the advection–diffusion (Eq. 1) is often written in the form [23]

$$\frac{\partial \varphi}{\partial t} + \mathbf{U} \cdot \nabla \varphi + \sigma\varphi - \nabla \cdot \mu \nabla \varphi = f(r, t), \quad r \in D, \quad t \in (0, T). \quad (4)$$

The initial condition at $t = 0$ is simply the absence of oil on the sea surface:

$$\varphi(r, 0) = 0, \quad r \in D. \quad (5)$$

To obtain a well-posed problem according to Hadamard [23], care is required in setting conditions at the boundaries. Let U_n be the projection of the velocity \mathbf{U} on the outward normal n to the boundary S . We divide S into the outflow part S^+ , where $U_n \geq 0$ (oil flows out of the domain D) and the inflow part S^- where $U_n < 0$ (oil flows into D). The boundary conditions for Eq. 1 are

$$\mu \frac{\partial \varphi}{\partial n} - U_n \varphi = 0 \quad \text{at inflow boundary/coastline } S^-, \quad (6)$$

$$\mu \frac{\partial \varphi}{\partial n} = 0 \quad \text{at outflow boundary } S^+. \quad (7)$$

By Eq. 6, the combined diffusive plus advective oil flow is absent at the inflow part S^- , as no oil flows into D from the outside where the water is free of oil. Condition 7 means that at the boundary S^+ (that includes the coastline with $U_n = 0$), the diffusive oil flow is small compared to the advective oil outflow $\mu \partial \varphi / \partial n$ from D .

In the non-diffusion limit ($\mu = 0$), condition 6 is reduced to $\varphi = 0$ (there is no oil on the inflow boundary), while Eq. 7 vanishes, as it must. Indeed, the pure advection problem ($\mu = \sigma = 0$) does not require conditions at the outflow boundary, since its solution is predetermined by the method of the characteristics, cf. [10].

We note that condition 7 includes the coastline where $U_n = 0$. In particular, for a closed basin D everywhere bounded by the coastline, S^- is empty and $S = S^+$. Thus, Eqs. 6 and 7 include the coastline condition and approach the correct boundary conditions of the pure advection problem in the non-diffusion limit.

Another setting of boundary conditions, which is somewhat different from Eqs. 6 and 7, reads

$$\varphi = 0 \quad \text{at } S^-, \quad (8)$$

$$\frac{\partial \varphi}{\partial n} = 0 \quad \text{at } S_1^+, \quad \frac{\partial \varphi}{\partial n} = \alpha \varphi \quad \text{at } S_2^+, \quad (9)$$

where S_1^+ is the actual outflow part ($U_n > 0$), S_2^+ is the coastline part of the boundary ($U_n = 0$), and $\alpha \geq 0$ is the absorption coefficient of the coastline.

Next, we want to motivate some balance equations for this oil pollution problem that yield some physical insights. First, we integrate the 2D transport equation (Eq. 1) in space gives

$$\begin{aligned} \frac{\partial}{\partial t} \int_D \phi \, dr - \int_D \nabla U \cdot \phi \, dr + \int_D \sigma \phi \, dr \\ - \int_S \left(\mu \frac{\partial}{\partial n} \phi - U_n \phi \right) \, dS = F(t), \end{aligned} \tag{10}$$

and using the inflow and outflow conditions 6 and 7, we see that any solution of problems 1–7 satisfies the *oil balance equation*

$$\begin{aligned} \frac{\partial}{\partial t} \int_D \phi \, dr = F(t) + \int_D \nabla \cdot U \phi \, dr - \int_D \sigma \phi \, dr \\ - \int_{S^+} U_n \phi \, dS, \end{aligned} \tag{11}$$

that reduces to

$$\frac{\partial}{\partial t} \int_D \phi \, dr = F(t) - \int_D \sigma \phi \, dr - \int_{S^+} U_n \phi \, dS. \tag{12}$$

if the continuity Eq. 3 is fulfilled. Equation 12 describes the time evolution of the *total pollution concentration* $\int_D \phi \, dr$ that increases due to the emission $F > 0$, see Eq. 2, and decreases due to evaporation and the advective pollution transport across the outflow boundary S^+ .

Secondly, to obtain an estimate for the L^2 -norm of the solution ϕ , we multiply Eq. 1 by 2ϕ and integrate again

$$\begin{aligned} \frac{\partial}{\partial t} \int_D \phi^2 \, dr - \int_D \nabla \cdot U \phi^2 \, dr + 2 \int_D (\sigma \phi^2 + \mu |\nabla \phi|^2) \, dr \\ - \int_S \left(2\phi \mu \frac{\partial}{\partial n} \phi - U_n \phi^2 \right) \, dS = 2F(t)\phi(r_0, t), \end{aligned} \tag{13}$$

and with the boundary conditions 6 and 7, we obtain the integral equation

$$\begin{aligned} \frac{\partial}{\partial t} \int_D \phi^2 \, dr - \int_D \nabla \cdot U \phi^2 \, dr + 2 \int_D (\sigma \phi^2 + \mu |\nabla \phi|^2) \, dr \\ + \int_{S^+} U_n \phi^2 \, dS - \int_{S^-} U_n \phi^2 \, dS = 2F(t)\phi(r_0, t). \end{aligned} \tag{14}$$

Finally, if the continuity Eq. 3 is fulfilled, Eq. 14 reduces to

$$\begin{aligned} \frac{\partial}{\partial t} \int_D \phi^2 \, dr + 2 \int_D (\sigma \phi^2 + \mu |\nabla \phi|^2) \, dr \\ + \int_{S^+} U_n \phi^2 \, dS - \int_{S^-} U_n \phi^2 \, dS = 2F(t)\phi(r_0, t), \end{aligned} \tag{15}$$

where $\int_D \phi^2 \, dr$ is the norm squared in Hilbert space $L^2(D)$ of square-integrable functions in the domain D . If the oil spill from the damaged tanker has been stopped ($F = 0$), both quantities $\int_D \phi \, dr$ and $\int_D \phi^2 \, dr$ decrease with respect to time.

3 The Adjoint Problem

It is well-known that the *adjoint equation approach* [2, 6, 7, 12, 13, 20–22] is very useful in problems of estimating pollution concentration in sensitive zones and optimization problems of air pollution. In this work, we shall use this approach for the problem of identification of the point source location and the time of accident causing oil pollution. Since the location of the accident can be quickly determined from a satellite, as an alternative method for determining the intensity (not only invariable intensity) of the source, the method suggested in [25, 26] can be used. We refer to [1, 16] and the references therein for an overview of methods of pollution source identification.

Using the *Lagrange identity*, the adjoint problem for the main problems 1, 5, 6, and 7 in the domain D and the time interval $(0, T)$ can be written as

$$L^* \varphi^* \equiv -\frac{\partial \varphi^*}{\partial t} - \mathbf{U} \cdot \nabla \varphi^* + \sigma \varphi^* - \nabla \cdot \mu \nabla \varphi^* = p(r, t), \tag{16}$$

$$\varphi^*(r, T) = 0, \tag{17}$$

$$\mu \frac{\partial \varphi^*}{\partial n} + U_n \varphi^* = 0 \quad \text{at } S^-, \tag{18}$$

$$\mu \frac{\partial \varphi^*}{\partial n} = 0 \quad \text{at } S^+. \tag{19}$$

For the solutions of the main and adjoint problems, there holds the Lagrange identity

$$(L\varphi, \varphi^*) = (L^* \varphi^*, \varphi), \tag{20}$$

where we denote

$$(\varphi, \psi) = \int_0^T \int_D \varphi(r, t) \psi(r, t) \, dr dt.$$

Now, we introduce $\tau = T - t$ as the reversed time and set $\phi^*(r, T - \tau) = \Phi^*(r, \tau)$, $p(r, T - \tau) = P(r, \tau)$. Then the adjoint problem becomes

$$L_-^* \phi^* \equiv \frac{\partial \phi^*}{\partial \tau} - \mathbf{U} \cdot \nabla \phi^* - \nabla \cdot \mu \nabla \phi^* + \sigma \phi^* = P(r, \tau), \tag{21}$$

$$\phi^* = 0 \quad \text{at } \tau = 0, \tag{22}$$

$$\mu \frac{\partial \phi^*}{\partial n} - (-U_n) \phi^* = 0 \quad \text{on } S^+ \quad (\text{inflow for } -\mathbf{U}), \tag{23}$$

$$\mu \frac{\partial \phi^*}{\partial n} = 0 \quad \text{on } S^- \quad (\text{outflow for } -\mathbf{U}), \tag{24}$$

which is similar to the main problem with the reversed flow $(-\mathbf{U})$. Now we derive an important relation between the solutions of the main and the adjoint problems, which will be useful later. For this purpose, let us take

$$f(r, t) = Q\delta(r - r_0) \delta(t - t_0), \tag{25}$$

$$p(r, t) = Q\delta(r - r_1) \delta(T_d - t), \tag{26}$$

where Q denotes the power of instantaneous source of oil spill, which is located at the accident point r_0 at the time t_0 and at the point r_1 at some later time T_d , respectively. Here we suppose that $0 \leq t_0 < T_d \leq T$.

Proposition 1 *For the solution of the main problem and the adjoint problem, there holds the relation*

$$\phi^*(r_0, T - t_0) = \varphi(r_1, T_d), \tag{27}$$

or

$$\phi^*(r_0, \tau_0) = \varphi(r_1, T_d). \tag{28}$$

Proof Indeed, we have

$$\begin{aligned} (L\varphi, \varphi^*) &= (f, \varphi^*) \\ &= \int_0^T \int_D Q\delta(r - r_0) \delta(t - t_0) \varphi^*(r, t) \, dr dt \\ &= Q\varphi^*(r_0, t_0), \end{aligned} \tag{29}$$

$$\begin{aligned} (L^*\varphi, \varphi) &= (p, \varphi) \\ &= \int_0^T \int_D Q\delta(r - r_1) \delta(T_d - t) \varphi(r, t) \, dr dt \\ &= Q\varphi(r_1, T_d). \end{aligned} \tag{30}$$

Then from the Lagrange equality Eq. 20, it follows

$$\phi^*(r_0, t_0) = \varphi(r_1, T_d).$$

□

This is the same as Eq. 27 or Eq. 28.

4 Numerical Schemes for the Main and Adjoint Problems

For solving the main and adjoint problems for advection–diffusion–reaction equation, there exists a large number of numerical schemes. Mainly, they are based on splitting methods developed by Yanenko [29] and Marchuk [12]. These schemes are stable and possess good approximation properties, but they may lead to solutions with negative values that are meaningless. Therefore, it is desired to construct difference schemes that avoid this defect. These difference schemes must ensure that if all initial and boundary conditions are nonnegative, then the solution of the corresponding problem is nonnegative, too. The difference schemes of this type are called *monotone* (or *positive*) ones (cf. [4, 5]). Below, we present a monotone difference scheme for the main problem that was developed in [4] and used later in [5]. Throughout this paper, we shall use the standard difference notations of Samarskii [19].

We begin with the consideration of the *1D parabolic problem*

$$\begin{aligned} c(x, t) \frac{\partial \varphi}{\partial t} &= L\varphi + f(x, t), \quad 0 < x < 1, \quad 0 < t \leq T, \\ \varphi(0, t) &= \mu_1(t), \quad \varphi(1, t) = \mu_2(t), \\ \varphi(x, 0) &= \varphi_0(x), \end{aligned} \tag{31}$$

where

$$\begin{aligned} L\varphi &= \frac{\partial}{\partial x} \left(k(x, t) \frac{\partial \varphi}{\partial x} \right) + r(x, t) \frac{\partial \varphi}{\partial x} - q(x, t)\varphi, \\ 0 < c_1 &\leq k(x, t) \leq c_2, \quad c(x, t) \geq c_1, \quad q(x, t) \geq 0. \end{aligned} \tag{32}$$

We will construct a difference scheme for this problem on the uniform grid

$$\omega_{h\tau} = \left\{ x_i = ih, t_j = j\tau, \quad i = 0, 1, \dots, N, \right. \\ \left. j = 0, 1, \dots, J, \quad h = \frac{1}{N}, \tau = \frac{T}{J} \right\}.$$

First, we associate with the operator L a *perturbation operator*

$$\tilde{L}\varphi = \chi \frac{\partial}{\partial x} \left(k(x, t) \frac{\partial \varphi}{\partial x} \right) + r(x, t) \frac{\partial \varphi}{\partial x} - q(x, t)\varphi, \tag{33}$$

where

$$\chi = \frac{1}{1 + R}, \quad R = \frac{h|r|}{2k}$$

and approximate the later one by the difference operator

$$\tilde{\Lambda}\phi = \chi (a\phi_{\bar{x}})_x + b^+ a^{(+1)}\phi_x + b^- a\phi_{\bar{x}} - d\phi, \tag{34}$$

where

$$\begin{aligned} b^\pm &= \tilde{r}^\pm(x, t), & a &= k(x - 0.5h, t), \\ d &= q(x, t), & a_i^{(+1)} &= a_{i+1}, \\ r^\pm &= \frac{r \pm |r|}{2}, & \tilde{r}^\pm &= \frac{r^\pm}{k}, & \phi_{\bar{x}} &= \frac{\phi_i - \phi_{i-1}}{h}, \\ \phi_x &= \frac{\phi_{i+1} - \phi_i}{h}. \end{aligned}$$

Next, the problem 31 is replaced by the difference scheme

$$\begin{aligned} c(x, \bar{t})\phi_t &= \tilde{\Lambda}(\bar{t})\hat{\phi} + f, & \bar{t} &= t + \tau/2, \\ \phi(0, t) &= \mu_1(t), & \phi(1, t) &= \mu_2(t), \\ \phi(x, 0) &= \varphi_0(x). \end{aligned} \tag{35}$$

This scheme has a truncation error of order $O(h^2 + \tau)$ and is monotone. In this aspect, the Crank–Nicolson difference scheme for the problem 31 is not better than Eq. 35 although it is of order $O(h^2 + \tau^2)$ because the Crank–Nicolson method is monotone only if

$$\frac{\tau}{h^2} \leq \frac{1}{2 \min k + h \max |r|}.$$

The same conclusion holds for the so-called *optimal weighting scheme* of Wang and Lacroix [27].

If instead of a Dirichlet boundary condition there are Robin boundary conditions posed at the endpoints, for example,

$$\left(\alpha\varphi + \frac{\partial\varphi}{\partial x}\right)(1, t) = \mu_2(t),$$

then by using the difference boundary condition

$$\alpha\phi_N + \frac{\phi_{N+1} - \phi_{N-1}}{2h} = \mu_2,$$

we obtain a monotone difference scheme for the corresponding differential problem.

Now, we consider the two-dimensional main problems 1, 5, 6, and 7. For simplicity, we suppose that the domain D is a parallelepiped $[0, X] \times [0, Y]$. In order to construct a difference scheme for this main problem, we rewrite the equation in a convenient form

$$\frac{\partial\varphi}{\partial t} - (L_1 + L_2)\varphi = f \quad \text{in } D \times (0, T], \tag{36}$$

where

$$\begin{aligned} L_1\varphi &= \frac{\partial}{\partial x} \left(\mu \frac{\partial\varphi}{\partial x} \right) - u \frac{\partial\varphi}{\partial x}, \\ L_2\varphi &= \frac{\partial}{\partial y} \left(\mu \frac{\partial\varphi}{\partial y} \right) - v \frac{\partial\varphi}{\partial y} - \sigma\varphi. \end{aligned} \tag{37}$$

We employ on the domain D the uniform grid $D_h = \{x_i = ih_1, y_j = jh_2\}$ and approximate the above differential operators (Eq. 37) by the following monotone difference operators

$$\begin{aligned} \tilde{\Lambda}_1\phi &= \chi^{(x)}\mu\phi_{\bar{x}x} - u\phi_{\bar{x}}, \\ \tilde{\Lambda}_2\phi &= \chi^{(y)}\mu\phi_{\bar{y}y} - v\phi_{\bar{y}} - \sigma\phi, \end{aligned}$$

where

$$\begin{aligned} \chi^{(x)} &= \frac{1}{1 + R^{(x)}}, & R^{(x)} &= \frac{h_1 u}{2\mu}, \\ \chi^{(y)} &= \frac{1}{1 + R^{(y)}}, & R^{(y)} &= \frac{h_2 v}{2\mu}. \end{aligned}$$

Here, for simplicity, we assume that $\mu = \text{const.}$. Now we write the difference scheme for the Eq. 36 with the boundary conditions for the case that the wind velocity is directed from west-south. In this case, the part of boundary S^+ is the right and the top sides of the rectangle D , and the part S^- is the other sides of D .

$$\begin{aligned} \frac{\phi^{l+1/2} - \phi^l}{\tau} - \tilde{\Lambda}_1\phi^{l+1/2} &= 0, \\ \mu \frac{\phi_1^{l+1/2} - \phi_{-1}^{l+1/2}}{2h_1} - U_n\phi_0^{l+1/2} &= 0, \\ \phi_{I+1}^{l+1/2} - \phi_{I-1}^{l+1/2} &= 0, \\ \frac{\phi^{l+1} - \phi^{l+1/2}}{\tau} - \tilde{\Lambda}_2\phi^{l+1} &= f^{l+1}, \\ \mu \frac{\phi_1^{l+1} - \phi_{-1}^{l+1}}{2h_2} - U_n\phi_0^{l+1} &= 0, \\ \phi_{J+1}^{l+1} - \phi_{J-1}^{l+1} &= 0, \\ l &= 0, 1, \dots \end{aligned} \tag{38}$$

Here, for brevity, we write only one space index for the computation direction, omitting other index, for example ϕ_l stands for ϕ_{Ij} .

Due to the monotonicity of each component difference scheme in Eq. 38, it is possible to prove the positiveness of the solution of Eq. 38, its stability, and the convergence order $O(h^2 + \tau)$.

Let us remark that in practice the two-dimensional continuity Eq. 3 may be not satisfied although for

incompressible fluid the three-dimensional continuity equation

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0$$

always is valid. Moreover, due to the fact that in the surface layer of sea the vertical component of velocity of flow decreases with the depth $\partial w/\partial z \leq 0$, then

$$\xi = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \geq 0.$$

In this case, the term $\xi\varphi$ will be added to the left side of the main Eq. 4, and a corresponding term will be added to the difference scheme with the conservation of all properties.

5 A Method for the Identification of Location and Time of Oil Emission

Suppose that at some observation time T_d an oil pollution plume Ω is detected. The problem is to identify the location of the source of the oil plume and the time of the emission of oil. Here we assume that the pollution plume is generated by an accident from tanker traffic. To the authors' knowledge, the research of mathematical methods for this kind of problem are not published in literature although similar problems for groundwater pollution is intensively studied (see, e.g., [14] and the references therein). In [14] following the adjoint approach of Neupauer and Wilson [15] and in the terminology of location probability density function, the authors proposed a method for solving the groundwater pollution problem based on a *fundamental property* of the forward and backward location probability density functions, which is not proved analytically. The same method is also used in [3] for the identification of contaminant point source in surface waters although the authors of this work do not refer to [14].

It should be mentioned that all the authors of the three above-mentioned papers only proposed method for solving the problem from technical point of view, and a rigorous mathematical justification is absent there. Differently from these works, in this paper we propose a method for simultaneous identification of a single point-source location and time of oil emission, which is based on the above established relation 28.

Suppose that at the accident time t_0 from the location r_0 an oil emission with the power Q happened and at the observation time T_d an oil plume Ω is detected. Let the oil concentration in the pollution plume be denoted by $\varphi(r, T_d)$. It is, of course, the solution, evaluated at this time, of the main problems 1, 5, 6, and 7 with

$f(r, t)$ defined by Eq. 25. Now, let us take any k points r_1, \dots, r_k in the plume Ω and consider the adjoint problems 21–24 with

$$P(r, \tau) = Q\delta(r - r_i)\delta(\tau - (T - T_d)). \quad (39)$$

Then, by Eq. 28, we have

$$\phi_{r_i}^*(r_0, \tau_0) = \varphi(r_i, T_d), \quad (40)$$

where we supply ϕ^* with the subscript r_i in order to indicate that it depends on r_i due to the right-hand side of the adjoint equation given in the form (Eq. 39). Now, setting

$$\varphi(r_i, T_d) = C_i \quad i = 1, \dots, k \quad (41)$$

we obtain the following:

Proposition 2 All iso-contours $\phi_{r_i}^*(r, \tau_0) = C_i$, $i = 1, \dots, k$ intersect at the point r_0 .

This proposition immediately follows from the relations 40 and 41.

Proposition 3 Let r_{\max} be the point in the pollution plume with maximal concentration, i.e.,

$$\varphi(r_{\max}, T_d) = \max_{r \in \Omega} \varphi(r, T_d).$$

Then, the iso-contour

$$\phi_{r_{\max}}^*(r, \tau_0) = \varphi(r_{\max}, T_d)$$

shrinks to a point r_0 .

Proof Each point in the pollution plume corresponds to a contour $\phi_{r_i}^*(r, \tau_0) = \varphi(r_i, T_d)$, and due to the fact that oil spills and is transported from the point sources, then the contour corresponding to r_i with the greater concentration will be smaller. Therefore, the contour $\phi_{r_{\max}}^*(r, \tau_0) = \varphi(r_{\max}, T_d)$ corresponding to the point r_{\max} with maximal concentration is the smallest, i.e., is a point. This point is r_0 because as was pointed in the previous proposition, the contour passes r_0 . Thus, the proposition is proved. \square

Except for the relations between the solution of the main and the adjoint problems established above, we shall deduce below a property of the solution of the adjoint problem, which is also useful for identification of location and time of an accident in the case if the mass of oil is conserved in the process of propagation.

For this purpose, we use the adjoint problems 16–19 with the right-hand side

$$p(r, t) = \delta(T_d - t) \mathbf{1}_\Omega(r)$$

or the problems 21–24 with

$$P(r, \tau) = \delta(\tau - (T - T_d)) \mathbf{1}_\Omega(r),$$

where $\mathbf{1}_\Omega(r)$ is the indicator or characteristic function of the set Ω , i.e.,

$$\mathbf{1}_\Omega(r) = \begin{cases} 1 & \text{if } r \in \Omega, \\ 0 & \text{if } r \notin \Omega. \end{cases}$$

Proposition 4 *For the solution of the adjoint problem with the above right-hand side, there holds the equality*

$$\phi^*(r_0, \tau_0) = 1. \tag{42}$$

Proof Let $\varphi(r, t)$ be the solution of the main problem with the right-hand side given by Eq. 25. Then as in the Proposition 1, we have

$$(L\varphi, \varphi^*) = Q\varphi^*(r_0, t_0).$$

Meanwhile, we have in the new context

$$\begin{aligned} (L^*\varphi^*, \varphi) &= (p, \varphi) = \int_0^T \int_D \delta(T_d - t) \mathbf{1}_\Omega(r) \varphi(r, t) \\ &\quad \times dr dt = \int_\Omega \varphi(r, T_d) dr. \end{aligned} \tag{43}$$

Therefore, taking into account that the mass of oil is conserved, i.e.,

$$\int_\Omega \varphi(r, T_d) dr = Q$$

from the Lagrange identity, we get $\varphi^*(r_0, t_0) = 1$ as the same as the required equality. \square

The above proposition gives a very general relation that the source location and the backward time of an accident must satisfy. Therefore, it can be used for predicting the possible area and time, where an accident may be happened if a oil slick is detected and no information of the pollution plume has not collected yet.

In the case if some concrete information of the pollution plume is known, we propose a method for finding the location and the time of emission with the use of Propositions 2 and 3. Here we assume that by monitoring the pollution plume the total oil in the

plume Q can be estimated, e.g., by using a *modified Fay-type spreading formula* [9, 11].

In the case if the center r_{\max} of the pollution plume is found and the concentration C_{\max} of oil at this point at the detected time T_d is known, then it suffices to solve only one adjoint problem 21–24 with the right-hand side

$$P(r, \tau) = Q \delta(r - r_{\max}) (\tau - (T - T_d)).$$

At each time τ_j after finding $\phi_{r_{\max}}^*(r, \tau_j)$, we plot the contour

$$\phi_{r_{\max}}^*(r, \tau_j) = C_{\max}$$

until the contour shrinks to a point. Due to Proposition 3, this point is the location r_0 and the corresponding time is the sought accident time τ_0 .

Next we consider the situation when it is difficult to determine the center r_{\max} of the pollution plume, and instead of this, we know the oil concentration C_i at the three points r_i , ($i = 1, 2, 3$) in the observed pollution plume. In this case, we have to solve three adjoint problems (21)–(24) with the right-hand side

$$P(r, \tau) = Q \delta(r - r_i) (\tau - (T - T_d)).$$

At each time τ_j after finding $\phi_{r_i}^*(r, \tau_j)$, we plot the contours

$$\phi_{r_i}^*(r, \tau_j) = C_i$$

until the three contours will intersect in a point. Due to Proposition 2, this point is the sought accident location r_0 , and the corresponding accident time is τ_0 .

6 Numerical Results

Below we show the simulation results for an example for demonstrating the effectiveness of the above stated method. The domain of the problem is the east sea offshore of the south of central part of Vietnam from the longitude 108° E to 112° E and latitude 10° N to 14° N. Let a source of oil emission located at 113° E, 13° N with the power $Q = 10,000$ kg. The solution of the main problem with known flow starting from 06:00 01th April 2011 is given in Fig. 1. Here we take the diffusivity $\mu = 3$ m²/s, the space grid of 201 × 201 nodes, and the time step $\tau = 300$ s.

First, suppose that we detect the pollution plume as depicted in Fig. 1 without any concrete information

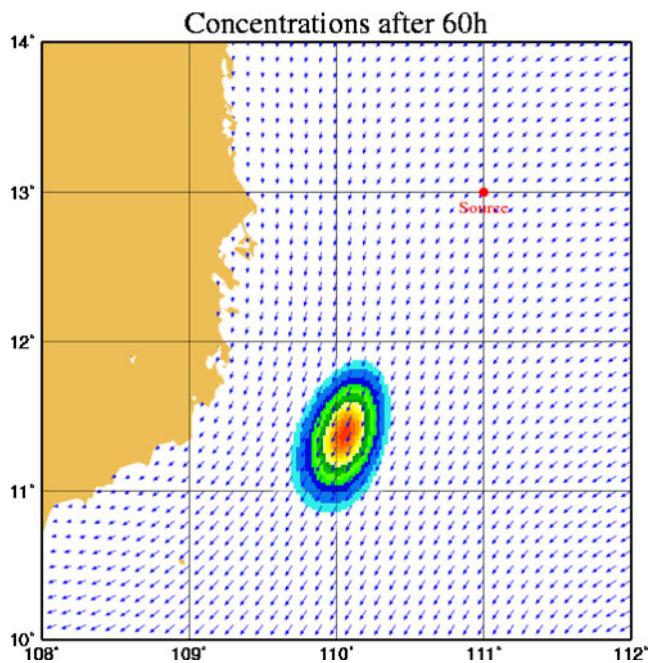


Fig. 1 Solution of the main problem with diffusivity $\mu_1 = 3 \text{ m}^2/\text{s}$ after 60 h

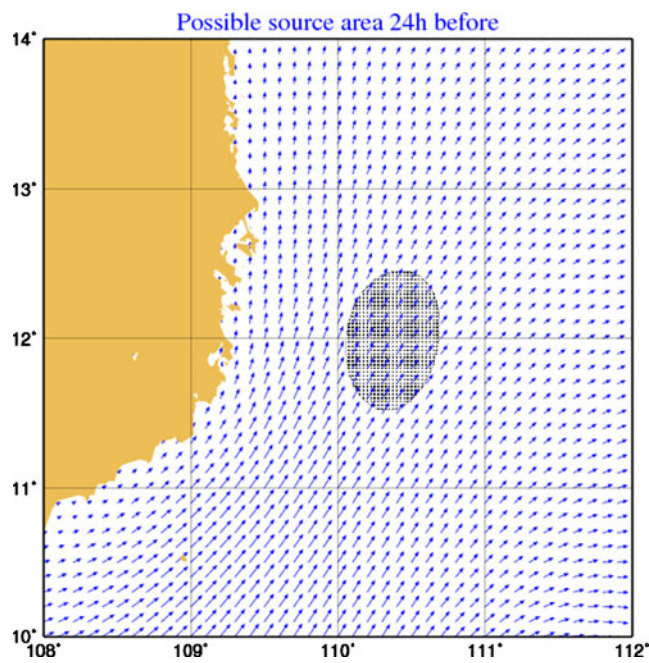


Fig. 3 Possible area of source 24 h before detection

about concentration. Then using Proposition 4, we can predict the possible area of a source location before some time. Figures 2, 3, 4, and 5 show the possible area of a source location before 12, 24, 42, and 60 h before the moment of detection. From Fig. 5, we see that the

predicted possible area of a source location before 60 h is an area that is not large and that contains the actual source location.

In order to demonstrate the effectiveness of the method for identification of the location and the time of the accident when some concrete information of the

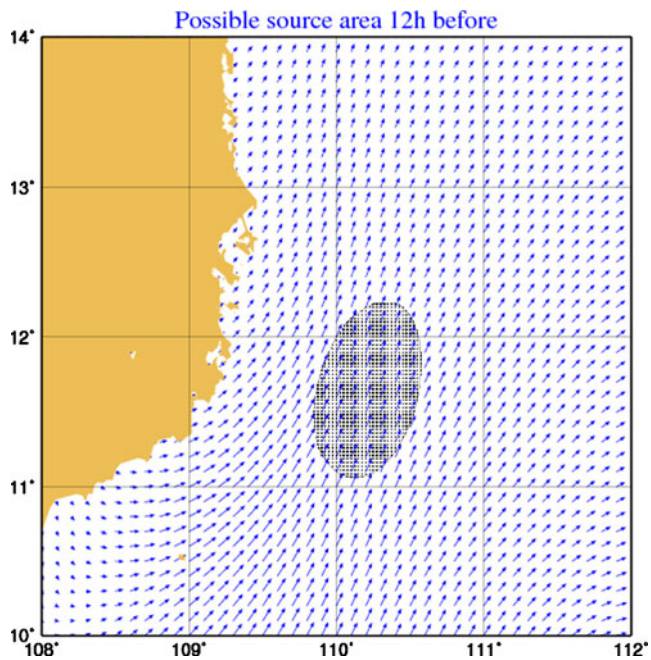


Fig. 2 Possible area of source 12 h before detection

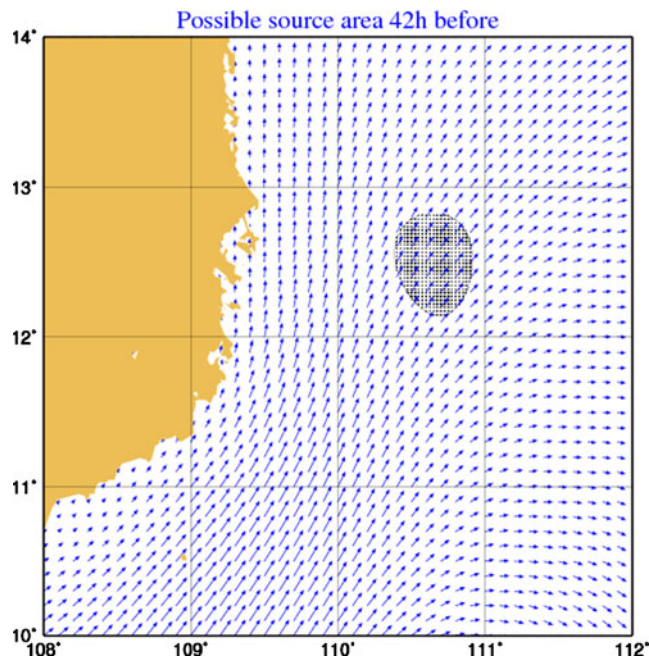


Fig. 4 Possible area of source 42 h before detection

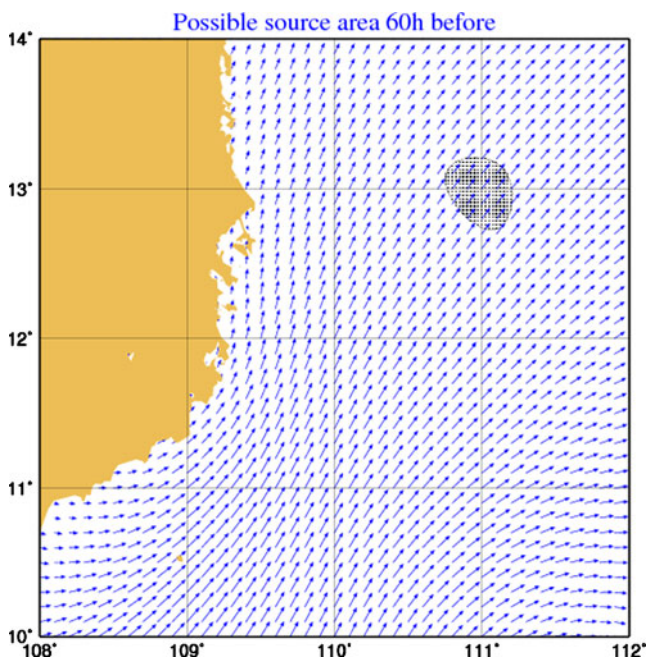


Fig. 5 Possible area of source 60 h before detection

pollution plume is known, we perform the following steps:

1. Take the center of the pollution plume as S_1 , and take 4 other points: S_2 left, S_3 right, S_4 below and S_5 upper S_1 by 0.002° . The color of $S_1, S_2, S_3,$

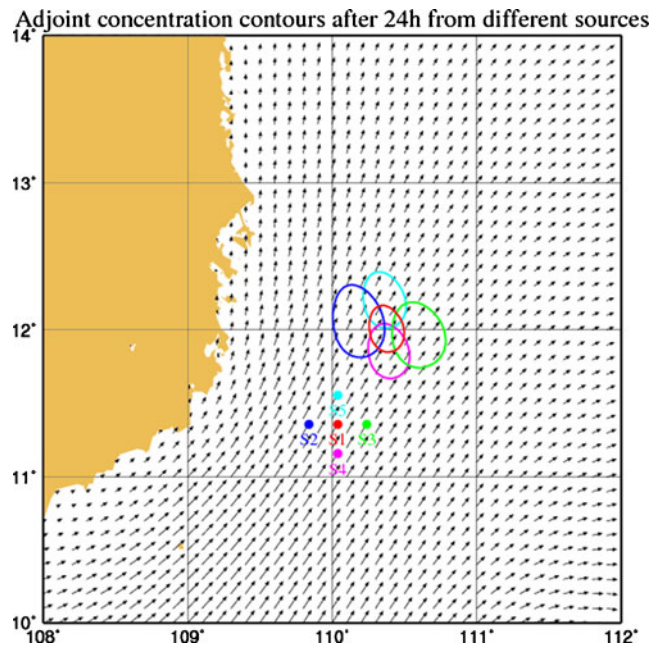


Fig. 7 Contours $\phi_{S_i}^*(r, \tau_j) = \varphi(S_i, T_d)$ for $\tau_j = 24$ h

$S_4,$ and S_5 are red, blue, green, magenta, and cyan, respectively.

2. Calculate values of the concentration at these points at the time of observation $T_d = 60$ h from the main problem, i.e., $\varphi(S_i, T_d)$. They are 24.715, 6.503, 7.404, 16.542, and 15.420 kg/m^3 , respectively.
3. Solve the adjoint problems for $r_1 = S_i$.

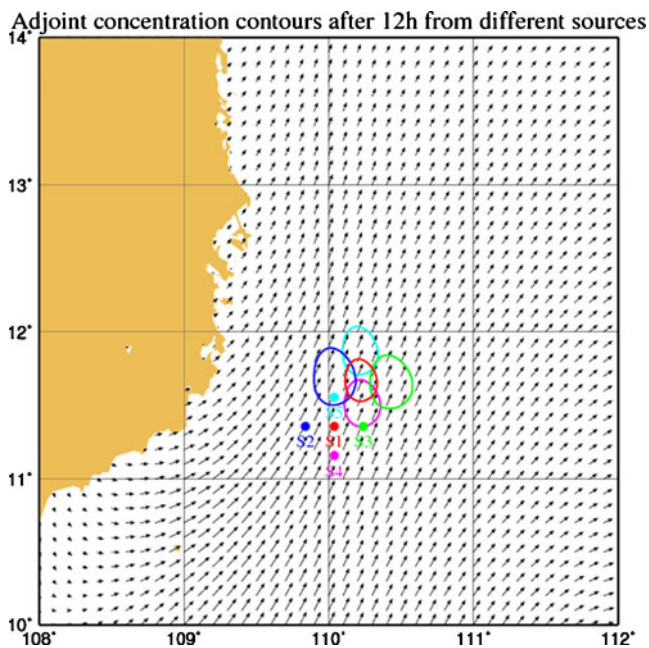


Fig. 6 Contours $\phi_{S_i}^*(r, \tau_j) = \varphi(S_i, T_d)$ for $\tau_j = 12$ h

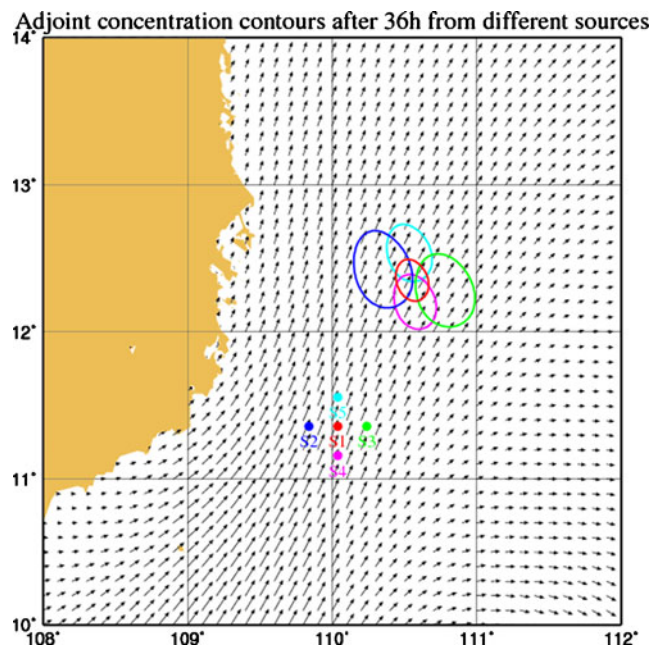


Fig. 8 Contours $\phi_{S_i}^*(r, \tau_j) = \varphi(S_i, T_d)$ for $\tau_j = 36$ h

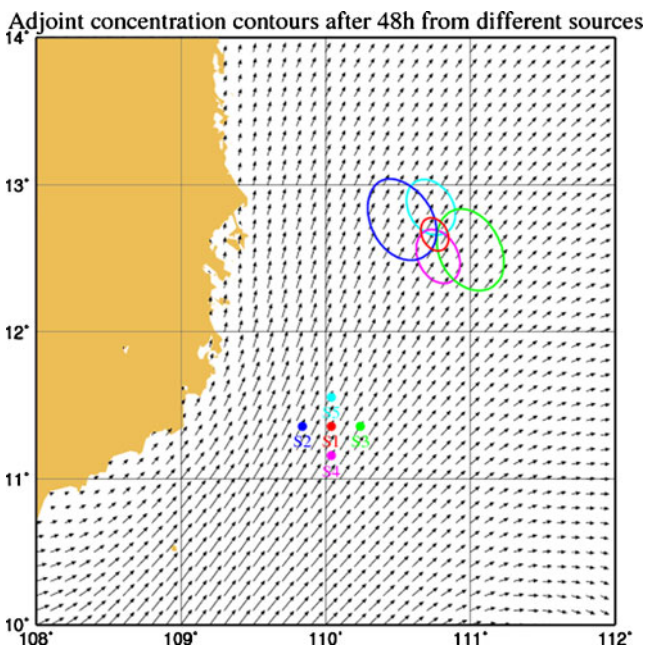


Fig. 9 Contours $\phi_{S_i}^*(r, \tau_j) = \varphi(S_i, T_d)$ for $\tau_j = 48$ h

- Plot contours $\phi_{r_i}^*(r, \tau_j) = \varphi(r_i, T_d)$, for $\tau_j = 6, 12, \dots, 60$ h, where $\varphi(r, t)$ is the solution of the main (forward) problem.

Figures 6, 7, 8, 9, and 10 show the contours for $\tau_j = 12, 24, 36, 48, 60$ h. The colors of the contours are the same of the corresponding source points S_i .

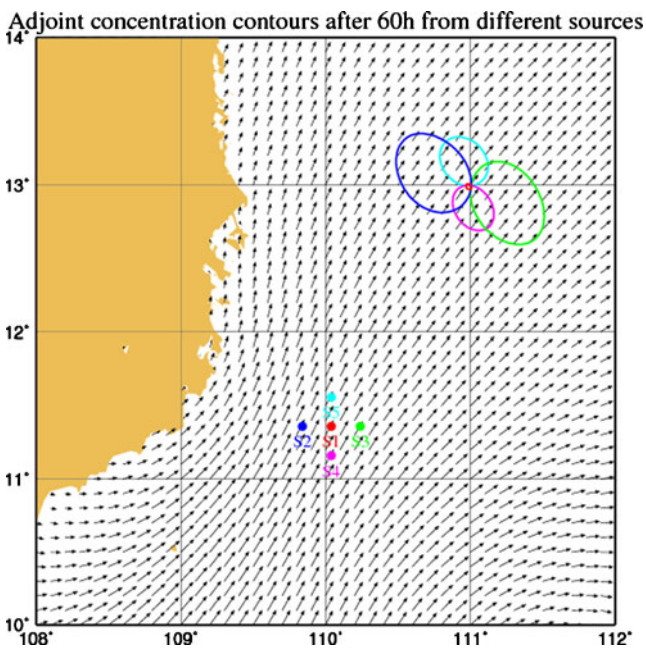


Fig. 10 Contours $\phi_{S_i}^*(r, \tau_j) = \varphi(S_i, T_d)$ for $\tau_j = 60$ h

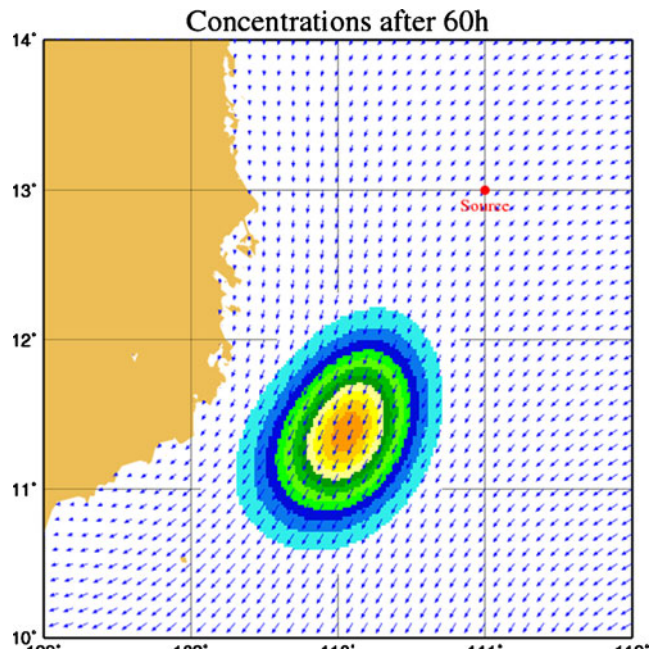


Fig. 11 Solution of the main problem with diffusivity $\mu_2 = 3,000 \text{ m}^2/\text{s}$ after 60 h

From the figures, we see that after 60 h the contour corresponding to S_1 shrinks to one single point, which is the source in the main problem, and all other contours intersect in this point, i.e., the results of simulations completely confirm the theoretical results of the previous section.

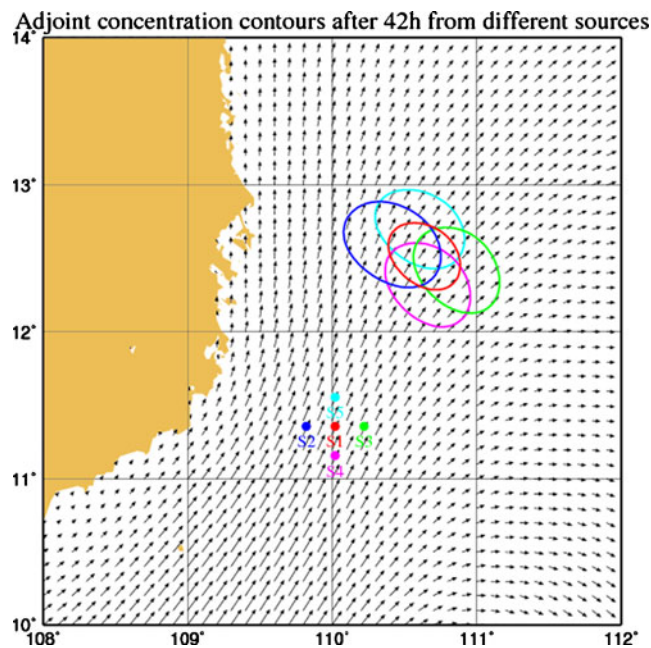


Fig. 12 Contours $\phi_{S_i}^*(r, \tau_j) = \varphi(S_i, T_d)$ for $\tau_j = 42$ h for μ_2

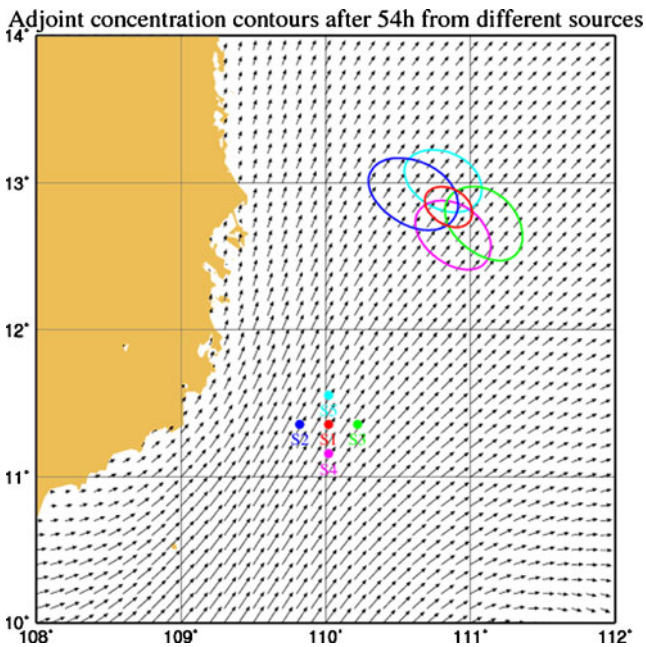


Fig. 13 Contours $\phi_{S_i}^*(r, \tau_j) = \varphi(S_i, T_d)$ for $\tau_j = 54$ h for μ_2

Below we present the results of a simulation when the diffusivity is very large $\mu_2 = 3,000 \text{ m}^2/\text{s}$. It is not real diffusivity but we perform the simulations only for the purpose of verification of effectiveness of our proposed method. The concentration distribution of oil after 60 h

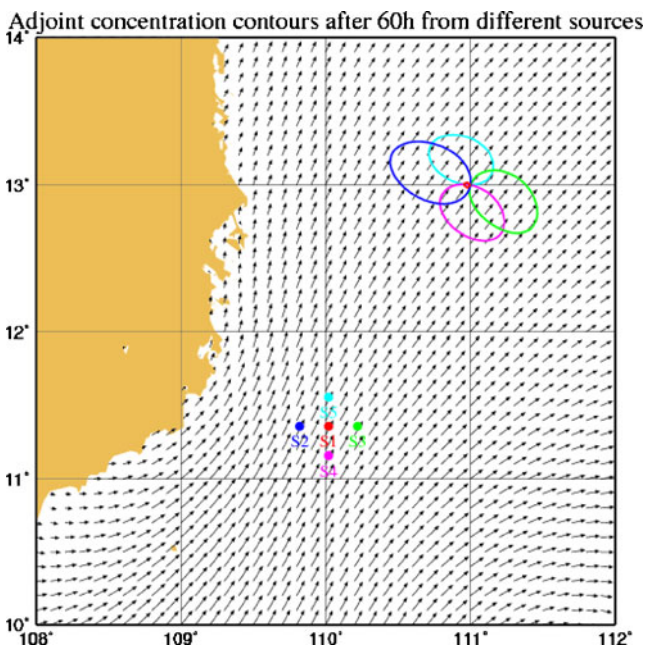


Fig. 14 Contours $\phi_{S_i}^*(r, \tau_j) = \varphi(S_i, T_d)$ for $\tau_j = 60$ h for μ_2

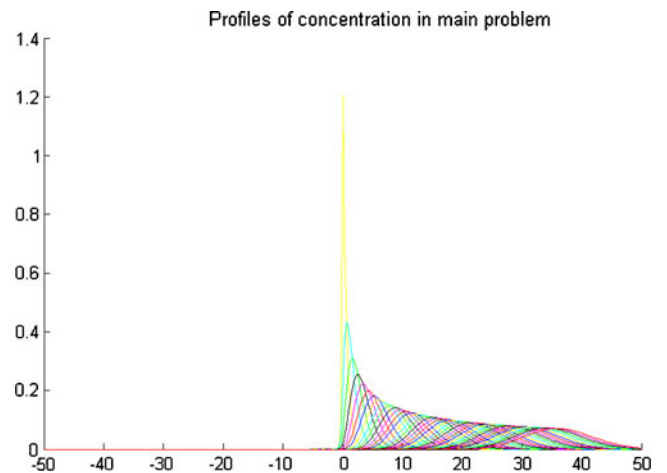


Fig. 15 Profiles of concentration caused by a source at $x = 0$

is depicted in Fig. 11, and the contours after 42, 54, and 60 h are given in Figs. 12, 13, and 14.

7 Remark on 1D Case

Now we illustrate the idea and results obtained in the 2D model by an 1D advection–diffusion equation, when we consider on the domain $(a, b) \times (0, T)$ the equation

$$L\varphi \equiv \frac{\partial \varphi}{\partial t} + \frac{\partial}{\partial x} (U\varphi) + \sigma\varphi - \mu \frac{\partial}{\partial x} \left(\mu \frac{\partial \varphi}{\partial x} \right) = f(x, t)$$

$$\varphi = 0, \quad t = 0,$$

$$\varphi = 0, \quad x = a, \quad \frac{\partial \varphi}{\partial x} = 0, \quad x = b$$

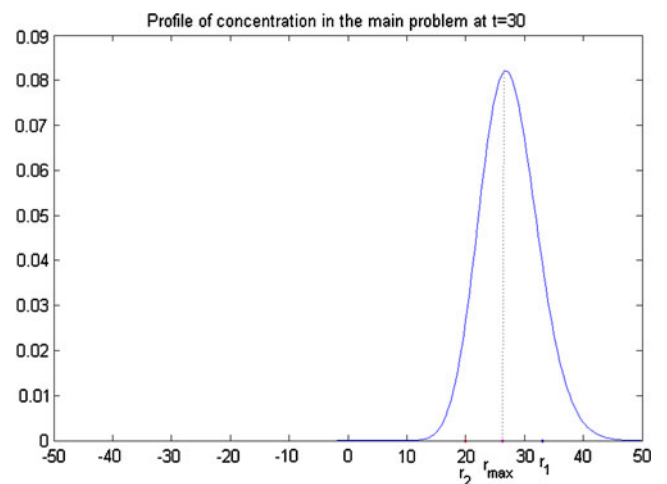


Fig. 16 Profile of concentration at the moment $t = 30$

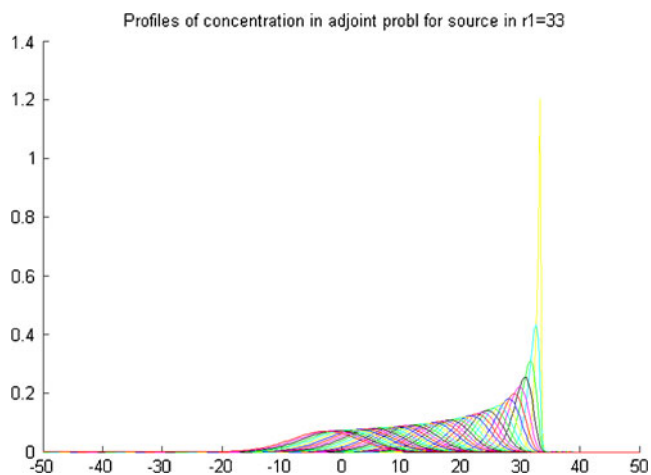


Fig. 17 Profile of concentration in adjoint mode for the source at r_1

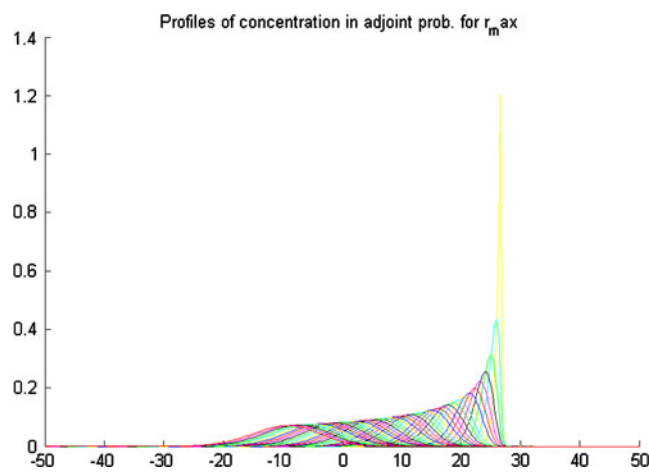


Fig. 19 Profile of concentration in adjoint mode for the source at r_{max}

under the assumption that the velocity is axially directed. In this, the adjoint problem in backward time for the above main problem has the form

$$L_-^* \phi^* \equiv \frac{\partial \phi^*}{\partial \tau} - U \frac{\partial \phi^*}{\partial x} + \sigma \phi^* - \mu \frac{\partial}{\partial x} \left(\mu \frac{\partial \phi^*}{\partial x} \right) = P(x, \tau)$$

$$\phi^* = 0, \quad \tau = 0,$$

$$\phi^* = 0, \quad x = a, \quad U \phi^* + \mu \frac{\partial \phi^*}{\partial x} = 0, \quad x = b.$$

By solving the main problem for the right-hand side $f(x, t) = \delta(x)\delta(t)$ on the interval $[-50, 50]$ with the diffusion coefficient $\mu = 0.1$, the velocity $u = 0.9$, space grid of 301 nodes, and time step $\Delta t = 0.5$, we obtain the profiles of concentration of substance caused by a point instantaneous source of the unit power located at $x = 0$,

which are depicted in Fig. 15. At the moment $t = 30$, the profile of concentration is given in Fig. 16.

On this Fig. 16, we see that the point with the maximal concentration is located at $r_{max} = 26.3$. Take two other points $r_1 = 33$ and $r_2 = 20$. The concentration at these points are 0.0817, 0.0395, and 0.0266, respectively. Now, putting the unit source at these points and solve the corresponding adjoint problems, we obtain the profiles of concentration as depicted in Figs. 17, 18, and 19.

In the 1D case, the contours $\phi_{r_i}^*(x, 30) = C_i$, where $C_i = \varphi(r_i, 30)$ are the abscissa of the points of intersection of the line $y = C_i$ and the profiles $y = \phi_{r_i}^*(x, 30)$. From the Fig. 20, we see that these contours meet at $x = 0$.

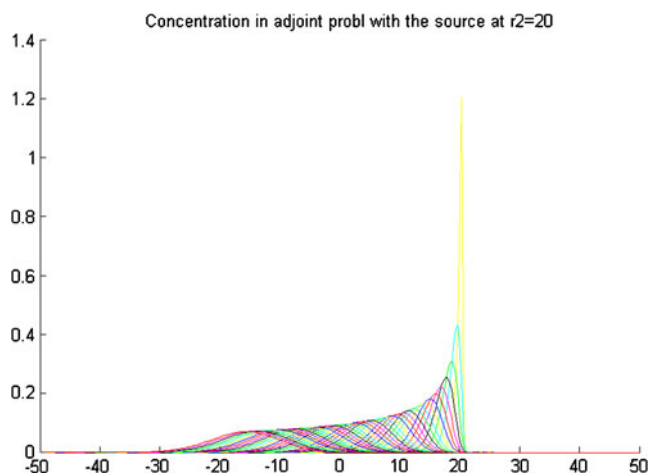


Fig. 18 Profile of concentration in adjoint mode for the source at r_2

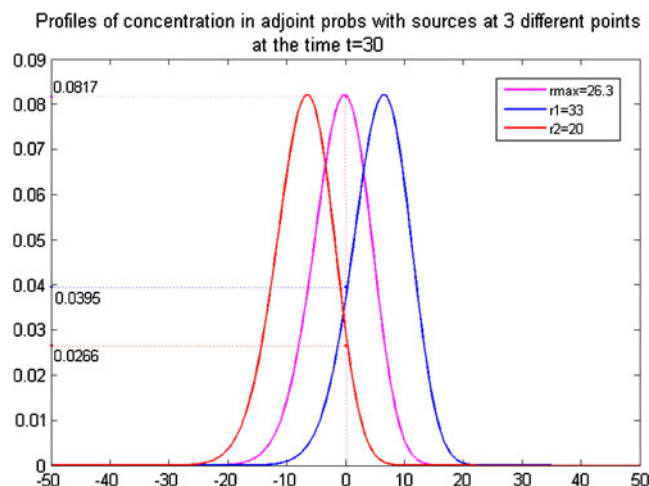


Fig. 20 Contours $\phi_{r_i}^*(x, 30) = C_i$ meet at $x = 0$

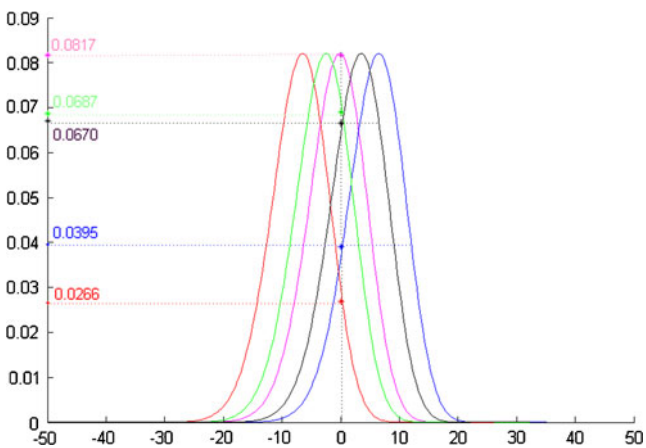


Fig. 21 Contours $\phi_{r_i}^*(x, 30) = C_i$ meet at $x = 0$

In addition to these three points, we take now the two points $r_3 = 24$, $r_4 = 30$ and plot the profiles $y = \phi_{r_i}^*(x, 30)$ for all five points $r_1, r_2, r_{\max}, r_3, r_4$ and define the contours $\phi_{r_i}^*(x, 30) = C_i = \varphi(r_i, 30)$ (see Fig. 21).

Once again we see that these contours meet at $x = 0$, which is the source location in the main problem. Thus, all results that are proved and demonstrated in the 2D case are verified in the 1D case.

8 Conclusion and Outlook

In this work, we considered a mathematical model of oil spill resulting from a tanker traffic accident and its numerical solution. For solving the problem of identification of the source of oil pollution, we use adjoint method. A fundamental equality between the solutions of the main and the adjoint problems was proved, and based on it, a method for the identification problem was proposed. Some numerical simulations demonstrated the effectiveness of the method.

Future research directions will include error analysis of the method and applicability of the method in the case of incomplete information of the total power of the source of emission. The case of non-instantaneous source also will be investigated.

Moreover, we will improve the coastline boundary conditions by including the shoreline interaction. Since only a certain maximum volume of oil can be deposited at the shoreline, we have consider different types of coastlines, cf. [18]

Acknowledgements This first two authors were supported partially by the bilateral German–Vietnamese project *OILPOLL*:

Mathematical Modelling and Numerical Algorithms for Simulation of Oil Pollution, financed by the International Buro of the BMBF. The third author was supported by the Vietnam National Foundation for Science and Technology Development (NAFOSTED).

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