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Simulation of Oil Pollution**

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# Mathematical Modelling and Numerical Algorithms for Simulation of Oil Pollution

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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.

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**Key words:** oil transport problems, oil spilling, weathering, adjoint equation approach, pollution source identification

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## 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 [26]. 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

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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 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

$$L\varphi \equiv \frac{\partial \varphi}{\partial t} + \operatorname{div}(\mathbf{U}\varphi) + \sigma\varphi - \nabla \cdot \mu \nabla \varphi = f(r, t), \quad r \in D, \quad t \in (0, T), \quad (2.1)$$

with the emission forcing function

$$f(r, t) = F(t) \delta(r - r_0), \quad (2.2)$$

where  $\mu(r, t)$  is the diffusion coefficient,  $\nabla$  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*

$$\nabla \cdot \mathbf{U} = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0, \quad (2.3)$$

the advection-diffusion equation (2.1) is often written in the form [23]

$$\frac{\partial \varphi}{\partial t} + \mathbf{U} \cdot \nabla \varphi + \sigma \varphi - \nabla \cdot \mu \nabla \varphi = f(r, t), \quad r \in D, \quad t \in (0, T). \quad (2.4)$$

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

$$\varphi(r, 0) = 0, \quad r \in D. \quad (2.5)$$

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 (2.1) are

$$\mu \frac{\partial \varphi}{\partial n} - U_n \varphi = 0 \quad \text{at inflow boundary / coastline } S^-, \quad (2.6)$$

$$\mu \frac{\partial \varphi}{\partial n} = 0 \quad \text{at outflow boundary } S^+. \quad (2.7)$$

By (2.6), 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 (2.7) 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 (2.6) is reduced to  $\varphi = 0$  (there is no oil on the inflow boundary), while (2.7) 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].

**Remark 2.1.** *We note that condition (2.7) 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 equations (2.6) and (2.7) 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 (2.6)–(2.7), reads

$$\varphi = 0 \quad \text{at } S^-, \quad (2.8)$$

$$\frac{\partial \varphi}{\partial n} = 0 \quad \text{at } S_1^+, \quad \frac{\partial \varphi}{\partial n} = \alpha \varphi \quad \text{at } S_2^+, \quad (2.9)$$

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 (2.1) in space gives

$$\frac{\partial}{\partial t} \int_D \phi \, dr - \int_D \nabla U \cdot \phi \, dr + \int_D \sigma \phi \, dr - \int_S \left( \mu \frac{\partial}{\partial n} \phi - U_n \phi \right) dS = F(t), \quad (2.10)$$

and using the inflow and outflow conditions (2.6) and (2.7) we see that any solution of problem (2.1)–(2.7) satisfies the *oil balance equation*

$$\frac{\partial}{\partial t} \int_D \phi \, dr = F(t) + \int_D \nabla \cdot U \phi \, dr - \int_D \sigma \phi \, dr - \int_{S^+} U_n \phi \, dS, \quad (2.11)$$

that reduces to

$$\frac{\partial}{\partial t} \int_D \phi \, dr = F(t) - \int_D \sigma \phi \, dr - \int_{S^+} U_n \phi \, dS. \quad (2.12)$$

if the continuity equation (2.3) is fulfilled. Equation (2.12) describes the time evolution of the *total pollution concentration*  $\int_D \phi \, dr$  that increases due to the emission  $F > 0$ , see (2.2), 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  $\phi$  we multiply (2.1) by  $2\phi$  and integrate again

$$\begin{aligned} \frac{\partial}{\partial t} \int_D \phi^2 \, dr - \int_D \nabla \cdot U \phi^2 \, dr + 2 \int_D (\sigma \phi^2 + \mu |\nabla \phi|^2) \, dr \\ - \int_S (2\phi \mu \frac{\partial}{\partial n} \phi - U_n \phi^2) \, dS = 2F(t)\phi(r_0, t), \end{aligned} \quad (2.13)$$

and with the boundary conditions (2.6) and (2.7) we obtain the integral equation

$$\begin{aligned} \frac{\partial}{\partial t} \int_D \phi^2 \, dr - \int_D \nabla \cdot U \phi^2 \, dr + 2 \int_D (\sigma \phi^2 + \mu |\nabla \phi|^2) \, dr \\ + \int_{S^+} U_n \phi^2 \, dS - \int_{S^-} U_n \phi^2 \, dS = 2F(t)\phi(r_0, t). \end{aligned} \quad (2.14)$$

Finally, if the continuity equation (2.3) is fulfilled (2.14) reduces to

$$\begin{aligned} \frac{\partial}{\partial t} \int_D \phi^2 \, dr + 2 \int_D (\sigma \phi^2 + \mu |\nabla \phi|^2) \, dr \\ + \int_{S^+} U_n \phi^2 \, dS - \int_{S^-} U_n \phi^2 \, dS = 2F(t)\phi(r_0, t), \end{aligned} \quad (2.15)$$

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. 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 problem (2.1), (2.5), (2.6) and (2.7) in the domain  $D$  and the time interval  $(0, T)$  can be written as

$$L^* \varphi^* \equiv -\frac{\partial \varphi^*}{\partial t} - \mathbf{U} \cdot \nabla \phi^* + \sigma \phi^* - \nabla \cdot \mu \nabla \phi^* = p(r, t), \quad (3.1)$$

$$\varphi^*(r, T) = 0, \quad (3.2)$$

$$\mu \frac{\partial \varphi^*}{\partial n} + U_n \varphi^* = 0 \quad \text{at } S^-, \quad (3.3)$$

$$\mu \frac{\partial \varphi^*}{\partial n} = 0 \quad \text{at } S^-. \quad (3.4)$$

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

$$(L\varphi, \varphi^*) = (L^*\varphi^*, \varphi), \quad (3.5)$$

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  $\varphi^*(r, T - \tau) = \Phi^*(r, \tau)$ ,  $p(r, T - \tau) = P(r, \tau)$ . Then the adjoint problem becomes

$$L_-^* \phi^* \equiv \frac{\partial \phi^*}{\partial \tau} - \mathbf{U} \cdot \nabla \phi^* - \nabla \cdot \mu \nabla \phi^* + \sigma \phi^* = P(r, \tau), \quad (3.6)$$

$$\phi^* = 0 \quad \text{at } \tau = 0, \quad (3.7)$$

$$\mu \frac{\partial \phi^*}{\partial n} - (-U_n) \phi^* = 0 \quad \text{on } S^+ \quad (\text{inflow for } -\mathbf{U}), \quad (3.8)$$

$$\mu \frac{\partial \phi^*}{\partial n} = 0 \quad \text{on } S^- \quad (\text{outflow for } -\mathbf{U}), \quad (3.9)$$

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

$$f(r, t) = Q \delta(r - r_0) \delta(t - t_0), \quad (3.10)$$

$$p(r, t) = Q \delta(r - r_1) \delta(T_d - t), \quad (3.11)$$

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 3.1.** *For the solution of the main problem and the adjoint problem there holds the relation*

$$\phi^*(r_0, T - t_0) = \varphi(r_1, T_d), \quad (3.12)$$

or

$$\phi^*(r_0, \tau_0) = \varphi(r_1, T_d). \quad (3.13)$$

*Proof.* Indeed, we have

$$(L\varphi, \varphi^*) = (f, \varphi^*) = \int_0^T \int_D Q \delta(r - r_0) \delta(t - t_0) \varphi^*(r, t) dr dt = Q \varphi^*(r_0, t_0), \quad (3.14)$$

$$(L^*\varphi, \varphi) = (p, \varphi) = \int_0^T \int_D Q \delta(r - r_1) \delta(T_d - t) \varphi(r, t) dr dt = Q \varphi(r_1, T_d). \quad (3.15)$$

Then from the Lagrange equality (3.5) it follows

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

This is the same as (3.12) or (3.13).

#### 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 [27] 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*

$$\begin{aligned} c(x, t) \frac{\partial \varphi}{\partial t} &= L\varphi + f(x, t), & 0 < x < 1, & \quad 0 < t \leq T, \\ \varphi(0, t) &= \mu_1(t), & \varphi(1, t) &= \mu_2(t), \\ \varphi(x, 0) &= \varphi_0(x), \end{aligned} \quad (4.1)$$

where

$$\begin{aligned} L\varphi &= \frac{\partial}{\partial x} \left( k(x, t) \frac{\partial \varphi}{\partial x} \right) + r(x, t) \frac{\partial \varphi}{\partial x} - q(x, t)\varphi, \\ 0 < c_1 \leq k(x, t) \leq c_2, \quad c(x, t) \geq c_1, \quad q(x, t) \geq 0. \end{aligned} \quad (4.2)$$

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

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

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

$$\tilde{L}\varphi = \chi \frac{\partial}{\partial x} \left( k(x, t) \frac{\partial \varphi}{\partial x} \right) + r(x, t) \frac{\partial \varphi}{\partial x} - q(x, t)\varphi, \quad (4.3)$$

where  $\chi = 1/(1 + R)$ ,  $R = 0.5h|r|/k$  and approximate the later one by the difference operator

$$\tilde{\Lambda}\phi = \chi(a\phi_{\bar{x}})_x + b^+a^{(+1)}\phi_x + b^-a\phi_{\bar{x}} - d\phi, \quad (4.4)$$

where

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

Next, the problem (4.1) is replaced by the difference scheme

$$\begin{aligned} c(x, \bar{t})\phi_t &= \tilde{\Lambda}(\bar{t})\hat{\phi} + f, \quad \bar{t} = t + \tau/2, \\ \phi(0, t) &= \mu_1(t), \quad y(1, t) = \mu_2(t), \\ \phi(x, 0) &= \varphi_0(x). \end{aligned} \quad (4.5)$$

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 (4.1) is not better than (4.5) although it is of order  $O(h^2 + \tau^2)$  because the Crank–Nicolson method is monotone only if  $\tau/h^2 \leq 1/(2 \min k + h \max |r|)$ . The same conclusion holds for the so-called *optimal weighting scheme* of Wang and Lacroix [25].

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

$$\alpha\varphi_N + \frac{y_{N+1} - y_{N-1}}{2h} = \mu_2,$$

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

Now, we consider the two-dimensional main problem (2.1), (2.5), (2.6) and (2.7). 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

$$\frac{\partial \varphi}{\partial t} - (L_1 + L_2)\varphi = f \quad \text{in } D \times (0, T], \quad (4.6)$$

where

$$\begin{aligned} L_1\varphi &= \frac{\partial}{\partial x} \left( \mu \frac{\partial \varphi}{\partial x} \right) - u \frac{\partial \varphi}{\partial x}, \\ L_2\varphi &= \frac{\partial}{\partial y} \left( \mu \frac{\partial \varphi}{\partial y} \right) - v \frac{\partial \varphi}{\partial y} - \sigma \varphi. \end{aligned} \quad (4.7)$$

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 (4.7) 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 equation (4.6) 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  $D$ .

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

$l = 0, 1, \dots$

(4.8)

Here, for brevity, we write only one space index for the computation direction, omitting other index, for example  $\phi_l$  stands for  $\phi_{Ij}$ .

Due to the monotonicity of each component difference scheme in (4.8) it is possible to prove the positiveness of the solution of (4.8), its stability and the convergence order  $O(h^2 + \tau)$ .

**Remark 4.1.** *Let us remark that in practice the two–dimensional continuity equation (2.3) 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 equation (2.4) 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  $\Omega$  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].

**Remark 5.1.** *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 (3.13).*

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  $\Omega$  is detected. Let the oil concentration in the pollution plume be denoted by  $\varphi(r, T_d)$ . It, of course, is the solution, evaluated at this time, of the main problem (2.1), (2.5), (2.6) and (2.7) with  $f(r, t)$  defined by (3.10). Now, let us take any  $k$  points  $r_1, \dots, r_k$  in the plume  $\Omega$  and consider the adjoint problem (3.6)–(3.9) with

$$P(r, \tau) = Q\delta(r - r_i)\delta(\tau - (T - T_d)). \quad (5.1)$$

Then, by (3.13) we have

$$\phi_{r_i}^*(r_0, \tau_0) = \varphi(r_i, T_d), \quad (5.2)$$

where we supply  $\phi^*$  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 (5.1). Now, setting

$$\varphi(r_i, T_d) = C_i \quad i = 1, \dots, k \quad (5.3)$$

we obtain the following

**Proposition 5.1.** *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 (5.2) and (5.3).

**Proposition 5.2.** *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 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.

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 consider the adjoint problem (3.1)–(3.4) with the right hand side  $p(r, t) = \delta(T_d - t)$  or the problem (3.6)–(3.9) with  $P(r, \tau) = \delta(\tau - (T - T_d))$ .

**Proposition 5.3.** *For the solution of the adjoint problem with the above right hand side there holds the equality*

$$\phi^*(r_0, \tau_0) = 1. \quad (5.4)$$

*Proof.* Let  $\varphi(r, t)$  be the solution of the main problem with the right hand side given by (3.10). Then as in the Proposition 3.1 we have

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

Meanwhile, we have in the new context

$$(L^*\varphi, \varphi) = (p, \varphi) = \int_0^T \int_D \delta(T_d - t)\varphi(r, t) dr dt = \int_D \varphi(r, T_d) dr. \quad (5.5)$$

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 obtain  $\varphi^*(r_0, t_0) = 1$  as the same as the required equality.

The above proposition gives a very simple method for determining the accident location  $r_0$  and the accident time  $t_0 = T - \tau_0$  of oil emission. For this goal we have to solve the adjoint problem only once for incremental  $\tau_j = j\Delta\tau \leq T$  and for each  $\tau_j$  to search a point  $r_0$ , such that  $|\phi^*(r_0, \tau_j) - 1| \leq TOL$ , where  $TOL$  is a some given tolerance, until a pair  $(r_0, \tau_j)$  is found.

Now we consider a method for finding the location and the time of emission in the general case with the use of Propositions 5.1 and 5.2. 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 (3.6)–(3.9) with the right hand side  $P(r, \tau) = Q \delta(r - r_{\max})(\tau - (T - T_d))$ . At each time  $\tau_j$  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 5.2 this point is the location  $r_0$  and the corresponding time is the sought accident time  $\tau_0$ .

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 (3.6)–(3.9) with the right hand side  $P(r, \tau) = Q \delta(r - r_i)(\tau - (T - T_d))$ . At each time  $\tau_j$  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 5.1 this point is the sought accident location  $r_0$  and the corresponding accident time is  $\tau_0$ .

## 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  $108^\circ\text{E}$  to  $112^\circ\text{E}$  and latitude  $10^\circ\text{N}$  to  $14^\circ\text{N}$ . Let a source of oil emission located at  $113^\circ\text{E}$ ,  $13^\circ\text{N}$  with the power  $Q = 10000\text{kg}$ . The solution of the main problem with known flow starting from 06:00 01th April 2011 is given in Figure 1. Here we take the diffusivity  $\mu = 3\text{m}^2/\text{s}$ , the space grid of  $201 \times 201$  nodes and the time step  $\tau = 300\text{s}$ .

In order to demonstrate the effectiveness of the method for identification of the location and the time of the accident we perform the following steps

1. Take the center of the pollution plume as  $S_1$ , and take 4 another points:  $S_2$  left,  $S_3$  right,  $S_4$  below and  $S_5$  upper  $S_1$  by 0.002 degrees. The colour of  $S_1, S_2, S_3, S_4, S_5$  are red, blue, green, magenta and cyan, respectively.
2. Calculate values of the concentration at these points at the time of observation  $T_d = 60\text{h}$  from the main problem, i.e.,  $\varphi(S_i, T_d)$ . They are 24.715, 6.503, 7.404, 16.542, 15.420  $\text{kg}/\text{m}^3$ , respectively.

3. Solve the adjoint problems for  $r_1 = S_i$ .
4. 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 2–6 show the contours for  $\tau_j=12, 24, 36, 48, 60$  h. The colours of the contours are the same of the corresponding source points  $S_i$ .

From the figures we see that after 60 hours 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.

Below we present the results of a simulation when the diffusivity is very large  $\mu_2 = 3000\text{m}^2/\text{s}$ . 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 hours is depicted in Figure 7, the contours after 42, 54 and 60 hours are given in Figures 8-10.

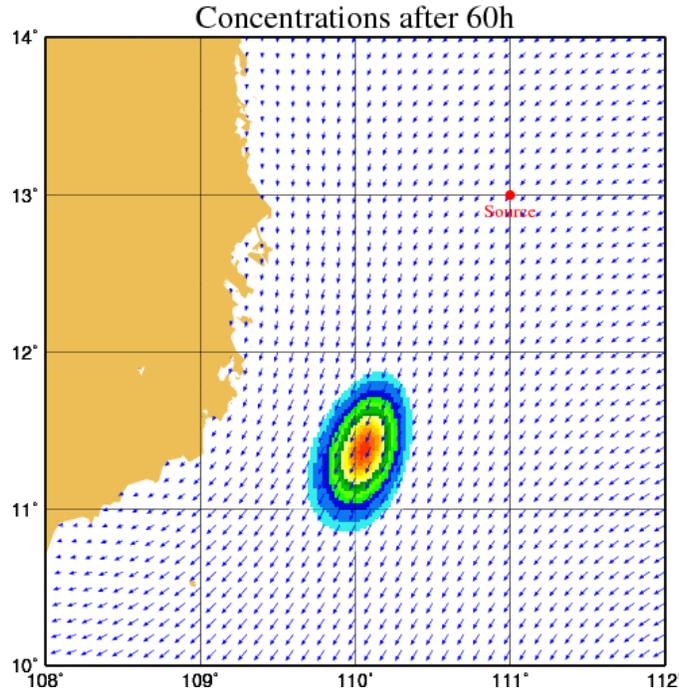


Figure 1: Solution of the main problem with diffusivity  $\mu_1=3\text{m}^2/\text{s}$  after 60h.

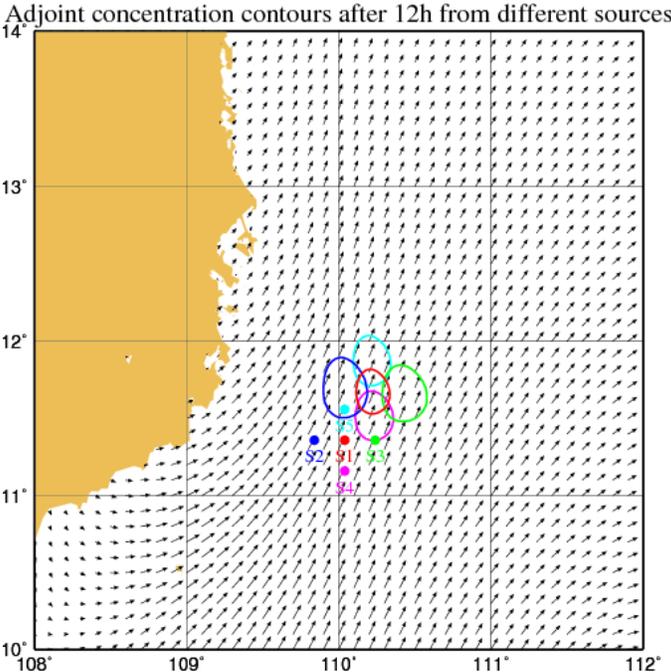


Figure 2: Contours  $\phi_{S_i}^*(r, \tau_j) = \varphi(S_i, T_d)$  for  $\tau_j = 12h$ .

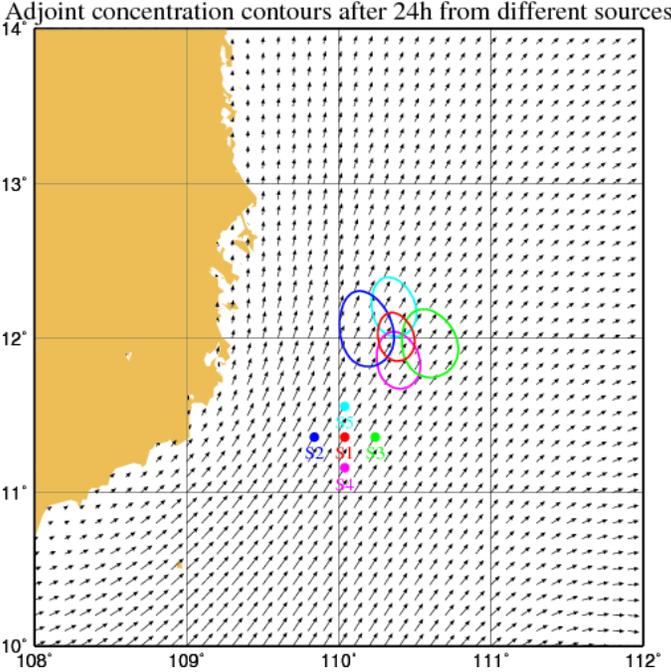


Figure 3: Contours  $\phi_{S_i}^*(r, \tau_j) = \varphi(S_i, T_d)$  for  $\tau_j = 24h$ .

Adjoint concentration contours after 36h from different sources

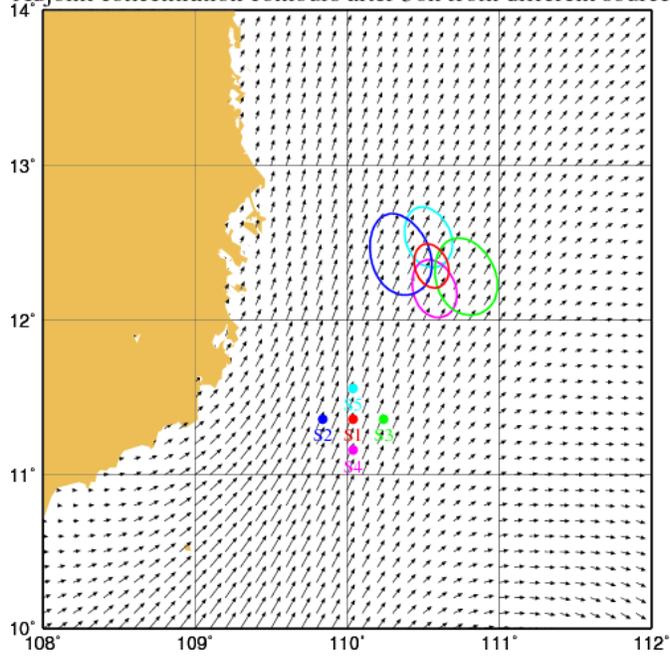


Figure 4: Contours  $\phi_{S_i}^*(r, \tau_j) = \varphi(S_i, T_d)$  for  $\tau_j = 36h$ .

Adjoint concentration contours after 48h from different sources

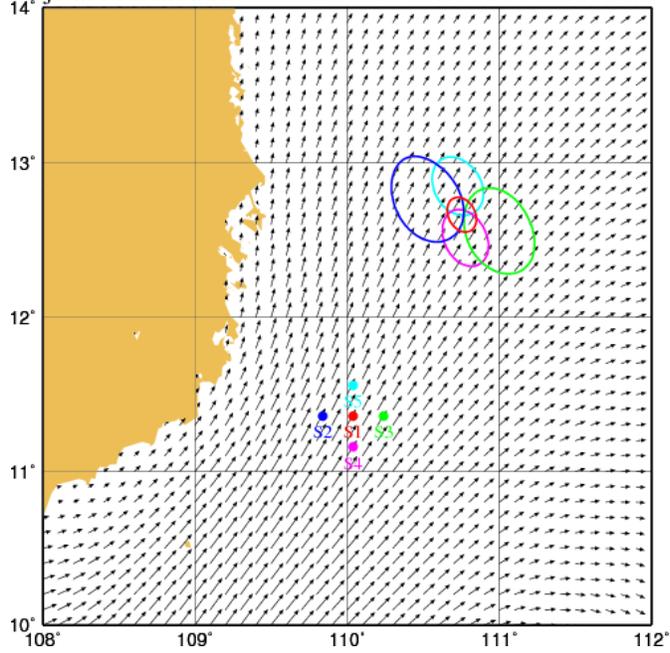


Figure 5: Contours  $\phi_{S_i}^*(r, \tau_j) = \varphi(S_i, T_d)$  for  $\tau_j = 48h$ .

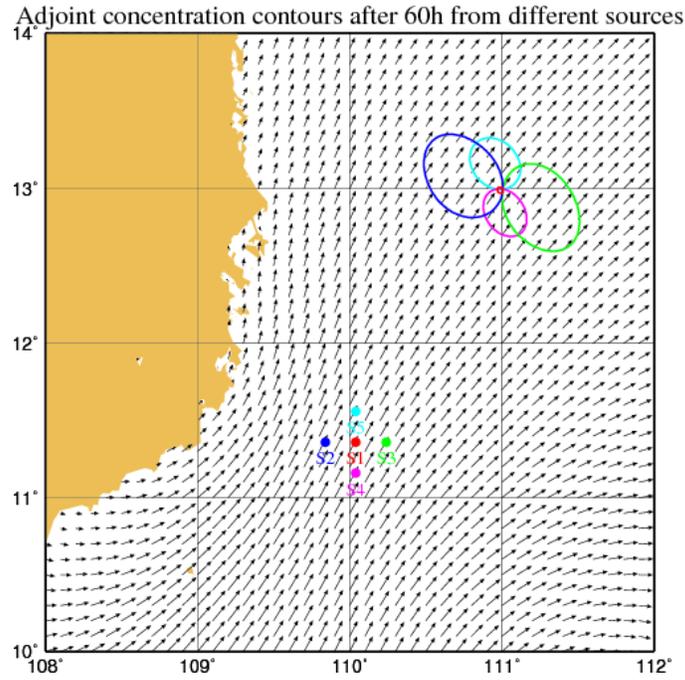


Figure 6: Contours  $\phi_{S_i}^*(r, \tau_j) = \varphi(S_i, T_d)$  for  $\tau_j = 60h$ .

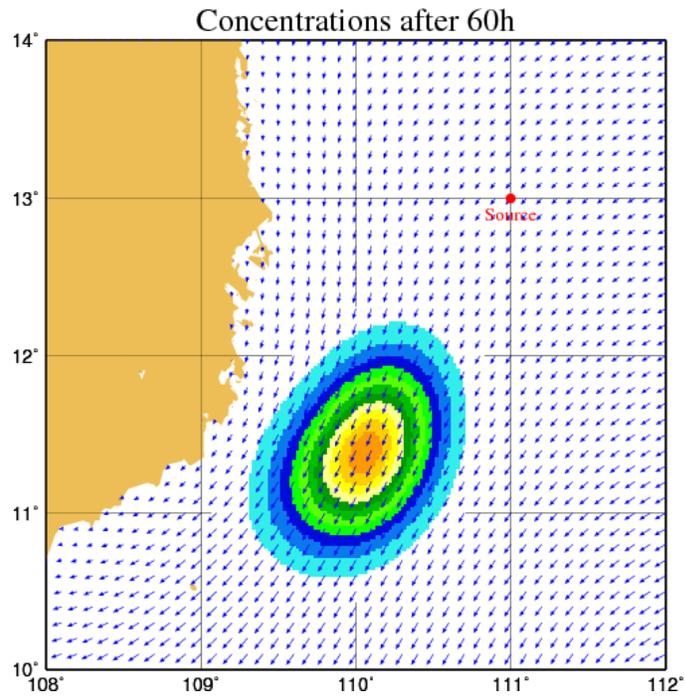
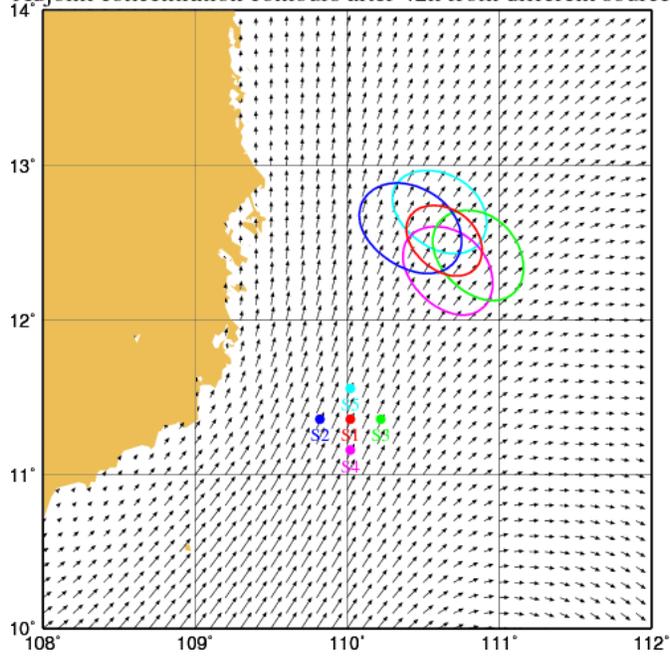
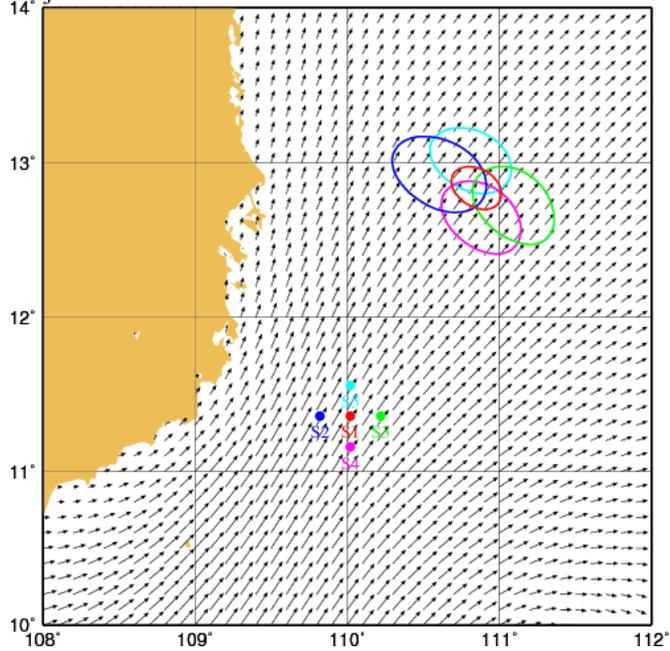


Figure 7: Solution of the main problem with diffusivity  $\mu_2=3000m^2/s$  after 60h.

Adjoint concentration contours after 42h from different sources

Figure 8: Contours  $\phi_{S_i}^*(r, \tau_j) = \varphi(S_i, T_d)$  for  $\tau_j = 42h$  for  $\mu_2$ .

Adjoint concentration contours after 54h from different sources

Figure 9: Contours  $\phi_{S_i}^*(r, \tau_j) = \varphi(S_i, T_d)$  for  $\tau_j = 54h$  for  $\mu_2$ .

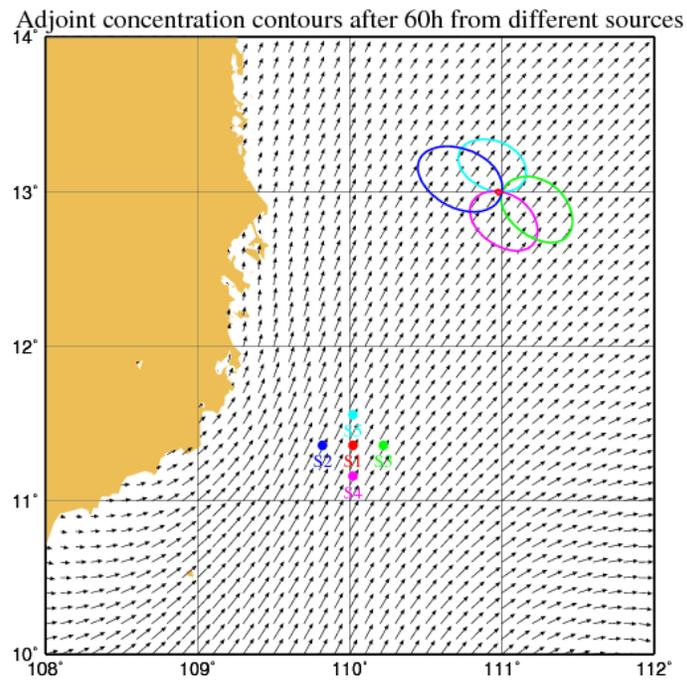


Figure 10: Contours  $\phi_{S_i}^*(r, \tau_j) = \varphi(S_i, T_d)$  for  $\tau_j = 60h$  for  $\mu_2$ .

### 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

$$\begin{aligned} L\varphi &\equiv \frac{\partial \varphi}{\partial t} + \frac{\partial}{\partial x}(U\varphi) + \sigma\varphi - \mu \frac{\partial}{\partial x} \left( \mu \frac{\partial \varphi}{\partial x} \right) = f(x, t) \\ \varphi &= 0, \quad t = 0, \\ \varphi &= 0, \quad x = a, \quad \frac{\partial \varphi}{\partial x} = 0, \quad x = b \end{aligned}$$

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

$$\begin{aligned} L_-^* \phi^* &\equiv \frac{\partial \phi^*}{\partial \tau} - U \frac{\partial \phi^*}{\partial x} + \sigma \phi^* - \mu \frac{\partial}{\partial x} \left( \mu \frac{\partial \phi^*}{\partial x} \right) = P(x, \tau) \\ \phi^* &= 0, \quad \tau = 0, \\ \phi^* &= 0, \quad x = a, \quad U\phi^* + \mu \frac{\partial \phi^*}{\partial x} = 0, \quad x = b. \end{aligned}$$

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, 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 Figure 11. At the moment  $t = 30$  the profile of concentration is given in Figure 12.

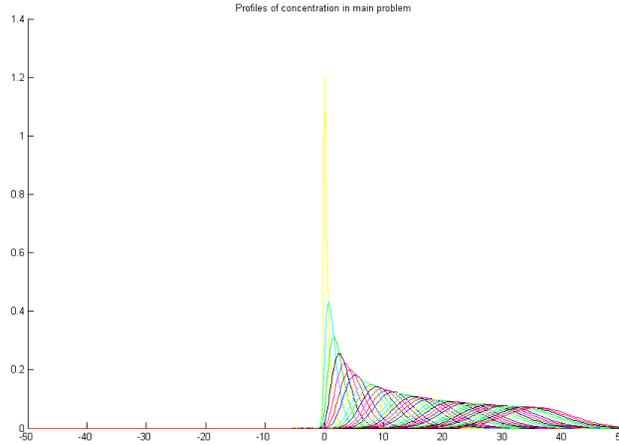


Figure 11: Profiles of concentration caused by a source at  $x = 0$ .

On this Figure 12 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

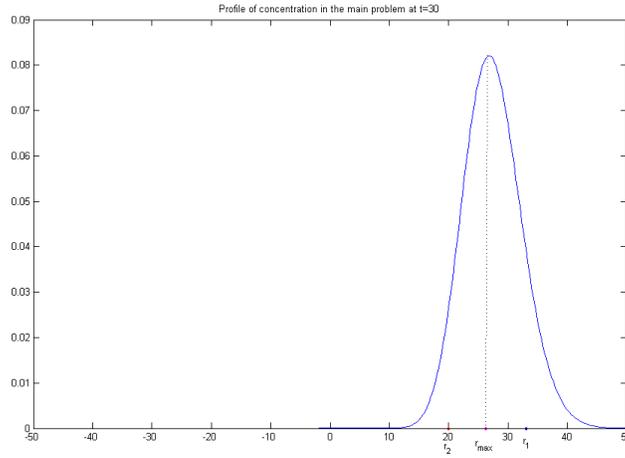


Figure 12: Profile of concentration at the moment  $t = 30$ .

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 Figures 13, 14.

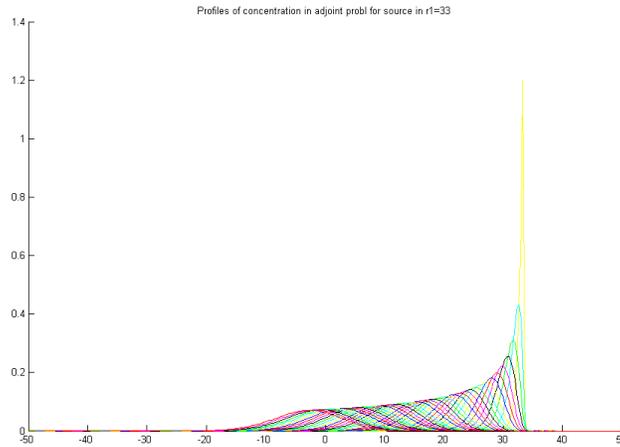


Figure 13: Profile of concentration in adjoint mode for the source at  $r_1$ .

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 Figure 16 we see that these contours 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 Figure 17).

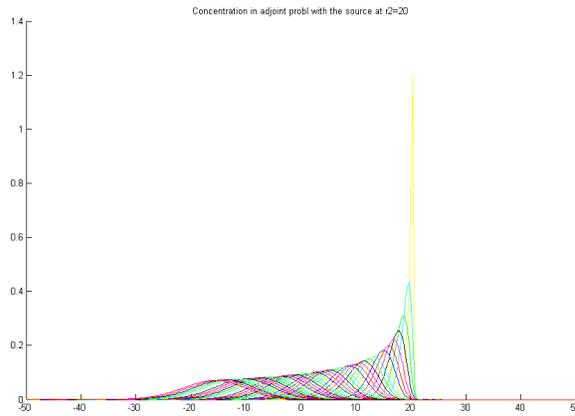


Figure 14: Profile of concentration in adjoint mode for the source at  $r_2$ .

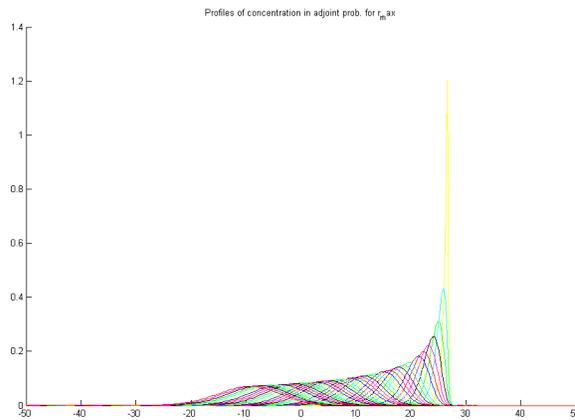


Figure 15: Profile of concentration in adjoint mode for the source at  $r_{\max}$ .

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.

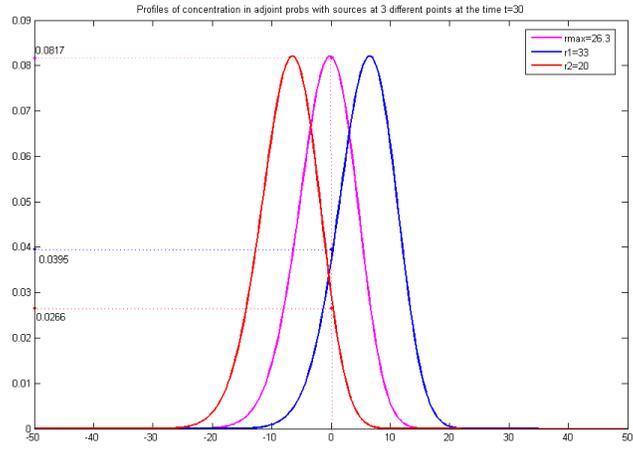


Figure 16: Contours  $\phi_{T_i}^*(x, 30) = C_i$  meet at  $x = 0$ .

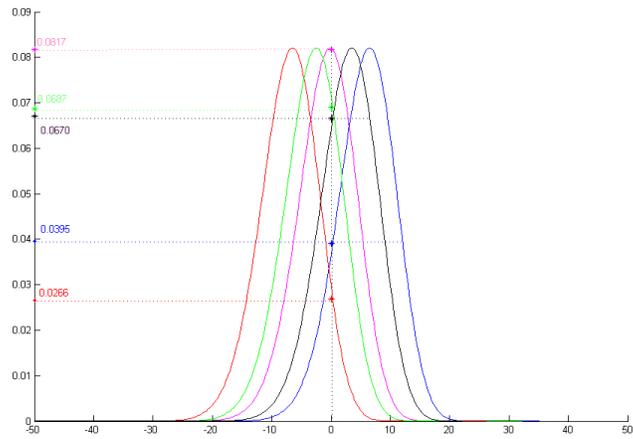


Figure 17: Contours  $\phi_{T_i}^*(x, 30) = C_i$  meet at  $x = 0$ .

## 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 the 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 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]

## References

- [1] A.C. BAGTZOGLU AND J. ATMADJA *Mathematical Methods for Hydrologic Inversion: The Case of Pollution Source Identification*, Handb. Environ. Chem., 5 (2005), pp. 65-96.
- [2] D.G. CACUCI AND M.E. SCHLESINGER, *On the application of the adjoint method of sensitivity analysis to problems in the atmospheric sciences*, *Atmósfera* 7 (1994), 47–59.
- [3] W.P. CHENG AND Y. JIA, *Identification of Contaminant Point Source in Surface Waters Based On Backward Location Probability Density Function Method*, *Adv. Water Resources*, 33 (2010), pp. 397-410.
- [4] Q. A DANG, *Monotone difference schemes for solving some problems of air pollution*, *Adv. Natural Sci.*, 4 (2002), pp. 297-307.
- [5] Q. A DANG AND M. EHRHARDT, *Adequate numerical solution of air pollution problems by positive difference schemes on unbounded domains*, *Math. Comput. Modelling*, 44 (2006), pp. 834-856.
- [6] Q. A DANG, M. EHRHARDT, G.L. TRAN AND D. LE, *On the numerical solution of some problems of environmental pollution*, Chapter 8 in: C.B. Bodine (ed.), *Air Pollution Research Advances*, Nova Science Publishers, Inc., NY, 2007, pp. 171-200.
- [7] I. DIMOV AND Z. ZLATEV, *Optimization Problems in Air-Pollution Modeling*, In: P.M. Pardalos and M.G.C. Resende (eds.), *Handbook on Applied Optimization*, Oxford University Press, 2002.
- [8] J.W. DOERFFER, *Oil Spill Response in the Marine Environment*, Pergamon Press, Oxford, 1992.
- [9] J.A. FAY, *Physical processes in the spread of oil on a water surface*, In: Proc. Conf. Prevention and Control of Oil Spills, 15-17 June, American Petroleum Institute, Washington, DC, 1971, pp 463-467.
- [10] H.-O. KREISS AND J. LORENZ, *Initial-Boundary Value Problems and the Navier–Stokes Equations*, Academic Press, 1989.
- [11] W.J. LEHR, R.J. FRAGA, M.S. BELEN AND H.M. CEKIRGE, *A New Technique to Estimate Initial Spill Size Using a Modified Fay-type Spreading Formula*, *Marine Pollution Bulletin*, 15 (1984), pp. 326-329.
- [12] G.I. MARCHUK, *Mathematical Models in Environmental Problems*, Elsevier, New York, 1986.
- [13] G.I. MARCHUK, *Adjoint Equations and Analysis of Complex Systems*, Kluwer, Dordrecht, 1995.

- [14] E. MILNES AND P. PERROCHET *Simultaneous identification of a single pollution point-source location and contamination time under known flow field conditions*, *Adv. Water Resources*, 30 (2007), pp. 2439-2446.
- [15] R.M. NEUPAUER AND J.L. WILSON, *Adjoint method for obtaining backward-in-time location and travel time probabilities of a conservative groundwater contaminant*, *Water Resources Research*, 35 (1999), pp. 3389-3398.
- [16] J.A. PUDYKIEWICZ, *Application of adjoint tracer transport equations for evaluating source parameters*, *Atmos. Environ.* 32 (1998), pp. 3039-3050.
- [17] M. REED, Ø. JOHANSEN, P.J. BRANDVIK, P. DALING, A. LEWIS, R. FIOCCO, D. MACKAY AND R. PRENTKI, *Oil Spill Modeling towards the Close of the 20th Century: Overview of the State of the Art*, *Spill Science & Technology Bulletin*, 5 (1999), pp. 3-16.
- [18] M. REED, *Technical Description and Verification Tests of OSCAR2000, A Multi-Component 3-Dimensional Oil Spill Contingency and Response Model*, SINTEF Applied Chemistry Report, 2001.
- [19] A.A. SAMARSKII, *The theory of difference schemes*, Dekker, New York, 2001.
- [20] Y.N. SKIBA, *Direct and adjoint estimates in the oil spill problem*, *Rev. Int. Contam. Ambient.*, 11 (1995), pp. 69-75.
- [21] Y.N. SKIBA, *Dual oil concentration estimates in ecologically sensitive zones*, *Environmental Monitoring and Assessment*, 43 (1996), pp. 139-151.
- [22] Y.N. SKIBA, *The derivation and applications of the adjoint solutions of a simple thermodynamic limited area model of the Atmosphere-Ocean-Soil system*, *World Resource Review*, 8 (1996), pp. 98-113.
- [23] Y.N. SKIBA, *Direct and adjoint oil spill estimates*, *Environmental Monitoring and Assessment*, 59 (1999), pp. 95-109.
- [24] Y.N. SKIBA AND D. PARRA-GUEVARA, *Mathematics of oil spills: existence, uniqueness, and stability of solutions*, *Geofísica Internacional*, 38 (1999), pp. 117-124.
- [25] H.Q. WANG AND M. LACROIX, *Optimal weighting in the finite difference solution of the convection-dispersion equation*, *J. Hydrology*, 200 (1997), pp. 228-242.
- [26] S.-D. WANG, Y.-M. SHEN AND Y.H. ZHENG, *Two-dimensional numerical simulation for transport and fate of oil spills in seas*, *Ocean Engineering*, 32 (2005), pp. 1556-1571.
- [27] N.N. YANENKO, *The method of fractional steps*, Springer-Verlag, 1971.