DIRECT AND ADJOINT ESTIMATES IN THE OIL SPILL PROBLEM

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ABSTRACT

The movement and spreading of oil from a damaged oil tanker are described by the 2-D oil transport equation in a limited sea area when there is an oil flux across the boundaries. Dual estimates of the average oil concentration in ecologically sensitive zones are derived. Whereas the first estimate uses the oil transport equation solution (the direct method), the second estimate based on the adjoint oil transport equation solution, represents a simple integral formula relating the average oil concentration with the oil expense from the tanker (the adjoint method). The main and adjoint oil transport problems are shown to be well-posed, i.e., any solution of these problems is unique and stable to initial perturbations. These properties are achieved by setting special boundary conditions. Advantages of each of the methods are illustrated with several examples. The adjoint method is readily generalized to the 3-D oil transport problem.

RESUMEN

El movimiento y la difusión del petróleo de un buque petrolero dañado se describen por la ecuación bidimensional de transporte de petróleo en un área limitada cuando existen flujos de petróleo a través de las fronteras. Se derivan las estimaciones duales de la concentración promedio del petróleo en zonas ecológicamente sensibles. Mientras que la primera estimación utiliza la solución de la ecuación de transporte del petróleo (el método directo), la segunda estimación se basa en la solución de la ecuación de transporte del petróleo y representa una fórmula integral simple que relaciona la concentración promedio de petróleo en la zona con el gasto de petróleo del buque (el método adjunto). Se demuestra que los dos problemas de transporte del petróleo, el principal y el adjunto, están bien condicionados, es decir, cualquier solución de los problemas es única y estable con respecto a las perturbaciones iniciales. Estas propiedades se logran mediante la declaración de las condiciones especiales de frontera. Las ventajas de cada uno de los dos métodos se ilustran con ejemplos. El método adjunto se generaliza fácilmente al problema tridimensional de transporte del petróleo.

INTRODUCTION

Defining the wind velocity as the result of using the dynamic modelling or climatic data, the main and adjoint pollutant transport equations can be applied to solve such theoretically and practically important problems as:

1) optimal location of new industries in a given region with the aim to minimize the pollution concentration in certain ecologically sensitive zones (Marchuk 1986);

2) optimization of the levels of emissions from operating industries (Marchuk 1982, Penenko and Raputa 1983);

3) detection of industrial plants violating sanitary regulations (Penenko and Raputa 1982);

4) analysis of the emissions originated by vehicles (Heidorn et al. 1991),

and others.

In this work we apply the above mentioned approach to the oil transport problem in the case of the oil spill from a

The 2-D oil transport-diffusion equation is used to describe the movement of the oil slick in a limited sea area. Dual estimates of the average oil concentration in ecologically sensitive zones are derived. The first classic estimate uses the oil transport equation (the direct method), and hence, is used to solve the oil transport problem repeatedly if the accident site or/and the oil volume spilled from the tanker in a unit time are changed. The second estimate is based on the adjoint oil transport equation and represents a simple integral formula relating the average oil concentration in an ecologically sensitive zone with the rate of the oil leak from the tanker (the adjoint method). The main idea of this method was given by Skiba (1995). The important difference of the adjoint method from the direct one is that the solution of the adjoint oil transport problem depends only on the oil propagation velocity and ecologically sensitive zone selected and is independent of the accident site and the oil expense from the tanker. It allows to solve the adjoint problem independently of a particular accident with the oil tanker, especially if the oil velocity is determined on the basis of a climatic (seasonal or monthly) sea surface currents and winds. In this case, the adjoint oil transport equation can be solved individually for each of the ecologically sensitive zones and kept in the computer memory. Besides, according to the adjoint estimate formula, it is sufficient to keep in the computer the adjoint solution values only for the grid points that lie on the oil tanker way. Then in an emergency, to make rapid preliminary estimates of the average oil concentration in an ecologically sensitive zone by the adjoint method, the only thing to be done is to choose the adjoint solution that corresponds to the zone, and by using the information about the accident site and the rate of the oil spill from the tanker, integrate over time the product of the oil spill rate and the adjoint solution values at the accident site.

The main and adjoint oil transport problems are shown to be well-posed, i.e., any solution of these problems is unique and stable to initial perturbations. These properties are achieved by setting special boundary conditions depending on the sign of the normal component of the velocity vector in each point of the boundary (Skiba 1993). Advantages of each of the two methods are illustrated with several examples. In particular, the adjoint method is preferable in the sensitivity study of oil concentration characteristics in a sea zone, to variations in the tanker accident site and the oil spill rate from the tanker. We stress once again that its application is especially simple when the oil propagation velocity is determined on a basis of the climatic currents and winds. Indeed, then the same adjoint solution taken out of the computer memory for the analyzed zone can be used repeatedly not only for all possible accident sites (that is, for each of the grid points lying on the tanker sea way) and different oil spill rates, but also for various initial moments of the accident. Thus, the two estimates complement each other nicely in studying the consequences of the oil spill. They are generalized to the 3-D oil transport problem.

**THE OIL PROPAGATION PROBLEM**

Assume that a point $r_0=(x_0, y_0)$ indicates the site of an accident with an oil tanker in a two-dimensional oceanic domain $D$ with the boundary $S$ (Fig.1), and $t=0$ is the point in time at which the accident happened. Besides, let $Q(t)$ be an oil spill rate, i.e., the oil amount spilling from the tanker in a unit time, and $\phi(r, t)$ denotes the thickness of the oil film on the sea surface at the point $r=(x, y)$ of the domain $D$ and instant $t>0$. Then, in the first approximation, the oil propagation in the domain $D$ and time interval $(0, T)$ can be described by the transport-diffusion equation

$$\frac{\partial}{\partial t} \phi + \nabla \phi \cdot U = \sigma \phi - \nabla \cdot \mu \nabla \phi = Q(t) \delta(r - r_0)$$

where $\mu$ is the diffusion coefficient, $\nabla$ is the 2-D gradient, the parameter $\sigma$ characterizes decreasing of $\phi(r, t)$ because of different physical and chemical processes, and $\delta(r)$ is the Dirac mass at the point $r$. It is assumed here that the resulting velocity vector $U(r, t) = (u(r, t), v(r, t))$ of the oil propagation is known and satisfies the continuity equation

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

This vector can be calculated by using the climatic (seasonal or monthly) sea surface currents and winds, or by using the currents and winds obtained from special dynamic models. If the domain $D$ is an open basin then an oil flux across the liquid boundaries is possible. Therefore the choice of mathematically and physically appropriate boundary conditions is very important to set the well-posed problem whose solutions are unique and stable to initial perturbations (Skiba 1993). To achieve this goal we now apply Marchuk's (1986) idea.

Let $U_0$ be a projection of the known velocity vector $U$ on the outward normal $n$ to the boundary $S$. We divide $S$ into the "outflow" part $S^+$ where $U_n>0$ and the oil flows out of the domain $D$, and the "inflow" part $S^-$ where $U_n<0$ and the current vector $U$ is directed from the outside to the inside of $D$ (Fig.1). As the initial and boundary conditions for Eq.(1) in the time interval $(0, T)$ and domain $D$ we take

$$\phi(r, 0) = 0 \quad \text{at} \quad t = 0 \quad (3)$$
THE ADJOINT PROBLEM

We now apply the adjoint approach to show two different but equivalent ways to estimate the average oil concentration level in an ecologically sensitive zone. Using the Lagrange identity (Marchuk and Skiba 1990) the adjoint transport-diffusion problem in the domain $D$ and the time interval $(0,T)$ can be written as

$$-\frac{\partial}{\partial t} g - U \cdot \nabla g + \sigma g - \nabla \cdot \mu \nabla g = P(r,t)$$

under the boundary conditions

$$\mu \frac{\partial}{\partial n} g = 0 \quad \text{on } S^-$$

$$\mu \frac{\partial}{\partial n} g + U_n g = 0 \quad \text{on } S^+$$

and with a forcing $P(r,t)$ which will be defined later. The velocity $U$ is the same as in Eq.(1). Similar to (6), it can be shown that the adjoint problem (8)-(10) is well-posed if, and only if, it is solved backward in time: from $t=T$ to $t=0$ (Skiba 1993). Therefore, unlike (3), the initial condition for the adjoint problem is set at the instant $t=T$:

$$g(r,T) = 0$$

Note that the zero initial function in (11) is essential for deriving the oil concentration estimate (see formula (13) in the next section). Also, if we put $P(r,t)=0$ and $Q(t)=0$ then the substitution $t'=T-t$ shows that Eq.(8) differs from Eq.(1) only by the sign of the velocity $U$. That is why the boundary conditions (4) and (5) of the main problem (1)-(5) are transformed to the conditions (9) and (10) for the adjoint problem (8)-(11).

Let us consider a standard combination of the main and adjoint equations (see, e.g. Marchuk 1982): the equations (1) and (8) are multiplied by $g$ and $\phi$ respectively, and the expressions obtained are integrated over the domain $D$ and time interval $(0,T)$. Taking into account the zero initial conditions (3),(11), the boundary conditions (4),(5),(9),(10), and subtracting the final results one from another, we obtain that the oil concentration

$$J_v (\phi) = \int_0^T \int_D P(r,t) \phi(r,t) \, dr \, dt$$

Thus, it is assumed that there is no oil on the sea surface in $D$ at the initial moment. The boundary condition (4) means the absence of the combined (turbulent and advective) oil flux from the outside of the domain $D$ at the inflow boundary $S^-$, whereas (5) signifies that the turbulent flux at the outflow boundary $S^+$ is negligible as compared with the advective outflow $U_n \phi$ from the domain $D$. In the limiting case when there is no diffusion ($\mu=0$), (4) is reduced to the reasonable condition $\phi=0$ (the absence of the oil at the inflow part of the boundary), while the condition (5) vanishes. The last fact is also natural, since for a pure advection equation, no condition is required at the outflow boundary where the solution is defined by the method of the characteristics (Godunov 1971). We also put $U_n=0$ at the part of $S$ coinciding with the coast line. Thus (4) and (5) not only generalize the well-known condition $\mu \{ \partial \phi / \partial n \} = 0$ usually set at the boundary of the closed sea basin, but also approach, in the non-diffusion limit, the boundary conditions of the pure advection equation.

Multiplying (1) by $\phi$ and integrating over the domain $D$ we obtain

$$\frac{1}{2} \frac{\partial}{\partial t} \int_D \phi^2 \, dr + \int_D \left[ \sigma \phi^2 + \mu |\nabla \phi|^2 \right] \, dr$$

$$+ \frac{1}{2} \left[ \int_{S^-} U_n \phi^2 \, ds - \int_{S^+} U_n \phi^2 \, ds \right] = Q(t)\phi(r_s,t)$$

(6)

where $ds$ is the infinitesimal element of the boundary line $S$. Since $U_n$ is negative on $S^-$, the second, third and fourth integrals in the left-hand side of (6) are positive. From (6), it is evident that the solution $\phi(r,t)$ is unique and stable to initial perturbations, i.e., the problem (1)-(5) is well-posed in the sense of Hadamard (Skiba 1993).

Integration of (1) over $D$ leads to the balance equation

$$\frac{\partial}{\partial t} \int_D \phi \, dr = Q(t) - \int_D \sigma \phi \, dr - \int_{S^-} U_n \phi \, ds$$

(7)

Thus the average oil concentration in the domain $D$ increases because of non-zero source $Q$, and decreases by reason of the dissipation ($\sigma > 0$) and the advective oil outflow across $S^+$.

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Thus the average oil concentration in the domain $D$ increases because of non-zero source $Q$, and decreases by reason of the dissipation ($\sigma > 0$) and the advective oil outflow across $S^+$.
ESTIMATION OF THE OIL CONCENTRATION IN ECOLOGICALLY SENSITIVE ZONE

Let $\Omega$ be an ecologically sensitive zone in the domain $D$ (Fig.1) in which we want to estimate the average oil concentration

$$J(\phi) = \frac{1}{\tau|\Omega|} \int_{T-\tau}^{T} \int_{\Omega} \phi(\mathbf{r}, t) d\mathbf{r} dt$$

within a time interval $[T-\tau, T]$ of the length $\tau$ $(0<\tau<T)$. Here $|\Omega|$ is the area of $\Omega$, and $\tau$ may be a few hours to one day.

According to the direct method, the problem (1)-(5) has to be solved, and then the integral (14) must be calculated. It is easily seen that the oil characteristic (14) is a special case of (12) when the forcing $P(r, t)$ is defined by

$$P(r, t) = \begin{cases} \frac{1}{|\Omega|}, & \text{if } r \in \Omega \land t \in [T-\tau, T] \\ 0, & \text{elsewhere} \end{cases}$$

i.e., $P(r, t) = 1/(\tau|\Omega|)$ if the point $r$ belongs to $\Omega$ and $t$ belongs to the interval $[T-\tau, T]$, and $P(r, t) = 0$ elsewhere. By the dual estimates derived in the previous section, the average pollution characteristic (14) can also be computed from the formula (13), that is, by the adjoint method. Besides, the solution $g(r_0, t)$ to the adjoint problem (8)-(11) at the accident point $r_0$ has to be calculated with the forcing (15).

Let us divide the whole time interval $(0, T)$ into uniform subintervals $(t_n, t_{n+1})$ of sufficiently small length $\Delta t$ where $n=1, \ldots, N$, $t_0 = 0$ and $t_N = T$. Then the formula (13) can be approximated by

$$J(\phi) = \Delta t \sum_{n=1}^{N} g(r_0, t_n) Q(t_n)$$

where $g(r_0, t_n)$ and $Q(t_n)$ are the values obtained by averaging $g$ and $Q$ over the subinterval $(t_n, t_{n+1})$. Thus, if at least one of the values $g(r_0, t_n)$ and $Q(t_n)$ is zero (or small) for some $n$ then their product is also zero (small), and hence, there is no (there is a small) contribution of the subinterval $(t_n, t_{n+1})$ to the sum (16). Note that the value $g(r_0, t_n)$ may be zero or small if the subinterval $(t_n, t_{n+1})$ is not too far from the instant $t=T$, since during the interval $[T-\tau, T]$, the nonzero values of the adjoint solution are located near the zone $\Omega$, and it takes time for them to reach the accident site $r_0$ (see Fig.1). Obviously the zero value $Q(t_n)$ means stopping the oil spilling from the tanker.

Fig.1. The domain $D$ with the ecological zone $\Omega$. The point $r_0$ is the oil tanker accident site. Isolines of the solution $\phi$ are represented schematically by the solid lines, whereas those of the adjoint solution $g$ are shown by the long-dashed lines. The points $r$ denote the grid points lying along the oil tanker route (the short-dashed line). The points $A$ and $B$ belong to the boundary parts $S$, and $S'$ respectively, and $U_{\perp}$ is the orthogonal projection of the velocity vector $U$ on the unit normal $n$ to the boundary $S$.

Each of the two (direct and adjoint) methods has its own advantages and disadvantages, and will be preferable
depending on the assumptions and aims of a concrete study. Several examples given below explain how to decide between the two methods discussed here.

Example 1. Climatic sea current and wind velocities

Assume that the oil velocity vector $U$ in the domain $D$ and time interval $(0,T)$ has been calculated through the use of climatic (monthly or seasonal) sea surface currents and winds. Then the application of the adjoint method is more convenient. Indeed, in contrast to the main problem (1)-(5) linked with the accident site $r_0$ and oil escape rate $Q(t_0)$, the adjoint problem (8)-(11),(15) depends only on the ecologically sensitive zone $\Omega$. Therefore its solution $g(r,t)$ can be calculated in the interval $(0,T)$ for each zone $\Omega$ regardless of any concrete accident. Moreover, since the formula (16) requires the values $g(r_0,t_n)$ solely at the accident point $r_0$, it is sufficient to keep in the computer only the values $g(r,t_n)$ of the adjoint solution in the grid points $r$ lying along the tanker way (Fig.1). Indeed, any of these grid points (and only such points) may be a possible site $r_0$ of the accident point. Then in an emergency, when the tanker accident site $r_0$ and oil escape rate $Q(t_n)$ are known, the only thing to be done is to estimate the oil concentration (14) in $\Omega$ and interval $[T-\tau, T]$, is to take the adjoint solution corresponding to the zone $\Omega$ out of the computer, and then calculate the sum (16) using as $g(r_0,t_n)$ the values $g(r,t_n)$ in the grid point $r$ nearest to the accident site $r_0$. Note that the distance between the two points, $r$ and $r_0$, can be made arbitrarily small by reducing the size of the grid mesh in the domain $D$. This approach provides a preliminary estimate of the oil concentration in the zone $\Omega$. The estimate may be improved if a more accurate solution of the adjoint problem (8)-(11),(15) is used in (16). For example, the adjoint problem can be solved with the oil velocity $U$ calculated using the present current and wind velocities rather than the climatic ones.

Example 2. Time-independent oil escape from the tanker

Within the limits of Example 1, and with the additional assumption that the oil escape rate $Q(t)$ from the tanker is time-independent in the interval $(0,T)$, say, equal to $Q$, the formulas (13) and (16) are simplified:

$$J_P(\phi) = Q \int_0^T g(r, t) dt \quad (17)$$

and

$$J(\phi) = Q \Delta t \sum_{n=1}^N g(r_0, t_n) \quad (18)$$

Then one may keep in the computer either the adjoint solution values $g(r_i, t_n)$ in each of the grid points $r_i$ on the tanker way in $D$, or the set of the sums $\sum_{n=1}^N g(r_i, t_n)$ for $N=1,2,...$.

Example 3. Estimation of the time available to take precautions against polluting the zone

One of the important questions is how long it takes for oil to reach the ecologically sensitive zone $\Omega$. In our case, the question can be restated as how long the average oil concentration (14) in $\Omega$ will not exceed a small number $\epsilon$. In order to estimate this time by the direct method, one has to run the problem (1)-(5), being (14) smaller than $\epsilon$; the integral (14) should be taken at each time step of the numerical algorithm. Let $T_{\text{max}}$ be the maximum of such $T$ that $J(\phi) \leq \epsilon$. Then $T_f = T_{\text{max}} - \tau$ is the time available to take precautions against polluting the zone $\Omega$.

The adjoint approach with the formula (16) does not require any integration over the domain $\Omega$. It is more convenient when the adjoint solution $g(r_0,t_n)$ is kept in the computer memory for $n=1,2,...,N$ (see example 1). Then $T_f = N \Delta t$ where $N$ is maximum number of the subintervals for which the sum (16) (or (18)) is smaller than $\epsilon$.

Example 4. Search of the most dangerous part of the oil tanker way

Let us assume that the ecologically sensitive zone $\Omega$, the oil velocity $U$, the oil escape rate $Q(t)$ from the damaged tanker, the time interval $(0,T)$, and the value $\tau$ are fixed, and let us try to answer the question: which part of the oil tanker way is more dangerous from the point of view of polluting the zone $\Omega$? Suppose that there are $K$ grid points $r_i$ lying on the oil tanker way in the domain $D$ (Fig.1). Following to the direct method, the problem (1)-(5) must be solved $K$ times with the forcing $Q(t)$ successively located in each of the grid points $r_i$. The integral (14) is then calculated with each such solution $\phi(i=1,2,...,K)$. A neighborhood of the point $r$ corresponding to the maximal value of this integral, is believed to be the most dangerous part of the oil tanker way for the zone $\Omega$.

However, the use of the adjoint method is preferable here. Indeed, there is no need to solve the problem (1)-(5) at all, and the adjoint problem (8)-(11),(15) should be solved only once. Then the sum (16), with the values $g(r_i,t_n)$ instead of $g(r_0,t_n)$, is taken $K$ times for each grid point $r_i$ lying on the oil tanker way ($i=1,2,...,K$). The maximum value among these $K$ sums corresponds to the highest oil concentration level in the zone $\Omega$, and hence, determines the most dangerous point $r_i$ on the oil tanker way.
Example 5. The $Q(t)$-dependence of the estimate (14)

Assume that the ecologically sensitive zone $\Omega$, the oil velocity $U$, the time interval $(0,T)$, the value $\tau$, and the accident site $r_0$ are fixed, and we want to study the sensitivity of the oil concentration (14) in $\Omega$ with respect to variations in the oil source $Q(t)$ of the damaged tanker. With this in mind, we should analyze the values $J(\phi)$ obtained with different oil sources $Q_i(t)$ ($i=1,\ldots,I$). Following the direct method, the transport problem (1)-(5) is solved for each $Q_i(t)$ ($i=1,\ldots,I$), and then the integrals (14) calculated for each solution $\phi_i$ are compared. However, if the number $I$ is large, then the adjoint method is more efficient (affordable), since there is no need to solve the problem (1)-(5) at all. The adjoint problem (8)-(11), (15) is solved only once, and then the adjoint solution $g$ is used to take the simple integral (13) (or the sum (16)) repeatedly for each $Q_i(t)$.

In particular, if $(0,t_f)$ is the time interval over which the oil is spilling from the damaged tanker ($t_f \leq T$), the adjoint aproach is convenient to study the relationship between the oil concentration (14) in the zone $\Omega$ and the oil spill time $t_f$. Indeed, since $Q(t)=0$ if $t_f < t \leq T$, the integral (13) and the sum (16) are reduced to

$$J_s(\phi) = \int_0^\tau g(r_0,t)Q(t)dt$$

(19)

and

$$J(\phi) = \Delta t \sum_{n=1}^{N_f} g(r_0,t_n)Q(t_n)$$

(20)

respectively, where the union of $(t_n,t_{n+1})$ over $n$ from 1 to $N_f$ coincides with $(0,t_f)$.

FINAL CONCLUSIONS

The 2-D oil transport-diffusion equation is considered here to describe the movement and spreading of the oil spilling from a damaged oil tanker. The problem is studied in a limited sea area when there is an oil flux across the boundaries of the domain. The direct and adjoint methods are suggested to obtain dual estimates of the average oil concentration in an ecologically sensitive zone $\Omega$. As the direct estimate is based on the oil transport problem solution, the adjoint estimate requires a knowledge of the adjoint oil transport problem solution. It is shown that the both problems are well posed in the sense of Hadamard, that is, each of their solutions is unique and stable to initial perturbations. It was made possible by setting special boundary conditions (4), (5) and (9), (10). The two types of estimates complement each other nicely in studying the consequences of the tanker oil spill. Examples given demonstrate the advantages of the application of one or the other of these estimates. Evidently that the direct method is preferable if a comprehensive information about the oil concentration is required in each point of the domain $D$. At the same time, the adjoint estimate presented by the simple integral formula (13) or, by the approximate formula (16), directly relates the average oil concentration in the zone $\Omega$ (being only a subset of $D$) with the oil escape rate $Q(t)$ from the damaged tanker, and hence, is very convenient for the sensitivity study of the model.

Note that several ecologically sensitive zones are analyzed in perfect analogy to what is considered here. The adjoint method can be applied also to any oil spill problem regardless the oil source, and is readily generalized to the 3-D oil transport problem.

The main and adjoint oil transport problems considered here can be solved with the help of balanced and absolutely stable finite-difference schemes and numerical algorithms developed by Skiba (1993) and Skiba et al. (1995) for the 2-D and 3-D pollutant transport problem. In the absence of the dissipation and pollutant sources each of the schemes has two conservation laws. The implicit numerical schemes constructed are based on the splitting method when the solution of the main as well as of the adjoint multi-dimensional problems are obtained by solving several simple 1-D split problems. Symmetric version of the splitting-up method leads to the schemes of the second order approximation in time and space. Since the original (unsplit) operators, as well as each of the split operators of the main and adjoint problems are positive semidefinite both in the differential and finite-difference forms, the application of the splitting-up method is justified.

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