Advances in Dynamical Systems and Applications
ISSN 0973-5321, Volume 8, Number 1, pp. 75–84 (2013)
http://campus.mst.edu/adsa

Numerical Simulation of Hydrocarbons Dispersion in Tangier Bay

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Abstract

This study focuses on modeling the transport and the distribution of pollutants into Tangier Bay. These pollutants come mainly from harbor activities, urban or industrial wastes. The mathematical model used for the prediction of pollutant concentrations is based on convection and dispersion equations. This model is linked to hydrodynamic processes based on Navier–Stokes equations for incompressible flow. Numerical tests are carried out using finite element methods.

AMS Subject Classifications: 65N22, 76R05.
Keywords: Concentration, pollutant, convection, dispersion, Navier–Stokes equations, Tangier bay, finite element method.

Received June 27, 2012; Accepted November 15, 2012
Communicated by Delfim F. M. Torres

1 Introduction

The marine environment is a precious asset. Oceans and seas provide 99% of the available living space on the planet. They cover 71% of earth's surface and contain 90% of the biosphere and consequently contain more biological diversity than terrestrial and freshwater ecosystems. The marine environment is essential to life on earth and plays a key role in climate and weather patterns. It is also an important factor in economic prosperity, social wellbeing and quality of life. However, the ecological balance of this medium is often threatened.

Conscious of pollution problems in the coastal marine environment and their direct impact on the socioeconomic life of the bordering countries, many studies have been conducted to modeling the behavior of pollutants after their marine spill. In [10], a numerical model has been developed to study the behavior of pollutants in Algeciras Bay. The model includes a hydrodynamic process and a sediment transport model. In [8], a hydrodynamic process coupled with a diffusion model was developed to simulate contaminant transport in the Bay of Daya in China. In [3], finite difference and finite element methods were applied to Sepetiba Bay. For the region of Tangier, a geochemical study was applied to Tangier Bay focussed on the evaluation of the aliphatic hydrocarbons concentrations in marine water (see [4, 5]).

In this paper, we target the key objective of developing a mathematical and a numerical model to estimate concentrations of hydrocarbons discharged in the Bay of Tangier. This estimation takes into account experimental measurements of concentrations published in [1]. The mathematical model is established by the coupling between hydrodynamic and transport models. The first one is based on Navier–Stokes equations, it considers all the factors influencing the flow such as velocity, Coriolis force, gravity and pressure, as well as physico-chemical properties of sea water (density and dynamic viscosity). The second is based on convection and dispersion equations. Numerical tests are carried out by using a finite element method using FreeFem++ software (see [9]).

The text is organized as follows. In Section 2, we describe the mathematical model defined for the simulation of the pollutants transport in the Bay of Tangier. Section 3 is devoted to the discretization scheme and to the variational formulation of the problem. Section 4 presents some numerical results related to the transport model in a two dimensional space. Finally, some conclusions and possible extensions of this work are presented in Section 5.

2 Mathematical Model

Several models have been proposed for the simulation of pollutant transport in the sea, all of them based on convection and diffusion equations. In this work, an incompressible fluid is considered and two mathematical models are coupled to simulate transport hydrocarbons in the Bay of Tangier. The first is the hydrodynamic model that provides the velocity field and water levels, it is based on Navier–Stokes equations. The second is based on a convection-dispersion equations which simulates the concentration field.

2.1 Transport Equations

In a domain $\Omega \subset \mathbb{R}^3$, the incompressible pollutant transport model is built on the convection and dispersion equations:

$$\frac{\partial C}{\partial t} + U \cdot \nabla C - \operatorname{div}(D\nabla C) = f, \quad (x,t) \in \Omega \times]0,T[\,, \tag{2.1}$$

where C is the concentration of hydrocarbons in the sea water, U the Darcy velocity, f a source term, T the final time of observation and D the diffusion-dispersion tensor. The tensor D is given by $D = d_m + |U|\,\{\alpha_L P(U) + \alpha_T(I-P)(U)\}$, where d_m is the molecular tensor diffusion coefficient, α_L and α_T are the longitudinal and transverse dispersion coefficients and P_L and $I - P_L$ are the projections in the direction of the flow and the direction orthogonal to the flow respectively, which allow to consider the influence of the transport speed of the current (in dimensions of space chosen) on the phenomenon of dispersion, with $P_L(U)_{ij} = U_i U_j\,|U|^{-2}$, where U_i, $i = 1 \leq 3$, are the components of U. In a two dimensional space, (2.1) can be simplified to

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} - \frac{\partial}{\partial x}\left(D_x\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y\frac{\partial C}{\partial y}\right) = f, \tag{2.2}$$

where u and v are two components of U in the directions x and y; the dispersion coefficients D_x and D_y depend upon the flow characteristics and vary according to the velocities u and v, see for instance [6].

2.2 Hydrodynamic Model

The hydrodynamic model is derived from the Navier–Stokes equations which couple mass conservation equations (continuity equations for incompressible flow) and momentum conservation equations. They are used to describe water movement in a marine environment taking into account all the factors affecting the rate of transport, namely, the pressure force, gravitational force, the Coriolis force and the friction force turbulent due to the viscosity. In our domain Ω we consider the following problem:

$$\begin{cases} \dfrac{\partial U}{\partial t} + U \cdot \nabla U + \dfrac{1}{\rho}\nabla P = \mu \triangle U + F - \dfrac{\tau^f}{h} & \text{in } \Omega \times]0,T[\,, \\ \dfrac{\partial h}{\partial t} + \nabla \cdot (hU) = 0. \end{cases} \tag{2.3}$$

Here, U is the velocity, it has two components u and v, μ is the horizontal eddy viscosity corresponding to the inverse Reynolds number, ρ is the density of sea water, P is the pressure from the water column under the law of hydrostatics, it corresponds to $P = \rho g h$

with g the acceleration of gravity and h the depth of the sea water. In equation (2.3), F represents the Coriolis force which describes the influence of earth rotation on the direction of currents. For the two-dimensional space, F has two components along the axes x and y:

$$\begin{cases} F_x = 2\psi \sin\phi . v = f v, \\ F_y = -2\psi \sin\phi . u = -f u, \end{cases}$$

where f is the Coriolis factor, ψ is the speed of rotation of the earth, and ϕ is the latitude of the geographical area of study. Finally, τ^f is the bottom shear stresses with two components:

$$\begin{cases} \tau_x^f = g\rho u \dfrac{N^2}{h^{1/3}} \sqrt{u^2+v^2}, \\ \tau_y^f = g\rho v \dfrac{N^2}{h^{1/3}} \sqrt{u^2+v^2}. \end{cases}$$

The developed form of hydrodynamic equations is the following:

$$\begin{cases} \dfrac{\partial u}{\partial t} + u\dfrac{\partial u}{\partial x} + v\dfrac{\partial u}{\partial y} + g\dfrac{\partial h}{\partial x} = \mu\left(\dfrac{\partial^2 u}{\partial x^2} + \dfrac{\partial^2 u}{\partial y^2}\right) + f v - g u\dfrac{N^2}{h^{4/3}}\sqrt{u^2+v^2} \\ \dfrac{\partial v}{\partial t} + u\dfrac{\partial v}{\partial x} + v\dfrac{\partial v}{\partial y} + g\dfrac{\partial h}{\partial y} = \mu\left(\dfrac{\partial^2 v}{\partial x^2} + \dfrac{\partial^2 v}{\partial y^2}\right) - f u - g v\dfrac{N^2}{h^{4/3}}\sqrt{u^2+v^2} \\ \dfrac{\partial h}{\partial t} + \dfrac{\partial (hu)}{\partial x} + \dfrac{\partial (hv)}{\partial y} = 0 \end{cases} \tag{2.4}$$

with initial condition the velocity $U(t=0) = U^0$ and suitable boundary conditions.

2.3 Boundary Conditions

The domain Ω mimics the bay of Tangier. As a consequence, the three dimensional geometry of the domain Ω is limited by the bottom, the free surface of the water, the coastline and some imaginary vertical wall on the sea at some reasonable distance of the shore. To simplify the numerical tests, we have considered a two dimensional setting neglecting the limits of the bottom and the free surface of the water. This transforms the dimensions of the domain Ω from $(3D)$ to $(2D)$. In this context, for the numerical resolution of the Navier–Stokes equation in $(2D)$, we neglect the parameters of the bottom shear stresses τ^f, and the depth of the sea water h. As a consequence, we work with a $(2D)$ Lipschitz domain Ω with Dirichlet boundary conditions on the coastline and Neumann conditions elsewhere.

3 Numerical Model

We now present the discretization scheme and the variational formulation of the problem. A classical way to compute an approximation to the Navier–Stokes equations is to discretize the variational problem via finite elements for the spacial variables and the characteristic approach to deal with the time evolution. With this characteristic approach, the convection term $\dfrac{\partial U}{\partial t} + U \cdot \nabla U$ is approximated by the following scheme:

$$\frac{U^{n+1} - U^n \circ X^n}{\Delta t} \simeq \frac{\partial U}{\partial t} + U \cdot \nabla U.$$

For a particle x that lives in Ω at time t^{n+1}, $X^n(x)$ gives the position at time $t^n = n\Delta t$, where this particle x comes from. So, we have $X^n(x) = \zeta_x(t^n)$ where $\zeta_x(t^n)$ is a solution of the differential equation $d\zeta/dt = U(t, \zeta_x(t))$ with inital condition $\zeta_x(t^{n+1}) = x$ and solved from t^{n+1} to t^n. Then, the time discretization scheme of the hydrodynamic model are the following equations:

$$\begin{cases} U^{n+1} - \nu \Delta t \Delta U^{n+1} + \Delta t \nabla P^{n+1} = U^n \circ X^n, \\ \nabla \cdot U^{n+1} = 0. \end{cases} \tag{3.1}$$

After multiplying by a test function ω, integrating on Ω and applying the boundary conditions, we obtain that

$$\frac{1}{\Delta t} \int_\Omega U^{n+1} \cdot \omega - \nu \int_\Omega \Delta U^{n+1} \cdot \omega + \int_\Omega \nabla P^{n+1} \cdot \omega = \frac{1}{\Delta t} \int_\Omega (U^n \circ X^n) \cdot \omega \tag{3.2}$$

for any vector function $\omega \in H^1(\Omega)^2$. Then, integration by parts, using $\mathbf{n}$ as the outward normal to $\partial\Omega$, gives

$$\int_\Omega \Delta U^{n+1} \cdot \omega = -\int_\Omega \nabla U^{n+1} \cdot \nabla \omega + \int_{\partial\Omega} \frac{\partial U^{n+1}}{\partial \mathbf{n}} \cdot \omega, \tag{3.3}$$

$$\int_\Omega \nabla P^{n+1} \cdot \omega = -\int_\Omega P^{n+1}\, div(\omega) + \int_{\partial\Omega} P^{n+1} (\mathbf{n} \cdot \omega). \tag{3.4}$$

Therefore,

$$\begin{cases} \dfrac{1}{\Delta t} \displaystyle\int_\Omega U^{n+1} \cdot \omega + \mu \int_\Omega \nabla U^{n+1} \cdot \nabla \omega + \mu \int_{\partial\Omega} \left(-\frac{\partial U^{n+1}}{\partial \mathbf{n}} + P^{n+1} \mathbf{n} \right) \cdot \omega, \\ \displaystyle\int_\Omega P^{n+1} div(\omega) = \frac{1}{\Delta t} \int_\Omega (U^{n+1} \circ X^n) \cdot \omega. \end{cases} \tag{3.5}$$

Now, we take $\partial\Omega = \partial\Omega_D \cup \partial\Omega_N$, where $\partial\Omega_N$ accounts for the boundary of the domain on the sea and $\partial\Omega_D$ represent the shore. Having a free flow on $\partial\Omega_N$ amounts to the boundary condition

$$\frac{\partial U}{\partial \mathbf{n}} - P\mathbf{n} = 0 \text{ on } \partial\Omega_N$$

and assuming flow at rest on the shore:

$$U = 0 \text{ on } \partial\Omega_D.$$

As a consequence, it makes sense to take

$$w = 0 \text{ on } \partial\Omega_D,$$

that respects the data of the sought solution U and also cancels the unknown normal contribution on $\partial\Omega_D$ of U. Then, all boundary terms are gone and if we take

$$\begin{cases} a(U^{n+1}, \omega) = \dfrac{1}{\Delta t} \displaystyle\int_\Omega U^{n+1}\omega + \mu \int_\Omega \nabla U^{n+1} \nabla\omega \\ b(\omega, P^{n+1}) = - \displaystyle\int_\Omega P^{n+1} \nabla\omega \\ l(\omega) = \dfrac{1}{\Delta t} \displaystyle\int_\Omega (U^{n+1} \circ X^n)\omega. \end{cases} \tag{3.6}$$

Then, the variational problem becomes a saddle point problem at each time step. For $n \geq 0$ and given $U^n \in V_h$, find $(U^{n+1}, P^{n+1}) \in V_h \times M_h$ such that:

$$\forall\omega \in V_h, \quad a(U^{n+1}, \omega) + b(\omega, P^{n+1}) = l(\omega), \tag{3.7}$$

$$\forall q \in M_h, b(U^{n+1}, q) = 0, \tag{3.8}$$

where V_h and M_h are finite element spaces for the velocity and pressure taken in the usual way and satisfying the standard discrete $\inf$-$\sup$ conditions, for instance, we could take the pair of spaces $\mathbb{P}_2 - \mathbb{P}_1$ or $\mathbb{P}_{1b} - \mathbb{P}_1$, see [2] or [7]. For example, in the simplest case $\mathbb{P}_2 - \mathbb{P}_1$, an idea on the definition of the spaces is the following one: given a regular triangulation of Ω, define $\Omega_h = \bigcup_{k=1}^{nbv} T_k$, and denote by υ^i, $i \in \{1, \ldots, nbv\}$, the vertices of the triangulation. Then define the discrete spaces V_h and M_h by:

$$V_h = \{\upsilon_h \in C^0(\Omega_h), \forall k \in \{1, \ldots, nbt\}, \upsilon_h \mid T_h \in \mathbb{P}_2\}, \tag{3.9}$$

$$M_h = \{\upsilon_h \in C^0(\Omega_h), \forall k \in \{1, \ldots, nbt\}, \upsilon_h \mid T_h \in \mathbb{P}_1\}, \tag{3.10}$$

where $\mathbb{P}_k$ designates the vector space of polynomials of two variables of the overall degree less or equal to k. The functions of V_h are entirely determined by their values in each summits υ^i, $i \in \{0, \ldots, nbv - 1\}$, and the midpoints of all edges of the mesh. The dimension of the space V_h is equal to the total number $nbv + nbe - 1$, where nbe is the number of edges of the nodes of the mesh. The functions of M_h are entirely determined by their values in each summits υ^i, $i \in \{0, \ldots, nbv - 1\}$. The dimension of M_h is equal to the total number nbv of vertices of the mesh.

4 Numerical Simulation

In this section, some results related to nonaromatic hydrocarbons discharged on the Bay of Tangier are investigated. The maps presented in the figures below are based on experimental measures published in [1], and are realized by ArcGIS 9 software. Figure 4.1

illustrates the spatial distribution of hydrocarbon concentrations while Figure 4.2 corresponds to the interpolation of these concentrations. After analyzing the maps, we deduce that the largest concentrations are located at the mouth of Mghogha river and in Tangier's harbor. However, the spatial interpolation model does not give the true distribution of concentrations because it does not take into account the natural factors influencing the distribution, namely current velocity, dispersion coefficient, and wind speed. Hence, the importance of establishing a numerical model which allows to take into account all these factors, and consequently to obtain a more realistic model. Since we use a finite element scheme for the resolution in space of equation (2.1), we build the triangulation τ_h of Ω shown in Figure 4.3. Time discretization is performed by a first order characteristic scheme implemented in FreeFem++ [9]. In Figure 4.4, we plot the concentration C at different instants of time for the numerical simulation of equation (2.1); the velocity is computed by solving Navier–Stokes equations with Dirichlet boundary conditions on the coastline and Neumann conditions elsewhere.

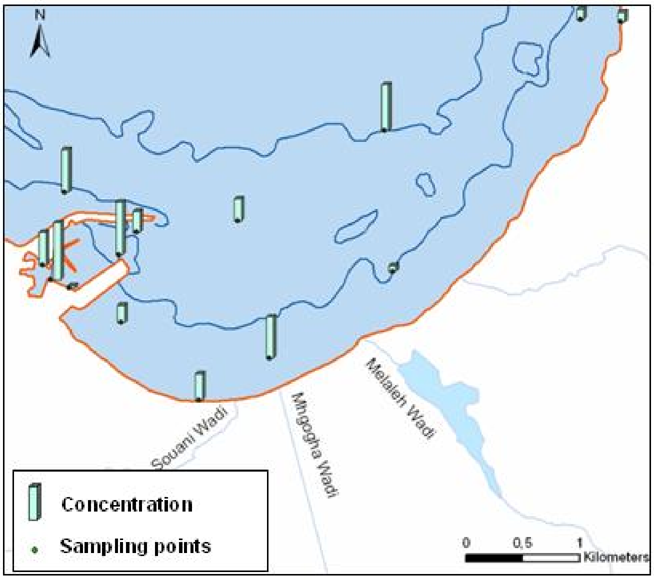

Figure 4.1: Map indicating the spatial distribution of hydrocarbons in Tangier Bay.

5 Conclusion and Perspectives

In this paper, a mathematical model for the evaluation of hydrocarbon concentrations in Tangier Bay was presented. The model was based on convection and dispersion equations. The flow velocity was calculated for the two dimensional incompressible Navier–Stokes equations. Numerical tests were carried out by using finite element method with the free software FreeFem++ [9]. Following some experimental measures given in [1],

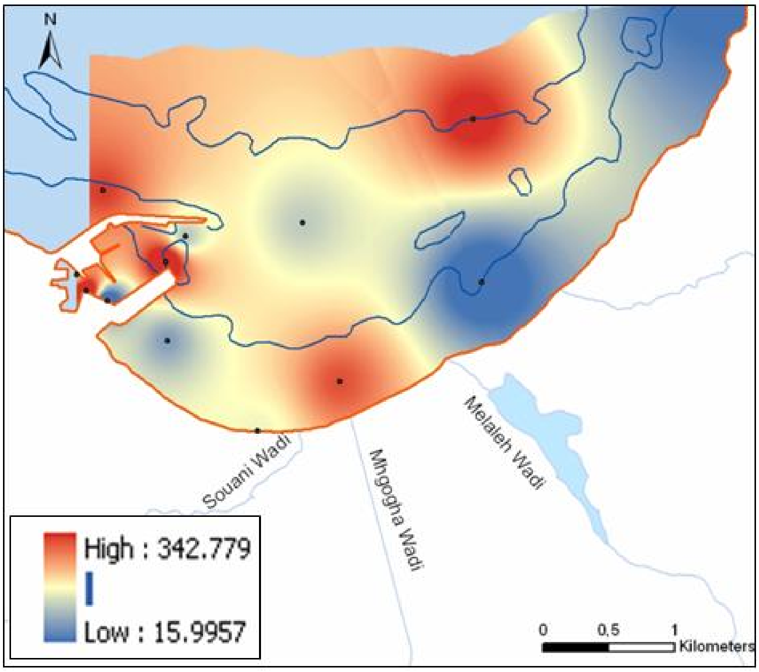

Figure 4.2: Interpolated concentrations elaborated by ArcGIS software.

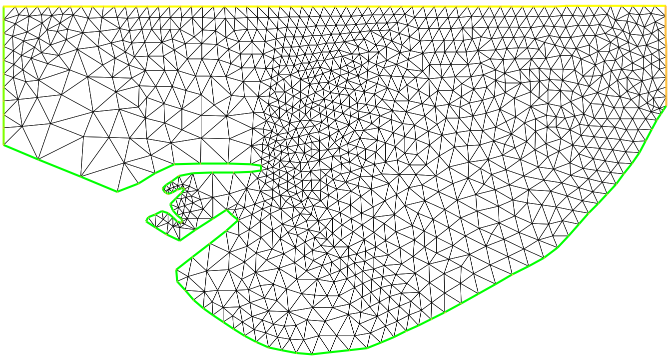

Figure 4.3: Finite element mesh of the study area.

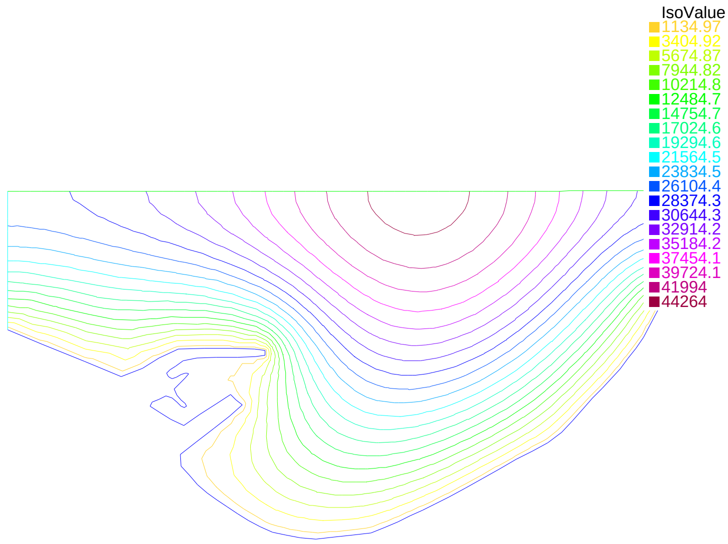

Figure 4.4: Concentrations of hydrocarbons on the Bay of Tangier.

and using ArcGIS 9 software, we established a spatial distribution of hydrocarbon concentrations and the corresponding interpolated values. Our approach may be extended to the 3-dimensional space taking into account the sea level variation. Finally, in order to construct a realistic numerical model, an inverse problem may be solved to adjust model parameters and to determine their associated uncertainty. Calibration results may show close agreement between simulated and expected concentrations.

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