

NUMERICAL MODELING OF MARINE POLLUTION: APPLICATION TO HYDROCARBONS DISTRIBUTION IN TANGIER BAY

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ABSTRACT. The study of marine pollution has become a major necessity and aims to offer solutions for the preservation of the marine environment. Our work attempts to make a contribution to solve this problem. More precisely, we are mainly concerned with a mathematical modeling and a numerical simulation of marine pollution in Tangier Bay which undergoes an alarming state. The mathematical model is built on convection and dispersion equations coupled with a hydrodynamic model based on incompressible Navier-Stokes equations. The numerical solving of the convection term uses the Characteristic–Galerkin method. Finally, some numerical tests based on a finite element discretization are presented here and are performed by **FreeFem++** software. The numerical results indicate that high concentrations of hydrocarbons are located at the mouth of Mghogha river, in the harbor sheltered areas and in the transitory ships boarding area.

1. INTRODUCTION

Many works dealing with modeling marine pollution threat are worldwide growing up. Some case studies are listed here in order to give a general idea about the state of the art on modelling the pollution of marine environments. In the Daya Bay, southeast of China, numerical modeling, using Monte Carlo method, has been carried out in order to predict the drift and the propagation of oil after the oil spill paroxysmal accident, [6]. In the Middle East, the Arabian Gulf is another area concerned by marine pollution due to the high petroleum transportation, the industrialization and the urban development along of its shores. This area was concerned by a numerical modeling of hydrocarbons discharges by using finite differences scheme, [8]. In [12], the investigation consisted of building a two dimensional non-linear hydrodynamic finite differences model and an advection-diffusion model in order to simulate the behavior of discharged pollutants into coastal lagoon system of Topolobampo, located in northwestern of Mexico. In the Atlantic Ocean, the Gibraltar Strait is a strategic transit pathway characterized by complex maritime routes (Algeciras-Ceuta, Algeciras-Tangier and Tarifa-Tangier), and by a hazardous transport of radioactive materials. In this context, this area has been

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subject of some modeling studies of the pollutants behavior and their dispersion into shallow marine environment, [3, 13]. Mathematical models were solved by applying a finite volume method and a Lagrangian approach. Recently the Algeciras Bay, in the northern side of Gibraltar Strait was the subject of a numerical study for understanding the pollutant dynamics and their spreading into the Bay. All equations were solved by explicit finite differences schemes, [15]. Eastward of the Gibraltar Strait, the Gulf of Cadiz was concerned by a recent study [14] where hydrodynamic, sediment and metal transport models were simulated by explicit finite differences schemes. In the southern side of the Gibraltar Strait, Tangier Bay object of this work undergoes an alarming pollution state due to Tangier-Med Harbor. Only seldom studies were realized for modeling the fate of pollutants dispersed in coastal and marginal marine environments near Tangier Bay, [2, 4]. Therefore, it becomes necessary to increase scientific investigation in order to quantify marine pollution and to suggest various reliable sustained remediations. In this context, the present work improves an already published research [9] in order to update it by more accurate results. The main objective is to define and to implement a new hydrodynamic model coupled with a transport model in order to simulate pollutants distribution in Tangier Bay using FreeFem++, [7]. We take into account the effect of the waves currents velocity in the study area and different sources of pollution coming from rivers and sea.

The paper is organized as follows. Section 2 describes the mathematical formulation of the problem. Section 3 presents a numerical formulation of the problem with a finite element method and section 4 relates some computational results. Section 5 closes the paper with a conclusion and some perspectives.

2. MATHEMATICAL FORMULATION OF THE PROBLEM

In this study, an incompressible fluid is considered and two models are presented in order to simulate contaminants transport in Tangier Bay. The first one is a hydrodynamic model based on Navier-Stokes equations, it provides the velocity field and water levels. The second one is based on convection-dispersion equations for the assessment of the concentration and its distribution.

The hydrodynamic model describes the water movement in a marine environment taking into account all the factors affecting the contaminant transport, namely, the pressure, the gravity, the Coriolis and the friction forces due to the viscosity, [5]. This model derives from Navier-Stokes equations coupled with mass conservation equations (continuity equations for incompressible flow) and momentum conservation equations. We consider the following problem where Ω denotes the domain of simulation. We impose Dirichlet conditions on the velocity field.

$$\begin{cases} \frac{\partial U}{\partial t} + U \cdot \nabla U + \frac{1}{\rho} \nabla P = \mu \Delta U - \frac{\tau}{h} \\ \frac{\partial h}{\partial t} + \nabla \cdot (hU) = 0, \text{ in } \Omega \times]0, T[\end{cases} \quad (2.1)$$

The function U corresponds to the velocity, μ is the viscosity corresponding to the inverse Reynolds number, ρ is the density of sea water, P denotes the pressure and it corresponds to $P = \rho gh$ with g is the gravity, h is the sea water depth and τ corresponds to the shear stress.

The transport model uses the velocity calculated by the hydrodynamic model. In $\Omega \subset \mathbb{R}^3$, the transport model is built on the basis of convection and dispersion equations as follows

$$\begin{cases} \frac{\partial c}{\partial t} + \text{div}(Uc - D\overrightarrow{\text{grad}}c) = f & \text{in } \Omega \times]0, T[\\ c(., 0) = c^0 & \text{in } \Omega \end{cases} \quad (2.2)$$

We denote the hydrocarbons concentration in sea water by c , f is a source term, T is the final time of observation and D is the dispersion tensor.

Boundary conditions: We can impose Neumann boundary conditions for the transport on $\partial\Omega$ like $(Uc - D\nabla c) \cdot n_\Omega = q$ with n_Ω the outward normal to the boundary $\Gamma = \partial\Omega$ or we can impose multiple Dirichlet boundary conditions on a number parts of $\partial\Omega$.

Moreover, the domain Ω is limited by the bottom, the free surface of water, the coastline and some imaginary vertical wall on the sea at some reasonable distance of the shore. For sake of simplicity, we consider a two dimensional setting neglecting the limits of the bottom and the free surface of water. This assumption transforms Ω from a three dimensional domain to a two dimensional one. Thus, for the numerical resolution of Navier-Stokes equations in the two dimensional domain, we neglect the parameters τ and h .

Comparing this study with those realized in the Gibraltar Strait [3, 13], Algeciras and Tangier bays [2, 4, 15], we note that only a hydrodynamic model was applied to calculate the tidal or the wave current velocities, while the studies on Algeciras Bay [15], Gibraltar Strait [13] and this study, deals with a hydrodynamic model jointly applied with the transport-dispersion model to modeling the transport-dispersion of pollutants into shallow marine environments. In the other hand, the Tangier bay hydrodynamic model [4] was applied simultaneously with a transport-diffusion model. The numerical resolution method for previous mathematical modeling used in the Gibraltar Strait and Tangier Bay is the finite volume method, whereas finite element method was applied for the current study.

3. FINITE ELEMENT DISCRETIZATION

The variational problem of the hydrodynamic model was described and the transport model was solved considering a constant velocity, [9]. In the present study, the velocity is variable; the hydrodynamic model is coupled with the transport model in order to quantify a two-dimensional distribution of hydrocarbons concentration. For the sake of simplicity, we assume that the dispersion tensor D is constant, then the model becomes

$$\frac{\partial c(x, y, t)}{\partial t} + U(x, y, t)\nabla c(x, y, t) - D\Delta c = 0, \quad (x, y, t) \in \Omega \times]0, T[\quad (3.1)$$

with an initial condition c^0 and multiple Dirichlet boundary conditions. It is important to mention that the convection term $\frac{\partial c}{\partial t} + U\nabla c$ is approximated by

$$\frac{c^{n+1}(x) - c^n \circ X^n(x)}{\Delta t} \quad (3.2)$$

where Δt is the time step and $X^n(x)$ is the characteristic line providing the position of a particle x at time t^n . The function $X^n(x)$ represents the unique solution of the ordinary differential equation

$$d\zeta/dt = U(t, \zeta_x(t)) \quad (3.3)$$

where we set $X^n(x) = \zeta_x(t^n)$.

Remark. *The numerical solving of the convection term is done by the Characteristic-Galerkin method implemented by FreeFem++ with a function named `convect`, [7].*

Now, by using an implicit Euler scheme and by injecting the equality (3.2) in the equation (3.1), we obtain the following discretization

$$\frac{c^{n+1} - c^n \circ X^n}{\Delta t} - D\Delta c^{n+1} = 0 \quad (3.4)$$

Consequently, the variational formulation of the equation (3.4) is

$$\forall \varphi \in H_0^1(\Omega), \frac{1}{\Delta t} \int_{\Omega} c^{n+1} \cdot \varphi - D \int_{\Omega} \Delta c^{n+1} \cdot \varphi = \frac{1}{\Delta t} \int_{\Omega} c^n \circ X^n \cdot \varphi \quad (3.5)$$

where we multiplied the equation (3.4) by a test function φ and we integrated on the domain Ω . Using a Green's formula on $\int_{\Omega} \Delta c^{n+1} \cdot \varphi$ with n the outward normal to $\partial\Omega$, we obtain the following equality

$$\int_{\Omega} \Delta c^{n+1} \cdot \varphi = - \int_{\Omega} \nabla c^{n+1} \cdot \nabla \varphi + \int_{\partial\Omega} \frac{\partial c^{n+1}}{\partial n} \cdot \varphi \quad (3.6)$$

Since the boundary term $\int_{\partial\Omega} \frac{\partial c^{n+1}}{\partial n} \cdot \varphi$ is always null ($\varphi \in H_0^1(\Omega)$), the equation (3.5) becomes:

$$\frac{1}{\Delta t} \int_{\Omega} c^{n+1} \cdot \varphi + D \int_{\Omega} \nabla c^{n+1} \cdot \nabla \varphi = \frac{1}{\Delta t} \int_{\Omega} c^n \circ X^n \cdot \varphi \quad (3.7)$$

Now, if we set

$$\begin{cases} a(c^{n+1}, \varphi) = \frac{1}{\Delta t} \int_{\Omega} (c^{n+1} \varphi + D \nabla c^{n+1} \cdot \nabla \varphi) \\ l(\varphi) = \frac{1}{\Delta t} \int_{\Omega} (c^n \circ X^n) \varphi \end{cases} \quad (3.8)$$

Approximation space Q_h : For the simplest case, let T_k be a regular triangulation of Ω , $k = 1, \dots, n_t$. If we set $\Omega_h = \bigcup_{k=1}^{n_t} T_k$, then the discrete space Q_h is defined by

$$Q_h = \{v \in C^0(\Omega_h) : \forall T_k \in \tau_h, v|_{T_k} \in \mathbb{P}_2(T_k)\} \quad (3.9)$$

where τ_h is a triangulation of Ω or mesh and \mathbb{P}_2 designates the space of polynomials of the degree less or equal to 2 on each triangle of τ_h . The vertices of T_k are the nodes of the mesh and the functions of Q_h are entirely determined by their values in each vertices. The dimension of Q_h is equal to the total number of vertices of the mesh.

then the discrete solution of the problem 3.1 is given at each time step by the following problem.

For a given Hilbert space Q_h and a concentration function $c^n \in Q_h$, find $c^{n+1} \in Q_h$ such that

$$a(c_h^{n+1}, \varphi_h) = l(\varphi_h), \quad \forall \varphi_h \in Q_h \quad (3.10)$$

Remark. The term $c^n \circ X^n$ in $l(\varphi)$ is approximated by the quantity $c^n(x + U^n(x)\Delta t)$.

Following the above, the existence and uniqueness of a solution of the variational problem (3.10) is a consequence of Lax-Milgram's lemma.

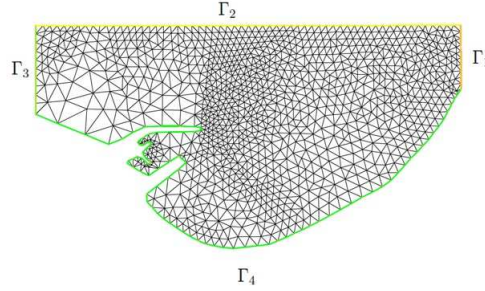
Finally, under Lax-Milgram's lemma hypothesis and as the form a is symmetric, we deduce that the solution of the problem (3.10) corresponds to the minimum of the functional

$$J(v) = \frac{1}{2}a(u, v) - l(v) \quad (3.11)$$

4. NUMERICAL SIMULATION

The problem 3.10 is solved by the Feefem++ software. The mesh of Ω is illustrated on Figure 1 where we divided the boundary Γ of Ω into four parts: $\Gamma = \Gamma_1 \cup \Gamma_2 \cup \Gamma_3 \cup \Gamma_4$.

FIGURE 1. Mesh of Tangier Bay

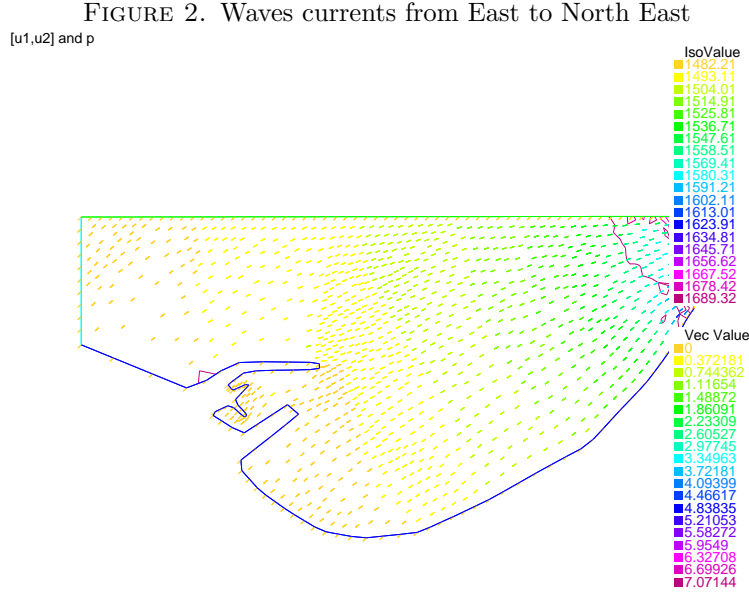


The hydrodynamic model solved in this paper takes into account only the effect of the waves currents derived from East and West (Figures 2 et 3). We remark that the results are in conformity with the actual data published in [10] where the velocity of the waves currents coming from the North East is approximately $v = 0.4m/s$, and the one coming from the North West is $v < 0.3m/s$. In the West extremity of the Bay, the estimated velocity is very low in the harbor protection area according to some published results in [1].

The results of the convection-dispersion model show that the highest concentrations are located near the coast line, especially in the protected area of the harbor characterized by a low hydrodynamic regime which promotes pollutants accumulation, (Figure 4).

Comparing our numerical simulation results with those obtained on the Algeciras bay and the Gibraltar Strait, it is noteworthy that in the Algeciras bay [15], the hydrodynamic model had given a tides realistic representation. On the other hand, the Zn, Cu and Ni distribution, in both, water and sediments calculated by the dispersion model matched well field data and observations. Similarly, the Gibraltar strait results [13], show that tide and current amplitudes were calculated in good

agreement with the field observations. Also, published results in [2] and performed in our study area allowed to visualize effluents dispersion taking into account the effect of tide movements (ebb and flow). Also, this study allows calculation of the main wave's current velocity and numerical simulation pollutants transport-dispersion. Thus, the obtained hydrodynamic model was enough realistic for the implementation of pollutants dispersion model and accordingly, obtained numerical results were fitting well both observations and field data.



5. CONCLUSION AND PERSPECTIVES

In this paper, we presented an overview of different studies made at various places in the world for modeling the fate of pollutants spilled into the marine environment. Regarding our study on Tangier Bay, we defined a mathematical model built on the basis of hydrodynamic Navier-Stokes equations and on a transport convection-dispersion equations. We solved the hydrodynamic model in order to calculate the transport velocity and then we solved the convection-dispersion equations in order to evaluate concentrations of pollutants discharged into Tangier Bay. We solved the discrete variational problem with a finite element method and we used **FreeFem++** software to perform the numerical simulation. The numerical results obtained indicate that the waves current coming from East to North-East are the most dominant, and that the most polluted areas are the mouth of Mghogha river and the harbor protected area. This simulation may be more realistic if we solve the hydrodynamic model taking into account the changes on the western part of the Bay after the construction of the new marina. These changes will have an impact on

FIGURE 3. Waves currents from West to North-West
[u1,u2] and p

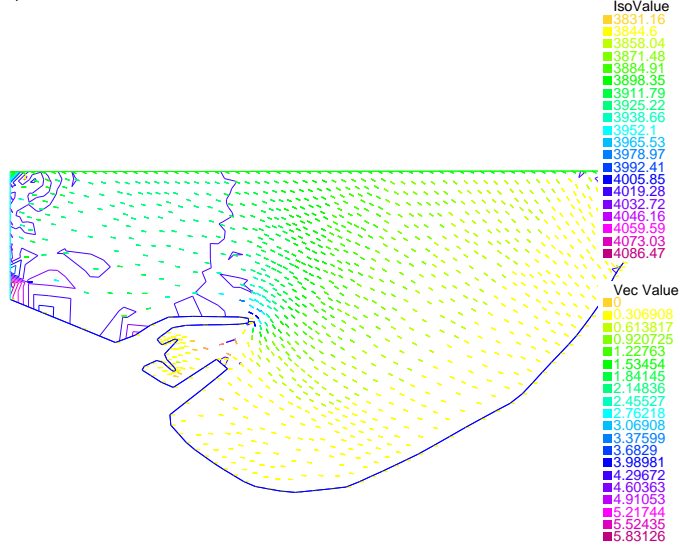
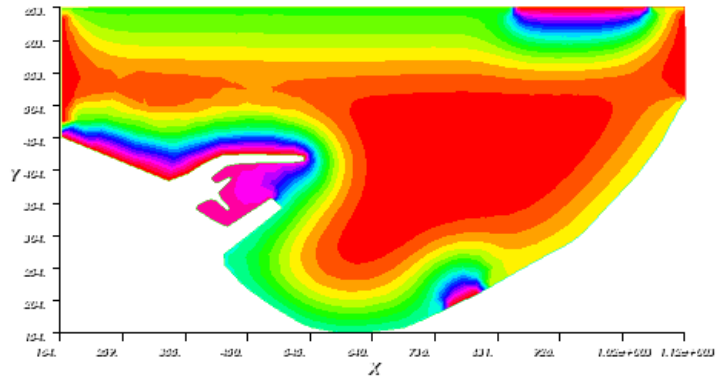


FIGURE 4. Concentration hydrocarbons in Tangier Bay



velocity and currents direction and consequently on the fate of pollutants discharged into Tangier Bay.

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