Hybrid Methods for the Simulation of Pollutant Transport in Estuaries

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Abstract: This paper deals with the simulation of the transport of a scalar non-interacting and non-dissipative pollutant in a shallow water environment. We present a hybrid method involving a classic finite difference scheme for the solution of the shallow water equations and a semi-Lagrangian method for the simulation of the time evolution of the scalar pollutant field.

Keywords: shallow water equations, semi-Lagrangian method, finite difference, transport of pollutants, numerical solutions.

1. Introduction

During the past years there has been an increasing concern about water management, involving not only potable water resources but also aspects of pollution on rivers, estuaries and coastal waters, which can have drastic consequences on life within its neighbourhood. Human activity has been causing severe damage to these masses of water through the discharge of huge quantities of effluents, either thermal or chemical, which are significantly altering the conditions of the ecosystem. Related to these activities is the risk of unpredictable events or disasters that alter dramatically in a short period of time the environment. Recently, a discharge of an enormous amount of chemical pollutants in Pomba and Paraíba do Sul rivers in the north of Rio de Janeiro state caused several problems to the population. One of the measures taken to improve these type situations is the effort to simulate the various physical, chemical and biological phenomena that take place in those environments, in order to predict its effects and identify corrective actions.

In the field of numerical simulation, the so-called Shallow Water Equations, SWE, are the main equations to be dealt with. These are a time-dependent two-dimensional system of non-linear partial differential equations of hyperbolic type. Two-dimensional solutions, either with horizontal or vertical grids, are generally applied to estuaries, bays, lagoons and coastal circulation. Channels, rivers and special situations on estuaries are treated with the one-dimensional model. Other fields of application of these equations include atmospheric and oceanic flows, among others.

The numerical solution of the SWE equations is still a computationally challenging task, even after the strong simplifying assumptions made in their derivation. The hyperbolic character of the equations, which admit discontinuous solutions, is the main responsible for the difficulties encountered.

For the 2-D case, Martinez and Santos (1993) present a numerical solution for the hydrodynamic problem based on the explicit method of Taylor-Galerkin, where the spatial domain is discretized using finite element techniques and time integration is achieved through Taylor expansion. Jin and Kranenburg (1993) developed a quasi-3D scheme which is employed on the solution of large scale circulation in water bodies, providing full spatial velocity distribution. Kikukawa *et alii* (1997) presented a solution for the hydrodynamic problem coupled to a salt conservation equation and to the energy equation for temperatures, in a 2-D vertical grid configuration using a finite difference scheme. As for 1-D, Soetaert and Herman (1995-a) presented a set of equations modelling the advective-diffusive transport of a conservative substance, which were solved by Runge Kutta techniques. In another work, the same authors (1995-b) extended their work to include the effects of chemical transformation of the conserved substance. Rentrop and Steinebach (1997) presented an analytical approximation of an advective-diffusive equation including an exchange term accounting for the transport of dissolved substances, that was solved by a numerical combination of the method of lines and stiff integrators of Rosenbrock-Wanner type.

A relevant issue is the simulation of the transport of a scalar, non-interacting pollutant. Such model can simulate the transport of pollutants as occurred in the recent disaster in Pomba and Paraíba do Sul rivers. In this paper we present a treatment of this problem using semi-Lagrangian finite difference scheme. Such scheme for the time evolution of the pollutant allows large time step and an adequate representation of the pollutant scalar field.

This paper is organised as follows. Section 2 presents the equations for modelling the transport of a non-degrading and non-diffusive scalar pollutant. Section 3 presents the finite difference scheme used for solving SWE while in section 4 we derive a semi-Lagrangian scheme for the transport equation for the pollutant. Finally in section 5 we present the results of the simulation.

2. Model of a Passive Scalar Pollutant

A model describing water flow under the effects of gravity and with a free surface, such as encountered in rivers and estuarine regions, can be represented by the shallow water equations. Let the bottom of the liquid region and the height of the water column be represented, respectively, by $z = b(x, y)$ and $h(x, y, t)$. Then the air-water interface is represented by the surface $z = b(x, y) + h(x, y, t)$; see figure 2.1.

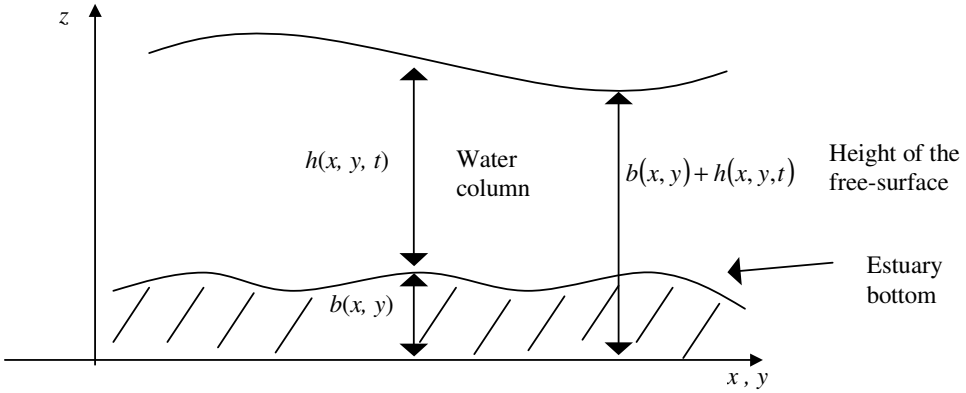

Figure 2.1. Representation of a free-surface flow in a estuarine region.

By assuming that the horizontal spatial scales are much larger than the water column one finds that the vertical acceleration of the fluid is negligible. Then let $(u, v) = (u(x, y, t), v(x, y, t))$ be the horizontal components of the fluid velocity field. The equations for *u*, *v* and *h* are (Stoker, 1958)

$$\begin{cases} h_t + (hu)_x + (hv)_y = 0 & (2.1) \\ u_t + uu_x + vu_y + gh_x = -gb_x & (2.2) \\ v_t + uv_x + vv_y + gh_y = -gb_y & (2.3) \end{cases}$$

for $0 \le x \le L, 0 \le y \le M$ and $t \ge 0$. Here *g* denotes the acceleration of gravity.

Equation (2.1) represents mass conservation and equations (2.2) and (2.3) represent momentum conservation. In this model we neglect turbulence and friction effects and consider that these are no contributions of sources or sinks neither in the mass nor in the momentum equation. The assumption of negligible vertical acceleration leads to a hydrostatic pressure distribution (shallow water theory hypothesis).

For simplicity we consider an estuary region which is slender and with a horizontal flat bottom. In this way, $v = b_x = b_y = 0$, the variables *u* and *h* depend only on *x* and *t*, and we keep only equations (2.1) and (2.2) which we rewrite with the stated simplifications:

$$\begin{cases} h_t + uh_x + hu_x = 0 & (2.4) \\ u_t + uu_x + gh_x = 0 & (2.5) \end{cases}$$

for $0 \le x \le L$ and $t \ge 0$.

Let now ϕ denote the concentration (mass of pollutant per unit volume of the fluid) of a scalar non-reacting (passive) non-diffusive pollutant. Then ϕ will be advected by the water-flow, as represented by

$$\phi_t + u\phi_x = 0. \quad (2.6)$$

for $0 \le x \le L$ and $t \ge 0$.

3. Numerical Solution of Shallow Water Equations

in this section we present a finite difference discretization of SWE, equations (2.4) and (2.5), as well as some discussion on boundary condition.

3.1. Lax-Friedrichs Method

Equations (2.4) and (2.5) can be rewritten in vector form as

$$\begin{pmatrix} h \\ u \end{pmatrix}_t + \overbrace{\begin{pmatrix} u & h \\ g & u \end{pmatrix}}^{A} \begin{pmatrix} h \\ u \end{pmatrix}_x = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \; 0 \le x \le L \text{ and } t \ge 0 \tag{3.1}$$

or, in conservation form, as

$$\begin{pmatrix} h \\ u \end{pmatrix}_t + \overbrace{\begin{pmatrix} hu \\ \dfrac{u^2}{2} + gh \end{pmatrix}}^{G(h,u)}_x = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \; 0 \le x \le L \text{ and } t \ge 0 . \tag{3.2}$$

The eigenvalues of A are $\lambda_{\pm} = u \pm \sqrt{hg}$ and when they have distinct signs (which is equivalent to $-\sqrt{hg} < u < \sqrt{hg}$) the flow is called subcritical (Rentrop & Steinebach, 1997). In this flow pattern, system (3.2) requires just one boundary condition at each boundary, $x = 0$ and $x = L$, which will be taken as the heights of the water columns,

$$h(0,t) = h_L(t); \;\; h(L,t) = h_R(t); \;\; t \ge 0 . \tag{3.3}$$

Initial conditions have also to be prescribed,

$$\begin{pmatrix} h(x,0) \\ u(x,0) \end{pmatrix} = \begin{pmatrix} h_0(x) \\ u_0(x) \end{pmatrix}; \; 0 \le x \le L . \tag{3.4}$$

Only smooth solutions of the evolution equation (3.2) will be considered which, together with the subcritical flow conditions, frames the set of applications admissible by the methodology presented. In this case, Lax-Friedrichs finite difference scheme (Sod, 1985) is appropriate to solve equation (3.2),

$$\begin{aligned} \begin{pmatrix} h_j^{k+1} \\ u_j^{k+1} \end{pmatrix} &= \frac{1}{2}\begin{pmatrix} h_{j-1}^k + h_{j+1}^k \\ u_{j-1}^k + u_{j+1}^k \end{pmatrix} - \frac{1}{2}\frac{\Delta t}{\Delta x}\left[G\begin{pmatrix} h_{j+1}^k \\ u_{j+1}^k \end{pmatrix} - G\begin{pmatrix} h_{j-1}^k \\ u_{j-1}^k \end{pmatrix} \right] \\ &= \frac{1}{2}\begin{pmatrix} h_{j-1}^k + h_{j+1}^k \\ u_{j-1}^k + u_{j+1}^k \end{pmatrix} - \frac{1}{2}\frac{\Delta t}{\Delta x}\begin{pmatrix} h_{j+1}^k u_{j+1}^k - h_{j-1}^k u_{j-1}^k \\ \dfrac{1}{2}\left(u_{j+1}^k\right)^2 + g h_{j+1}^k - \dfrac{1}{2}\left(u_{j-1}^k\right)^2 - g h_{j-1}^k \end{pmatrix} \end{aligned} \tag{3.5}$$

for $j = 1, \ldots, J-1$; $k = 0, 1, 2, \ldots$, where $j\Delta x$ is the spatial grid, $\Delta x = L/J$, and $k\Delta t$ is the temporal grid.

3.2. Boundary Conditions

Boundary conditions for the discrete equation (3.5) are taken to be constant height and constant velocity downstream and a function representing an increase of height of the water column (a bump) upstream,

$$h_0^{k+1} = \gamma_{k+1}, \; k = 0, 1, 2, \ldots . \tag{3.6}$$

For the numerical method, however, one needs a further boundary condition at $j = 0$. This comes from an analysis of the characteristics at the boundary point $x = 0$. We consider an approximation of equation (3.1) determined by freezing the coefficients of matrix A at $x = 0$ and $t = (k+1)\Delta t$, and we get

$$\begin{pmatrix} h \\ u \end{pmatrix}_t + \overbrace{\begin{pmatrix} u_0^{k+1} & h_0^{k+1} \\ g & u_0^{k+1} \end{pmatrix}}^{A_0} \begin{pmatrix} h \\ u \end{pmatrix}_x = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{3.7}$$

Now, by diagonalizing A_0 we get $A_0 = PDP^{-1}$ where

$$P = \begin{pmatrix} -h_o^{k+1} & h_0^{k+1} \\ \sqrt{h_0^{k+1} g} & \sqrt{h_0^{k+1} g} \end{pmatrix} \text{ and}$$

$$D = \begin{pmatrix} \lambda_- & 0 \\ 0 & \lambda_+ \end{pmatrix} = \begin{pmatrix} u_o^{k+1} - \sqrt{h_0^{k+1} g} & 0 \\ 0 & u_o^{k+1} + \sqrt{h_0^{k+1} g} \end{pmatrix}.$$

By a change of dependent variables,

$$\begin{pmatrix} \tilde{h} \\ \tilde{u} \end{pmatrix} = P^{-1} \begin{pmatrix} h \\ u \end{pmatrix} \tag{3.8}$$

equation (3.7) decouples into

$$\tilde{h}_t + \lambda_- \tilde{h}_x = 0 \text{ and } \tilde{u}_t + \lambda_+ \tilde{u}_x = 0 . \tag{3.9}$$

From equation (3.8) we have

$$\tilde{h}(x,t) = -\frac{1}{2h_0^{k+1}} h(x,t) + \frac{1}{2\sqrt{h_0^{k+1} g}} u(x,t) \tag{3.10}$$

and from equation (3.9) we have (since $\tilde{h}$ is constant along characteristics)

$$\tilde{h}(x,t) = \tilde{h}(x - \lambda_- \Delta t, t - \Delta t). \tag{3.11}$$

Substituting $\tilde{h}$ from equation (3.10) into equation (3.11) and evaluating equation (3.11) at $x = 0$ and $t = (k+1)\Delta t$ we get

$$-1 + \frac{u_0^{k+1}}{\sqrt{h_o^{k+1} g}} = -\frac{1}{h_o^{k+1}} h(-\lambda_- \Delta t, k\Delta t) + \frac{1}{\sqrt{h_o^{k+1} g}} u(-\lambda_- \Delta t, k\Delta t). \tag{3.12}$$

Equation (3.12) is the boundary condition for u_0^{k+1}. The values of *h* and *u* on the right hand side of equation (3.12) are interpolated linearly using h_0^k, h_1^k, u_0^k and u_1^k, and h_0^{k+1} is substituted by its value defined by the boundary condition equation (3.6). Finally we get,

$$u_0^{k+1} = \frac{\left[u_0^k + \sqrt{\gamma_{k+1} g} \cdot \left(1 - \beta - \frac{h_0^k}{\gamma_{k+1}} \right) \right]}{1 - \beta} \tag{3.13}$$

where

$$\beta = \frac{\Delta t}{\Delta x} \left[\left(u_o^k - u_1^k \right) + \frac{h_1^k - h_0^k}{\gamma_{k+1}} \sqrt{\gamma_{k+1} g} \right].$$

4. Semi-Lagrangian Scheme for the Scalar Pollutant

In this section we describe the scheme employed to integrate numerically the evolution equation for the transport of the scalar pollutant. This scheme uses a standard finite difference discretization for the spatial representation of the advected field and a semi-Lagrangian discretization for the time variable. First we present the main idea behind semi-Lagrangian time discretization schemes.

4.1. Time Advancing Characteristics Based Scheme

We recall (Lax, 1970) that the characteristics of the equation

$$\frac{\partial \phi}{\partial t} + u\frac{\partial \phi}{\partial x} = 0 \tag{4.1}$$

are defined by the solution of the ordinary differential equation

$$\frac{ds}{dt} = u(s(t),t),\ t \geq t_0\ ;\ s(t_0) = x^* \tag{4.2}$$

where x^* ($0 \leq x^* \leq L$) can be thought of as a material point in the spatial domain of interest. In this way, $s(t)$ is the trajectory of x^*. One can check that ϕ is constant along the trajectory of a particle,

$$\phi\left[s(t),t\right] = const. = \phi\left[s(t_0),t_0\right], \text{ for all } t. \tag{4.3}$$

This follows from verifying that the time derivative of $\phi\left[s(t),t\right]$ is null due to equations (4.2) and (4.1).

Using equation (4.3) one can propose a simple method for advancing ϕ in time. Assume ϕ is already known at time level $t_k = k\Delta t$ in the grid $x_j = j\Delta x,\ j = 0,1,\ldots,J$, and is represented by ϕ_j^k. To advance ϕ to the next level one finds the point x^* such that by evolving it by equation (4.2) with $t_0 = k\Delta t,\ s(t_0) = x^*$, it arrives at x_j in time $t = (k+1)\Delta t$, that is $s((k+1)\Delta t) = x_j$, see figure 4.1.

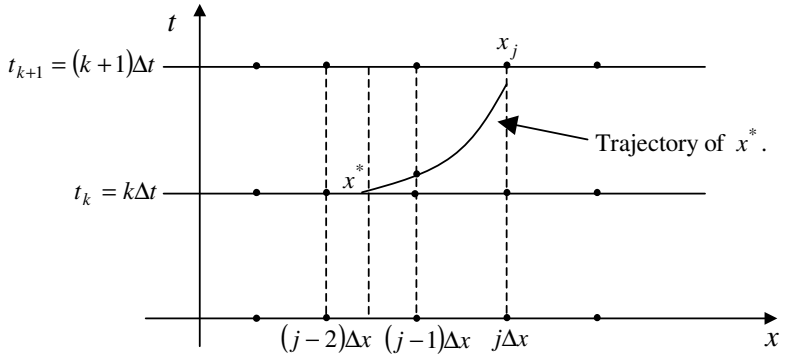

Figure 4.1. Time advancing of ϕ through the characteristics.

In this way one has

$$\phi_j^{k+1} = \phi(x^*, k\Delta t).$$

This is the basis of semi-Lagrangian methods (Russell, 1985). We now proceed to describe the two-level semi-Lagrangian scheme used to solve equation (4.1).

4.2. Two-Step Semi-Lagrangian Method

In order to get good accuracy (2^{nd} order) in the characteristics trajectory and, as a result, in the determination of the scalar field ϕ we use a two step method to solve equation (4.2) backwards in time, with initial condition x_j at time t_{k+1}, and with time step $\Delta t/2$:

$$\frac{s^{k+1}-s^k}{\Delta t}=u\left(s^{k+1/2},\left(k+1/2\right)\Delta t\right)$$
$$s^{k+1}=x_j \tag{4.4}$$

A further approximation is done by substituting $s^{k+1/2}$ in equation (4.4) by an average, $s^{k+1/2}=\left(s^{k+1}+s^k\right)/2$ which leads to

$$\frac{s^{k+1}-s^k}{\Delta t}=u\left(\frac{s^{k+1}+s^k}{2},\left(k+1/2\right)\Delta t\right)$$
$$s^{k+1}=x_j \tag{4.5}$$

Therefore, by substituting in equation (4.5) s^{k+1} by x_j and s^k by x^* we get

$$x^*=x_j-\Delta t\cdot u\left(\frac{x_j+x^*}{2},\left(k+1/2\right)\Delta t\right). \tag{4.6}$$

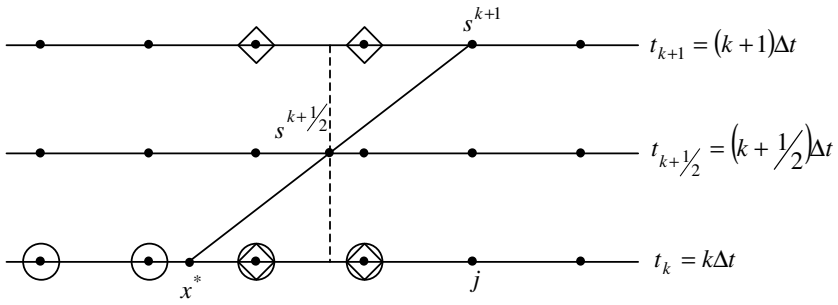

Figure 4.2. Determination of x^* by equation (4.6).

Given x_j, equation (4.6) is an implicit equation for x^* which we can solve by iteration,

$$x_{i+1}^*=x_j-\Delta t\cdot u\left(\frac{x_j+x_i^*}{2},\left(k+1/2\right)\Delta t\right)$$
$$x_0^*=x_j \tag{4.7}$$

where *i* is the iteration counter, $i=0,1,2,\ldots$.

We need to approximate in order to evaluate *u* in the right hand side of equation (4.7). We do this by interpolation as follows. We interpolate *u* between time levels t_k and t_{k+1} with the values of *u* on the grid points behind and ahead of $\left(x_j+x_i^*\right)/2$ (see diamond points on figure 4.2, when $\left(x_j+x_i^*\right)/2$ is already close to its converged value). Finally take an average of these linear interpolations.

The method to advance ϕ is then written as

$$\phi_j^{k+1}=\phi\left(j\Delta x,(k+1)\Delta t\right)=\phi\left(x^*,k\Delta t\right)$$

This step requires an interpolation of the values of ϕ and we do this by a cubic interpolation taking values on two grid points behind and two points ahead of x^*, (see circled points in figure 4.2).

We still have to consider initial and boundary conditions. For the advection problem, equation (4.1), the scalar field ϕ needs to be known at time $t=0$, $\phi(x,0)=\phi_0(x),\ 0\le x\le L$. Moreover, assuming that $u>0$, as for the intended application, a boundary condition on the field ϕ in the inlet boundary ($x=0$) is asked for, $\phi(0,t)=\phi_L(t),\ t\ge 0$.

5. Numerical Results

We use the methodology presented to simulate the transport of a pollutant which initially is concentrated on a small region. We tested the code using a constant velocity and constant height solution of the SWE when the pollutant is advected with constant velocity, see figure 5.1. The pollutant plume does not change its form as should be expected.

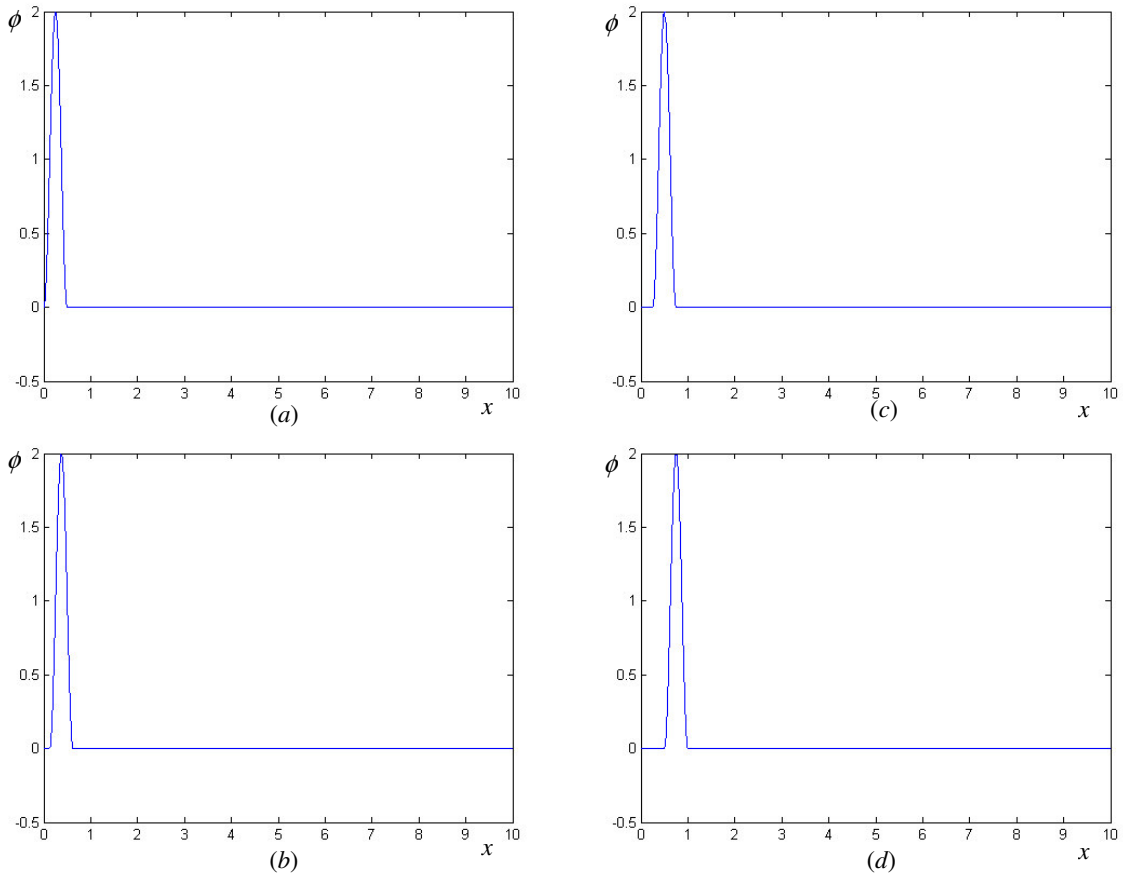

Figure 5.1. Evolution of pollutant concentration profile with constant velocity and water height: (*a*) $t = 0$; (*b*) $t = 1/4$ day; (*c*) $t = 1/2$ day; (*d*) $t = 1$ day.

Next, we consider the effect, on the transport of the same plume of pollutant, of a sudden rise of the water level due, possibly, to the collection of a peak of rain waters. Figure 5.2 shows the height profile on the left boundary along time, which is somewhat sharp. Time is measured in days. Figure 5.3 shows the numerical results of the water level at $t = 0$, $t = 1/4$ day, $t = 1/2$ day and $t = 1$ day of simulation. Figure 5.4 shows the velocity profile and figure 5.5 shows the pollutant distribution at the same time.

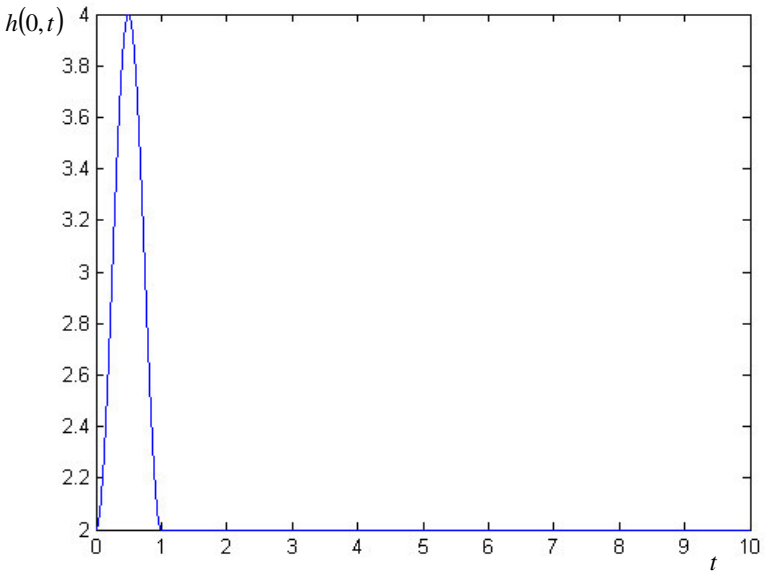

Figure 5.2. Boundary condition for the height of water at $x = 0$.

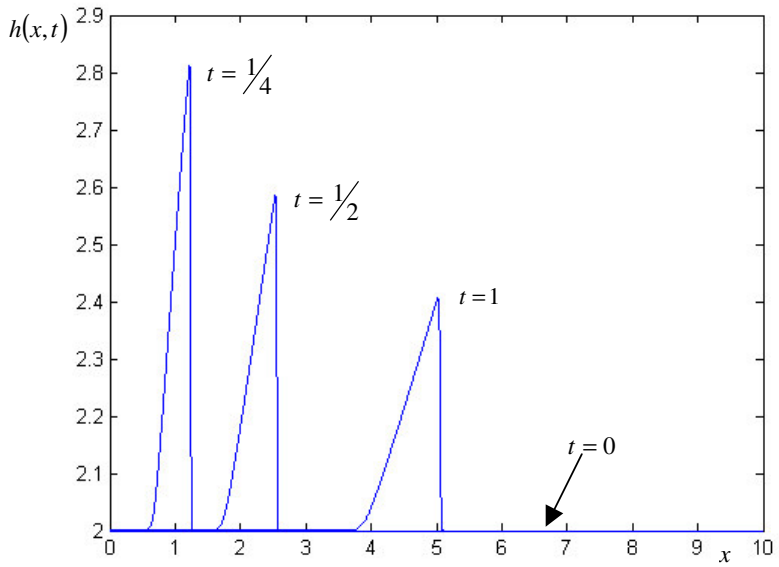

Figure 5.3. Evolution of height of water column.

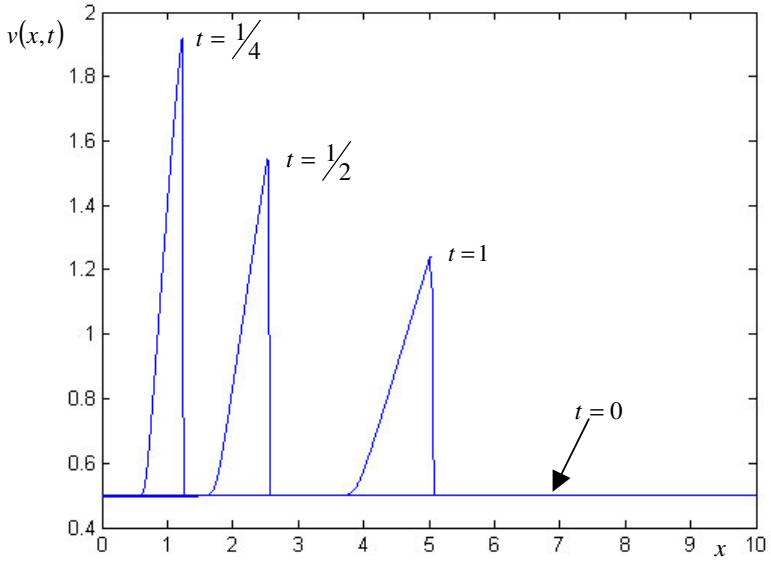

Figure 5.4. Evolution of velocity profile.

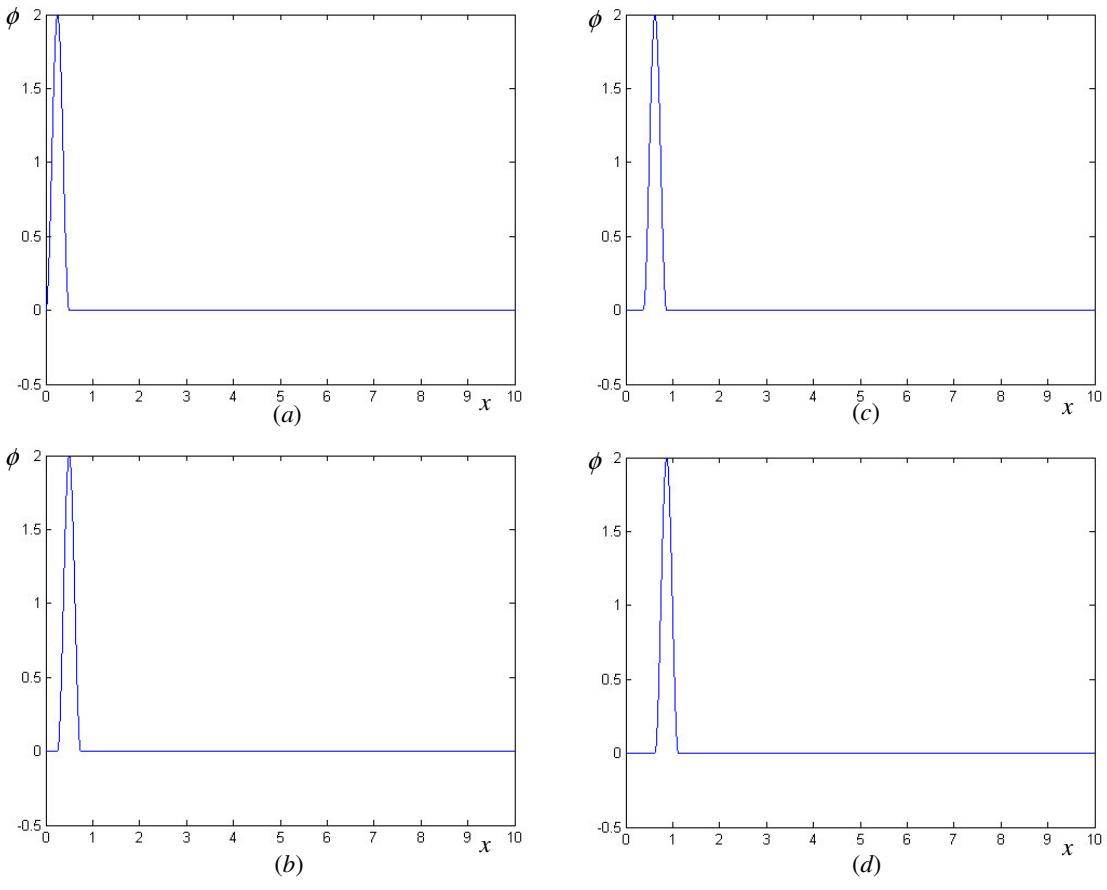

Figure 5.5. Pollutant concentration: (*a*) $t = 0$; (*b*) $t = 1/4$ day; (*c*) $t = 1/2$ day; (*d*) $t = 1$ day.

Conclusion

In this paper we presented the numerical solutions for the equations modelling the transport of a non-degrading and non-diffusive pollutant, in a one dimensional context, using Lax-Friedrichs method for the shallow water equations and the semi-Lagrangian method for the transport equation. The results thus obtained show good capability of these methods to deal with this models.

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