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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 semi-implicit semi-Lagrangian method for the discretization of the time variable involving the convective and advective terms coupled with a centered finite difference scheme for the space discretization of the shallow water equations together with an equation for a non-reacting and non-diffusive pollutant field. The linear terms, in the coupled equations for the perturbation of the water column, are responsible for the gravitational effects, and give rise to fast waves which can be handled by an implicit method resulting in a precise numerical scheme. This method allows the use of fine space resolution without incurring in severe time step restrictions (no CFL restriction). In this way reliable monitoring of pollutant fields is accomplished with low computational costs when compared with Eulerian methods.

ADDITIONAL INDEX WORDS: Shallow water equations, semi-Lagrangian method, finite difference, transport of pollutants, numerical solutions.

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 that can be taken to improve the outcome of these events 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 to resolve the hydrodynamics. 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 fast travelling waves and discontinuous solutions (even if these do not show up they impact the dynamics), is the main responsible for the difficulties encountered.

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 al. (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 Steinbach (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 a semi-implicit semi-Lagrangian finite difference scheme. Such scheme for the time evolution of the pollutant allows large time steps and an adequate representation of the pollutant scalar field with a low computational cost. This is very convenient since it can be run in PC’s in surveillance stations along large water bodies.

This paper is organised as follows. First we present the equations for modelling the hydrodynamics and the transport of a non-degrading and non-diffusive scalar pollutant. Next the numerical method is derived: a semi-Lagrangian scheme for the transport terms, semi-implicit for the linear terms and a finite difference scheme for the spatial derivatives for the resolution of the SWE and the equation for the pollutant. Finally the results of a simulation and a few conclusions are presented.

MODEL OF A PASSIVE SCALAR POLLUTANT

A model, describing the hydrodynamics of water flow under the effects of gravity and with a free surface, such as encountered in rivers and estuarine regions can be given by the shallow water equations. Let the bottom of the liquid region and the height of the water column be represented, respectively, by \( z = h(x,y) \) and \( h(x,y,t) \). Then the air-water interface is given by the surface \( z = h(x,y) + h(x,y,t) \).
Let $(u,v) = (u(x,y,t), v(x,y,t))$ be the horizontal components of the fluid velocity field. 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 the equations for $u$, $v$ and $h$ are (Stoker, 1992)

\begin{align}
\begin{cases}
h_t + (hu_x)_x + (hv_y)_y & = 0 \\
u_t + uu_x + vv_y + gh_x & = -gb_x \\
u_x + vv_x + vv_y + gh_y & = -gb_y
\end{cases}
\end{align}

for $0 \leq x \leq L$, $0 \leq y \leq M$ and $t \geq 0$. Here $g$ denotes the acceleration of gravity, $L$ represents the length of the section of the river under study, and $M$ its width.

Equation (1) represents mass conservation and Eqs (2) and (3) represent local momentum balance. In this model we neglect turbulence and friction effects and consider that there 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 that, moreover, has a horizontal flat bottom.

In this way, $v = b = h = 0$, the variables $u$ and $h$ depend only on $x$ and $t$, and we keep only Eqs (1) and (2) which are then rewritten as:

\begin{align}
\begin{cases}
h_t + u h_x + h u_x & = 0 \\
u_t + uu_x + gh_x & = 0
\end{cases}
\end{align}

for $0 \leq x \leq L$ and $t \geq 0$.

Let $\phi$ denote the concentration (mass of pollutant per unit volume of the fluid) of a scalar non-reacting (passive) non-diffusing pollutant. Then $\phi$ is advected by the water flow, which are represented by the following equation

$$\phi_t + u \phi_x = 0$$

for $0 \leq x \leq L$ and $t \geq 0$.

Equations (4) and (5) can be rewritten in vector form as

$$\begin{pmatrix}
h \\
u \\
g
\end{pmatrix}_t + \begin{pmatrix}
A \\
B \\
0
\end{pmatrix} \begin{pmatrix}
h \\
u \\
g
\end{pmatrix} = \begin{pmatrix}
0 \\
0 \\
0
\end{pmatrix}, \quad 0 \leq x \leq L \quad \text{and} \quad t \geq 0$$

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

$$h(0,t) = h_L(\ell), \quad h(L,t) = h_R(\ell), \quad \ell \geq 0$$

We consider flows going from left to right, which therefore implies that $\phi$ has to be prescribed on the left boundary. Initial conditions also have to be prescribed,

$$\begin{pmatrix} h(x,0) \\ u(x,0) \end{pmatrix} = \begin{pmatrix} h_0(x) \\ u_0(x) \end{pmatrix}, \quad 0 \leq x \leq L$$

$$\phi(x,0) = \phi_0(x)$$

Only smooth solutions of the evolution Eqs. (4-6) are treated which, together with the subcritical flow conditions, frames the set of applications admissible by the methodology presented here.

**SEMI-LAGRANGIAN SCHEME**

In this section we present the semi-implicit semi-Lagrangian finite difference discretization of the coupled pollutant hydrodynamic model. This method employs a standard central finite difference discretization for the spatial representation of convected and advected fields and a semi-implicit semi-Lagrangian discretization for the time variable. First we present the main idea behind semi-Lagrangian time discretization schemes and later the full discretization method.

**Time Advancing Characteristics Based Scheme**

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

$$\frac{\partial \gamma}{\partial t} + u \frac{\partial \gamma}{\partial x} = f(\gamma, x, t)$$

$$\gamma(x,t)$$ for $f$, where $f$ is a source term, are defined by the solutions of the ordinary differential equation

$$\frac{ds}{dt} = u(s(t), t), \quad t \geq t_0 \quad s(t_0) = x_D$$

where $x_D(0 \leq x_D \leq L)$ can be thought of as a material point in the spatial domain of interest, called the departure point. In this way, $s(t)$ is the trajectory of $x_D$. When $u$ is the velocity field of a body of fluid, $s(t)$ is the fluid particle trajectory. By defining the material derivative as

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + u \frac{\partial}{\partial x}$$

one gets that $\gamma$ satisfies

$$\frac{D\gamma}{Dt} = f$$

in particular in the case of $\gamma = \phi$, the scalar non-degrading and non-diffusing pollutant, $D\phi/Dt = 0$ which implies that

$$\phi(s(t), t) = \text{const} = \phi(s(t_0), t_0)$$

for all $t$.

Using Eq. (14) one can propose a simple method for advancing $\gamma$ in time. Assume $\gamma$ is already known at time level $t = n \Delta t$ in the grid $x = n \Delta x$, $i = 0, 1, ... , I$, and is represented by $\gamma_i$. To advance $\gamma$ to the next level one finds the departure point, $x_D$ such that by evolving it by Eq. (12) with $t = n \Delta t$, $s(t_D) = x_D$, it reaches $x$ (the arrival point) at time $t = (n+1) \Delta t$, that is $s((n+1) \Delta t) = x_D$.

A numerical approximation for $\gamma_i^{n+1}$ is given by

$$\gamma_i^{n+1} = \gamma(x_D, n \Delta t) + \Delta t \tilde{f}$$

where $\tilde{f}$ is some approximation of $f$ along the particle trajectory (to get an explicit method one could take $f$ evaluated at the departure point).

This is the basis of semi-Lagrangian methods (Russell, 1985; Ritchie, 1987; Durran, 1999). We now proceed to describe the computation of the departure point in a two-step method and semi-implicit semi-Lagrangian scheme used to solve Eq. (4-6).

**Computation of the Departure Point**

In order to get good accuracy ($2^\text{nd}$ order) in the characteristics trajectory and, as a result, in the determination of a general scalar field $\gamma$ we use a two step method to solve Eq. (12) backwards in time, with initial condition $x$ at time $t_{max}^-$ and with time step $\Delta t$.

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Two-Step Semi-Lagrangian Method

A further simplification is obtained by approximating \( s^{n+1} \) in Eq. (17) by an average, \( s^{n+1} = (s^n + s^+) \), which therefore implies that \( s^{n+2} = 2s^n - s^+ \), and substituting this in Eq. (17) leads to

\[
\begin{align*}
\frac{s^{n+2} - s^n}{2M} &= u(s^n, (n+1)\Delta t) \\
\frac{s^{n+1} - s^n}{\Delta t} &= u(s^n, n\Delta t) 
\end{align*}
\]

(18)

Therefore, by substituting in Eq. (18) \( s^{n+1} \) by its value \( x_i \) and \( s^{n+2} \) by \( x_M \), the middle point, which is the new unknown in place of the departure point \( x_M \), we get

\[
x_M = x_i - \Delta t u(x_M, (n+1)\Delta t) 
\]

(19)

Given \( x_i \), Eq. (19) is an implicit equation for \( x_M \), which we can solve by iteration,

\[
x_M^{(j+1)} = x_i - \Delta t u(x_M^{(j)}, (n+1)\Delta t) \\
x_M^{(0)} = x_i
\]

(20)

where \( j \) is the iteration counter, \( j = 0, 1, 2, \ldots \).

We need to approximate \( u \) in order to evaluate the right hand side of Eq. (20). We do this by linear interpolation of \( u \) in the neighbor grid points of \( x_M \).

Finally the point of departure is \( x_M = x_M^{(0)} = \beta x_i - x_M^{(0)} \).

**Two-Step Semi-Lagrangian Method**

We consider that \( h_i(t) = h_i(t-\Delta t) \), in Eq. (8), assumes a constant value, and we split the water column into \( h \) and a perturbation, \( h' \).

\[
h(x, t) = h^* + h'(x, t) 
\]

(21)

where \( h'(0, t) = h'(L, t) = 0 \), for \( t > 0 \). Since \( \partial h'/\partial t = \partial h'/\partial x = 0 \), and using Eq. (13), Eqs (4) and (5) can be rewritten as

\[
\frac{Dh'}{Dt} + h'u_x + h'u_x = 0 \\
\frac{Du}{Dt} + gh_x' = 0 
\]

(22)

(23)

Each equation in this coupled system is of the type given in Eq. (14). The method considered, which is a two step method, requires the knowledge of \( h \) and \( u \) at two time levels, \( t_{n+1} \) and \( t_n \), and advances \( h \) and \( u \) to the next time level \( t_{n+1} \). Using Eq. (21) we can recover \( h' \).

For simplicity we drop the superscript prime from \( h' \). By the method outlined before in Eq. (16), and denoting the evaluation of field variables at the departure, middle and arrival points, respectively by superscripts +, 0 and − and by appropriate choices in the evaluation of the ‘source’ terms in Eqs (22-23) we get:

\[
h^* = h^* - 2\Delta h^* \frac{u_x^* + u_x^+}{2} - 2\Delta t(hu_x)^0 \\
u^* = u^* - 2\Delta t(h^* + h^-) \\
F = h^* - \Delta t(h^* u_x^* - 2\Delta t(hu_x)^0) \\
G = u^* - \Delta tgh_x^* 
\]

(24)

(25)

(26)

(27)

which are known quantities (variables evaluated at preceding times, interpolated cubically using the values of the field variables at two grid points behind and two points ahead of the middle or of the departure points, whichever applies). Therefore, Eqs (24-25) can be rewritten as

\[
h^* = F - \Delta t u_x^+ \\
u^* = G - \Delta tgh_x^* 
\]

(28)

(29)

Differentiating Eq. (29) with respect to \( x \), substituting the result in Eq. (28) and rearranging it leads to a Helmholtz type of equation,

\[
(\Delta )^2 h_x^* - h^* = \Delta h^* G_x - F 
\]

(30)

Equations (29-30) are discretized by a finite difference scheme and Eq. (30) for \( h^* \) is solved first and finally using Eq. (29) one determines \( u^* \). This finishes the description of the semi-implicit semi-Lagrangian finite difference method for SWE.

The method to advance \( \phi \) is then written as

\[
\phi_i^{n+1} = \phi_i^n (n\Delta t) 
\]

(31)

This step requires an interpolation of the values of \( \phi \) and we do this by a cubic interpolation using four grid points closest to \( x_i \).

**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 constant velocity and height solution of the SWE in which the pollutant is advected with constant velocity; the pollutant profile is translated with constant velocity without change in its form as it should be. Another successful test involved an exact solution of a forced SWE.

Next, we consider the effect, on the transport of the same discharge of pollutant, of a sudden rise of the water level due, possibly, to the collection of a peak of rain waters. Figure 1 shows the initial conditions and the evolution of the height of water column, of the velocity field and of the concentration of pollutant. One feature of semi-Lagrangian schemes is that large time steps can be used avoiding CFL restrictions; (we use CFL=4.05).

**CONCLUSIONS**

In this paper we presented the numerical solution for the equations modelling the transport of a non-degrading and non-diffusive pollutant, in a one dimensional context, using a semi-implicit semi-Lagrangian finite difference 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 model problem in an efficient and accurate way.

LITERATURE CITED


