

CHAPTER 235

A modified method of characteristic technique combined with Galerkin finite element method to solve shallow water mass transport problems

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Abstract

In order to solve water circulation and solute transport-diffusion problems in two-dimensional hydrodynamical systems a comprehensive simulator, composed by two finite element models, has been developed. In particular the first model, which is of semi-implicit kind, solves hydrodynamical shallow water equations whereas the second, which is an Eulerian-Lagrangian method (ELM), is based on the Modified Method of Characteristics (MMOC) combined with Galerkin finite element method. Semi-implicit procedures for hydrodynamical models are sometimes used with finite differences but are quite rare with finite elements. Nevertheless they have a lot of advantages compared to the others, principally linked to a considerable time saving. This is determined by the fact that the systems of equations in the unknown levels and velocities are uncoupled and the time step is not constrained by Courant-Friedrichs-Levy stability criterion. It can be demonstrated that in the linear case the hydrodynamic model is indefinitely stable and good accuracy can be achieved for velocity field. On the other side, the proposed transport-dispersion model presents interesting features, among which the possibility to obtain good results in mass conservation and minimum numerical oscillations or grid orientation problems even under sharp front conditions. In these papers we shall discuss only the approximation method of transport-dispersion model, showing the theoretical fundamentals and some of its applications.

Introduction

The transport-dispersion equation constitutes one of the most difficult problem to solve by numerical methods, since the equation ranges from a parabolic to almost hyperbolic form, depending on the ratio of advection to dispersion, the Peclet number. In particular, when advection terms of the equation are dominant and concentration gradients very steep, using standard finite element many difficulties in the numerical solution arise, such as numerical dispersion, numerical oscillations, grid orientation influences and, even, mass conservation.

To treat this problem many approximations have been developed, but, nevertheless, three broad classes of methods can be identified.

The first group, based on using optimal test functions, is referred to as Optimal Spatial Methods (OMS). Examples of these approximations include the Quadratic Petrov-Galerkin Method (Christie et al., 1976; Bouloutas et al., 1988), the Optimal Test Function Method (OTF) (Celia et al., 1989). The limits of all these schemes consist in the variably upwinded nature of test functions which restrict the range of Peclet numbers allowable without numerical diffusion.

A second broad class is constituted by the Eulerian-Lagrangian methods (ELM), which appear to overcome the problems inherent to advection-dominated transport conditions. The approximations in this class of schemes have, as their common element, a Lagrangian treatment of advection processes. Again there are many examples from literature, including Operator Splitting Method (Baptista, 1987;

Wheeler et al., 1988), Eulerian-Lagrangian Method with the Method of Characteristics (Pinder et al., 1977), Eulerian-Lagrangian Method with the Modified Method of Characteristics (Ewing et al. 1984; Russel, 1985; Chiang et al., 1988). These methods can obtain significant reduction in numerical oscillations and in numerical diffusion even in presence of large Courant numbers. The principal drawbacks of ELM are, in some case, difficulty to conserve mass and to formulate general boundary conditions. However, material balance mass errors can be greatly reduced when an accurate velocity field from the solution of hydrodynamical equations is derived.

The third broad class (ELLAM) combines the ideas of OTF and ELM, by using space-time test functions satisfying a local adjoint condition that introduces a Lagrangian frame of reference (Celia et al., 1989; Zisman, 1988; Russel, 1990). Among other things, ELLAM schemes allow the solution of transport-dispersion equation in the conservative form unlike, for example, ELM methods where the obtained solution concerns the non-conservative form of the same equation. For this reason sometimes ELLAM approximations can achieve a better result in mass conservation than ELM themselves, even if at the expense of a non-irrelevant increase of computational effort.

Taking into account all these considerations, these papers present a comprehensive analysis of a numerical method adopting a Eulerian-Lagrangian Method with the Modified Method of Characteristics (MMOC), with interesting proceedings to evaluate the advection term of diffusion equation. Furthermore two brief reports, regarding a numerical validation and a real case application, are presented.

Governing equation

The general solute diffusion equation in a non-conservative form has been derived as follows:

$$\frac{\partial c}{\partial t} + \bar{v} \cdot \nabla c - \frac{1}{h} \nabla \cdot (hD \cdot \nabla c) = s \quad (1)$$

where

- c solute concentration, [kg/m³];
- D dispersion tensor, [m²/s];
- \bar{v} velocity vector, [m/s];
- h water depth, [m] ($h = Z - Z_f$ where Z , Z_f are surface and bottom levels, relative to a reference plane);
- s solute source or sink, [(kg/m³)/s].

The dispersion tensor D in two-dimensional flow fields is defined as (Peaceman, 1966):

$$D = \begin{pmatrix} D_{xx} & D_{xy} \\ D_{yx} & D_{yy} \end{pmatrix} = D_m I + \frac{hg^{1/2}}{C|\bar{v}|} \left\{ \alpha_l \begin{pmatrix} u^2 & uv \\ uv & v^2 \end{pmatrix} + \alpha_t \begin{pmatrix} v^2 & -vu \\ -vu & u^2 \end{pmatrix} \right\} \quad (2)$$

where

- D_m molecular isotropic diffusion coefficient, [m²/s];
- I unit tensor, dimensionless;
- α_l longitudinal dispersion coefficient, dimensionless;
- α_t transversal dispersion coefficient, dimensionless;
- u, v velocity components along coordinate axes, [m/s];
- g gravitational constant, [m/s²];
- C Chézy coefficient, [m^{1/2}/s].

The factors which determine diffusion processes are mainly two: the first, of advection kind, characterized by transport for the fluid base motion; the second, of dispersive nature, linked to whirling motions of turbulent origin internal to fluid masses.

Indeed equation (1) would range from a hyperbolic-type, if the hydrodynamic dispersion were null, to a parabolic-type, if the process were purely dispersive. Numerical proceedings which permit to solve suitably hyperbolic differential equations differ deeply from those applied in case of parabolic-type equations. It is well known that solution for hyperbolic-type equations can be represented from the initial data propagating over well-defined paths, called characteristics, over the surface in direction of flow. The solution of the overall equation (1) can be viewed as spreading or dispersion away from these characteristic curves, along which solute concentration is a smooth function (Douglas and Russel, 1982).

With regard to this, consider a domain Ω delimited by a boundary Γ where Dirichlet or null-flux boundary conditions are applied.

Defined the unit vector $\bar{v}(\bar{x}, t)$ in the characteristic direction, the directional derivative along a characteristic curve in \bar{x} at time t can be evaluated through the expression:

$$\frac{\partial}{\partial \tau} = \frac{1}{(|\bar{v}|^2 + 1)^{1/2}} \left(\frac{\partial}{\partial t} + \bar{v} \cdot \nabla \right) \quad (3)$$

where \bar{v} is the local velocity vector.

If we substitute expression (3) in equation (1), we will obtain:

$$(|\bar{v}|^2 + 1)^{1/2} \frac{\partial c}{\partial \tau} - \frac{1}{h} \nabla \cdot (h D \cdot \nabla c) = s \quad (4)$$

which constitutes the non-divergence form of diffusion equation.

Time discretization of diffusion equation

Many methods, based on characteristics, fix a point at the current time level and evaluate the final position at the advanced time level. MMOC method takes the opposite view, fixing a point at the advanced time level t^{n+1} and asking where it came from at the current time level t^n . Thus the solution grid at the advanced time level is controlled by the method, not the flow, so allowing a fixed finite element mesh to use.

In the mathematical model the derivative along characteristic curves can be approximated by a back-ward finite difference procedure, obtaining in this way:

$$(|\bar{v}|^2 + 1)^{1/2} \frac{\partial c}{\partial \tau} = (|\bar{v}|^2 + 1)^{1/2} \cdot \frac{c(\bar{x}, t^{n+1}) - c(\bar{x}^*, t^n)}{[(\bar{x} - \bar{x}^*)^2 + (t^{n+1} - t^n)^2]^{1/2}} + O(\Delta \tau) \quad (5)$$

If we would assign a precise physical meaning to the problem, \bar{x}^* might be interpreted as the initial position at time t^n where a particle, following the flow line, will arrive at time t^{n+1} from. During the time interval Δt within t^n and t^{n+1} , the relation linking \bar{x}, \bar{x}^* can be achieved, as first approximation, through the following cinematic expression:

$$\bar{x}^* = \bar{x} - \bar{v} \cdot \Delta t + O(\Delta t^2) \tag{6}$$

The backward difference in time makes the procedure implicit in nature and (5) becomes:

$$\left(|\bar{v}|^2 + 1\right)^{1/2} \frac{\partial c}{\partial \tau} = \frac{c(\bar{x}, t^{n+1}) - c(\bar{x}^*, t^n)}{\Delta t} + O(\Delta \tau) \tag{7}$$

The final form of the diffusion equation to solve, by using Galerkin weighted residual method, is thus the following (Neuman, 1981; 1983):

$$\frac{c(\bar{x}, t^{n+1}) - c(\bar{x}^*, t^n)}{\Delta t} - \frac{1}{h} \nabla \cdot (hD \cdot \nabla c^{n+1}) = s' \tag{8}$$

Considering equation (8), it can be noted that, in order to avoid the appearance of an artificial numerical diffusion mainly connected to large time steps often utilized in numerical simulations, the dispersion term is computed at advanced time level t^{n+1} .

Before proceeding to the mathematical formulation of the finite element method, it is necessary to define some notations. First of all denote the following surface and line integrals:

$$(u, v) = \int_{\Omega} (u \cdot v) d\Omega$$

$$\langle u, v \rangle = \int_{\Gamma} (u \cdot v) d\Gamma$$

where center dot is the inner product. Let $H^n(\Omega)$ be the Hilbert space of n-order defined in Ω . Let also $H_{\Gamma_1}^n(\Omega)$ be the Hilbert subspace of n-order defined in Ω of functions $u \in H^n(\Omega)$ which vanish on boundary Γ_1 where Dirichlet boundary conditions are applied.

The variational problem corresponding to differential equation (8), subject to boundary conditions just pointed out, is then the following:

$$\left(\frac{c(\bar{x}, t^{n+1}) - c(\bar{x}^*, t^n)}{\Delta t} - \frac{1}{h} \nabla \cdot (hD \cdot \nabla c^{n+1}) - s', \psi \right) = 0 \quad (\forall \psi \in H_{\Gamma_1}(\Omega)) \tag{9}$$

Integrating by parts against weight function ψ with Green formulas, we will obtain the Galerkin form of variational problem:

$$\left(\frac{c(\bar{x}, t^{n+1}) - c(\bar{x}^*, t^n)}{\Delta t}, \psi \right) + \frac{1}{h} (hD \cdot \nabla c^{n+1}, \nabla \psi) - (s', \psi) - \langle D \nabla c \cdot \bar{n}, \psi \rangle = 0 \quad (\forall \psi \in H_{\Gamma_1}(\Omega)) \tag{10}$$

Consider now a base φ_i ($i = 1, 2, \dots, N$) of a subspace $K_N \subset H_{\Gamma_1}^1(\Omega)$ and suppose unknown concentration c and weight function ψ to be approximated by C and φ_i respectively, belonging to such subspace K_N ; then equation (10) provides the following N linear equations in the unknown concentration $C^{n+1} = C(\bar{x}, t^{n+1})$:

$$\left(\frac{C^{n+1} - C(\bar{x}^*, t^n)}{\Delta t}, \varphi_i \right) + \frac{1}{h} (hD \cdot \nabla C^{n+1}, \nabla \varphi_i) - (S', \varphi_i) - \langle \frac{q_d^{n+1}}{h}, \varphi_i \rangle = 0 \quad (i=1, 2, \dots, N) \tag{11}$$

where q_d is the flux on the boundary, for unit length, of only dispersive nature.

Since, for hypothesis, boundary flux is null, developing equation (11) in its full form we will

obtain after all:

$$\begin{aligned} & \left(C^{n+1}, \varphi_i \right) + \frac{\Delta t}{h} \left\{ \left[h \left[D_{xx} \frac{\partial C^{n+1}}{\partial x} + D_{xy} \frac{\partial C^{n+1}}{\partial y} \right], \frac{\partial \varphi_i}{\partial x} \right] + \right. \\ & \left. + \left[h \left[D_{xy} \frac{\partial C^{n+1}}{\partial x} + D_{yy} \frac{\partial C^{n+1}}{\partial y} \right], \frac{\partial \varphi_i}{\partial y} \right] \right\} = \left(C(\bar{x}^*, t^n), \varphi_i \right) + (S', \varphi_i) \Delta t \quad (i=1,2,\dots,N) \end{aligned} \tag{12}$$

Equation (12) completes the procedure which combines the modified method of characteristics with finite element Galerkin method for the simulation of solute transport-dispersion equation. The integral relative to the function $C(\bar{x}^*, t^n)$ is computed through the well known quadrature formulas in a approximated way, since \bar{x}^* may belong to several elements as \bar{x} runs over a single element. Finally note that, being advection term $C(\bar{x}^*, t^n)$ moved to the right side of (12), the system of linear equations is symmetric and positive definite.

Backtracking algorithm

The integrals in (12) are standard in finite element schemes except for the inner product relative to $C(\bar{x}^*, t^n)$. The point \bar{x}^* does not lie, in general, at a precise node of the mesh, since it becomes necessary to utilize some particular procedure for its determination. In particular the integration involving $C(\bar{x}^*, t^n)$ is calculated by means of Gauss quadrature formulas, with a number of integration points in each element variable from three to twelve, in function of concentration front steepness and relative required solution precision. Consider then a point $P(\bar{x}_i, t^{n+1})$ within a finite element T_S at time t^{n+1} (fig. 1). Actually, even if particle path joining points $P(\bar{x}_i, t^{n+1})$ and $P(\bar{x}_i^*, t^n)$ could be determined, as first approximation, from equation (6) using the same time step considered for integration of overall diffusion equation, mainly for increasing method's precision particle path is calculated with a time step $\Delta t'$ shorter.

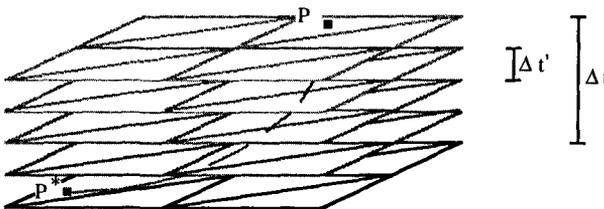


Fig. 1 - Path of a particle along a characteristic curve in the hydrodynamic system during a integration time Δt of dif-fusion equation. Integration time step $\Delta t'$ of characteristics is often much less than Δt , with the aim to increase method accuracy.

The particular attention reserved to the evaluation of corresponding points $P(\bar{x}_i, t^{n+1})$, $P(\bar{x}_i^*, t^n)$

resides fundamentally in the aim to evaluate correctly the advection term of transport-dispersion equation, fraction certainly of crucial importance especially in coastal and lagoon problems.

The cinematic differential equations governing particle motion are the following:

$$\frac{dx}{dt}=u(\bar{x},t) \quad , \quad \frac{dy}{dt}=v(\bar{x},t) \quad (13)$$

with initial conditions $\bar{x}=\bar{x}_i$ at $t=t^{n+1}$. The velocities $u(\bar{x},t)$, $v(\bar{x},t)$ inside a generic m -node finite element T_S will be calculated through the expressions:

$$\begin{cases} u(\bar{x},t)=\sum_1^m u_j(t;T_S)\cdot\phi_j(\bar{x};T_S) \\ v(\bar{x},t)=\sum_1^m v_j(t;T_S)\cdot\phi_j(\bar{x};T_S) \end{cases} \quad (14)$$

where u_j, v_j are j -th node velocities and ϕ_j j -th node shape function within an element T_S .

Generally nodal velocities u_j, v_j from hydrodynamical simulation are stored only at discreet regular intervals, so that it is necessary some type of interpolation to determine velocity values at each time, as required by integration of (13). In this case, to interpolate velocities, linear, quadratic and cubic polynomials are used, depending on number of velocity values available for such node in that particular phase of hydrodynamical simulation.

Boundary conditions

As we pointed out, one of the principal drawbacks of ELM procedures is the difficulty of formulating them for general boundary conditions. Indeed, during the early development of modified method of characteristics, a no-flow boundary condition was assumed for all boundaries (Neuman, 1981). Actually these schemes are suitable to reproduce both Dirichlet conditions at open boundaries Γ_1 (I° type) and no-flow conditions at closed boundaries Γ_3 (III° type).

For what concerns I° type conditions, it is necessary to distinguish, first of all, between inflow and outflow at open boundary Γ_1 . During inflow boundary conditions are imposed upon the system from the outside, so being sufficient to assign directly the concentration values on boundary nodes. The situation at an outflow boundary is altogether different, since boundary conditions are no longer influenced from the outside. In this case, neglecting dispersion and so making an approximation quite often reasonable in this kind of problems, the concentration value corresponds with that of the particle arriving in a boundary node from inside the system. Therefore it needs only to determine initial position of the particle by the backtracking procedure.

At last in the case of III° type condition, when \bar{x} reaches across the boundary, the hydrodynamical velocity field is used to reflect back the particle, implicitly imposing a no-flow boundary condition.

Model verification

The following presents an analysis of numerical results of the model. It is important to emphasize that, mainly in order to avoid completely the presence of negative concentrations, has been developed a particular procedure able to eliminate negative values and to conserve exactly solute masses without introducing any significant numerical diffusion, as it will be proved later in the numerical tests.

The model has been applied to cases from low to high Peclet numbers, in order to observe model's ability in handling steep concentration gradients. The diffusion equation was solved with a 2-D grid consisting of right isosceles 3-node elements of small legs Δx , where Δx was nodal spacing. Independent parameters include Peclet number $Pe = u \Delta x / D$, Courant number $Cu = u \Delta t / \Delta x$ and the number of elements N which the source is distributed in flow direction over.

It was analysed the following two sets, whose analytical solutions are known, having assumed in all cases seven integration points for each triangular element, utilized in Gauss quadrature formulas for integration of advection terms.

Instantaneous source in a uniform flow

The base one-dimensional equation is the following :

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} - D \frac{\partial^2 c}{\partial x^2} = 0$$

with initial condition $c(x) = C_0 \cdot \exp(-\sigma |x - x_0| / N \Delta x)$ for $t=0$.

From numerous tests, mass and phase appear exact for all runs and numerical diffusion, even with a very concentrated source and high Pe , is quite negligible. In the case of a particularly steep gradient ($N=2$), with parameters $Cu = 0.48$ and $Pe = \infty$, results are shown in Fig.2 for different time steps (0,10,20,30,40 and 50 Δt).

Breakthrough distribution in a uniform flow

The same analysis was carried for the case of a breakthrough distribution in a uniform flow.

The graphics in Fig.3 still show the case of a particularly steep gradient ($N=3$), $Cu = 0.48$ and $Pe = \infty$ for different time steps (0,10,20,30,40 and 50 Δt). It is possible to note only small oscillations in numerical results, however quickly damped in space, on either edges of the breakthrough curve. However, by numerical experiences, their maximum value and influence tends to decrease with increasing N and decreasing Pe .

Model application to Barbamarco lagoon (Rovigo - ITALY)

Among other things, the model has been set-up and applied to examine diffusion phenomena on Barbamarco lagoon, which is a small coastal lagoon on Delta Po. The hydrodynamical model has been verified on the base of tidal level measurements, caught in four gages all around the lagoon, and contemporary discharges, flowing through the two mouths and a controlled gate dug into Po river.

Because, unfortunately, there were no data measurements relating to diffusion phenomena in the lagoon, to evaluate the effectiveness of the projected canal network to dredge the results of the model were compared with those referring to real situation supposing a instantaneous source release of a conservative solute in different zones of hydrodynamical system, especially where water exchange is

particularly difficult.

The most interesting result is relative to a solute released near West Mouth (fig. 4). In fig. 4a the finite element mesh of Barbamarco lagoon and the Zoom of the zone interested to conservative solute diffusion are represented, while in fig. 4b the initial concentration distribution is shown. The following two pictures (fig. 4c, 4d) illustrate the distribution evolution during the first 12 hours, with 6 hours' time between representations. Finally the last four pictures (fig. 5a, 5b, 5c, 5d), which report the distribution isolines relative to four days from the beginning of hydrodynamical simulation, show the effects of slow plume migration towards East Mouth, so confirming the results obtained with hydrodynamical model where a residual current in the same direction, equal to roughly 10% of total volume exchanged during a tidal cycle, was noted.

Conclusion

A comprehensive simulator composed by two finite element models, the first solving hydrodynamical shallow water equations whereas the second the diffusion equation, has been developed. However, in this report only the diffusion model, based on the Modified Method of Characteristics (MMOC), is presented.

The important feature of the MMOC procedure is tracking the solution backward in time along the characteristics, in contrast to the forward front tracking or moving point methods. Thus the solution grid at the advanced time is controlled by the method, not the flow, and therefore a fixed grid system can be used for mathematical simulations. Among other advantages algebraic system is symmetric and positive definite.

Since diffusion equation is solved in a non-divergence form, it is required a very accurate velocity field to maintain good numerical material balance. On its hand, the two levels semi-implicit hydrodynamical model seems to furnish a solution accurate enough to assure overall mass conservation.

The accuracy of the model is analyzed through a comparison with analytical solutions. Good agreement between model results and analytical solutions is demonstrated. Furthermore the experiments demonstrate that large time steps can be taken without sacrificing much of MMOC model's solution accuracy. However, the model does require to consider a sufficient number of Gauss points in each finite element to resolve sharp concentration gradients increasing, in this case, computational effort.

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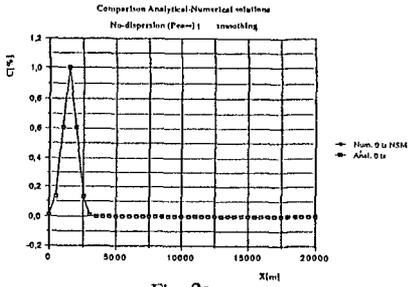


Fig. 2a

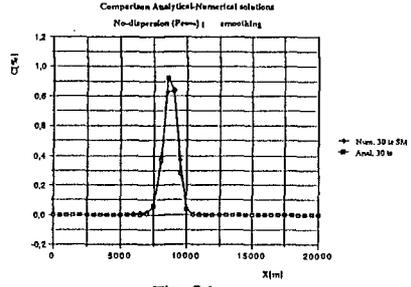


Fig. 2d

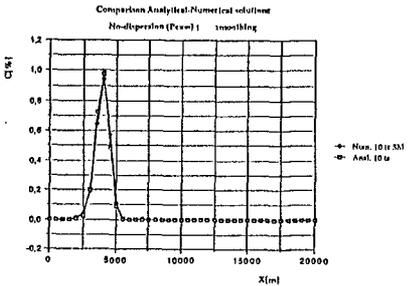


Fig. 2b

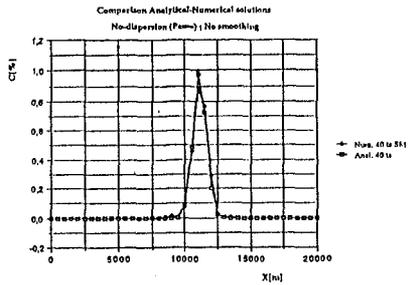


Fig. 2e

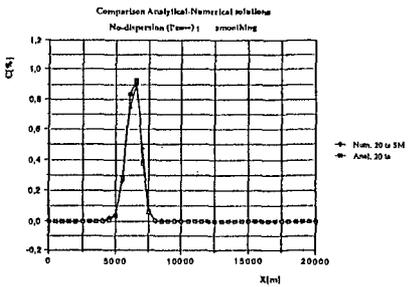


Fig. 2c

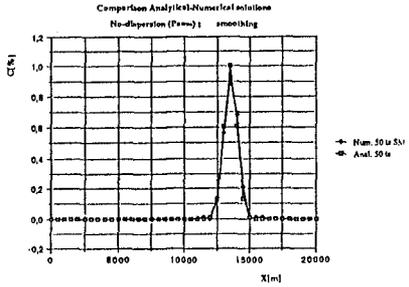


Fig. 2f

FIG. 2 - Instantaneous source in a uniform flow : comparison between analytical and numerical solutions in correspondence to different time steps [$0 \Delta t$ (fig.2a), $10 \Delta t$ (fig.2b), $20 \Delta t$ (fig.2c), $30 \Delta t$ (fig.2d), $40 \Delta t$ (fig.2e), $50 \Delta t$ (fig.2f)] with parameter values $N=2$, $Cu=0.48$ and $Pe = \infty$.

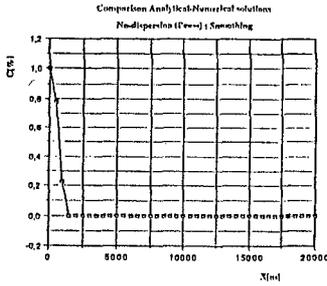


Fig. 3a

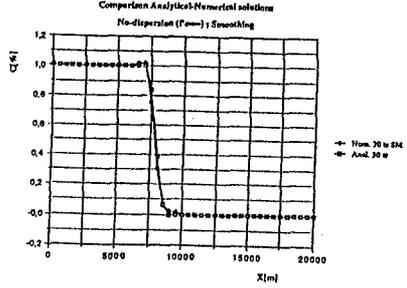


Fig. 3d

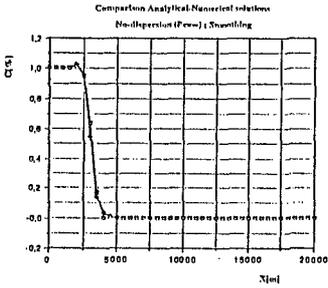


Fig. 3b

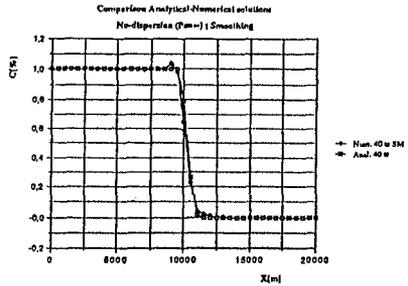


Fig. 3e

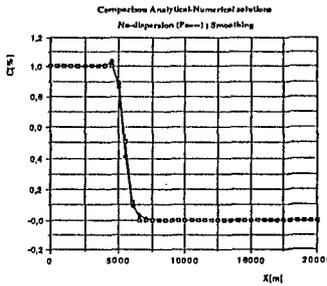


Fig. 3c

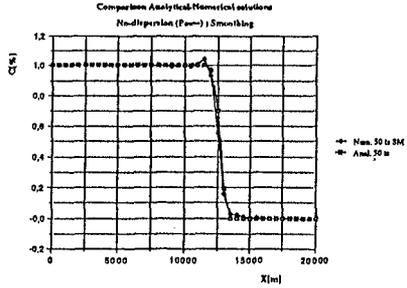


Fig. 3f

FIG. 3 - Breakthrough distribution in a uniform flow : comparison between analytical and numerical solutions in correspondence to different time steps [$0 \Delta t$ (fig.3a), $10 \Delta t$ (fig.3b), $20 \Delta t$ (fig.3c), $30 \Delta t$ (fig.3d), $40 \Delta t$ (fig.3e), $50 \Delta t$ (fig.3f)] with parameter values $N=2$, $Cu = 0.48$ and $Pe = \infty$.

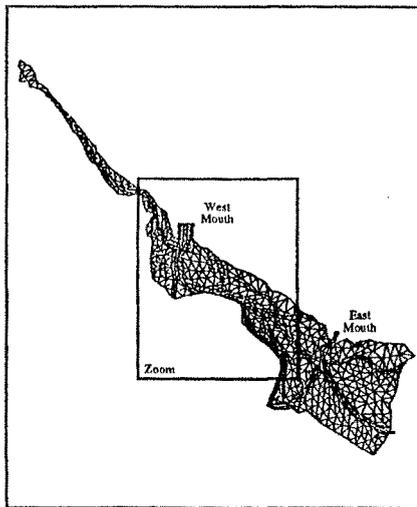


Fig. 4a - Barbamarco lagoon on Delta Po :
finite element mesh

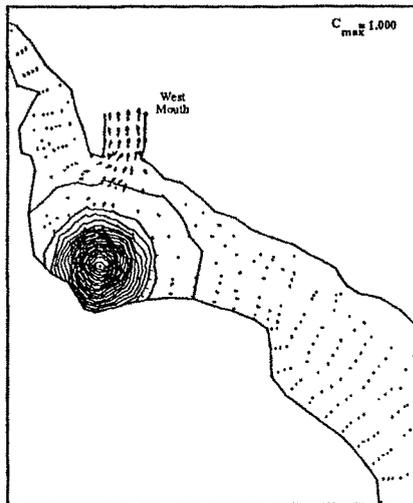


Fig. 4b : Barbamarco Lagoon on Delta Po :
representation of isoconcentration lines for a
instantaneous source of solute released near West
Mouth since 2 [h] from the beginning of simulation

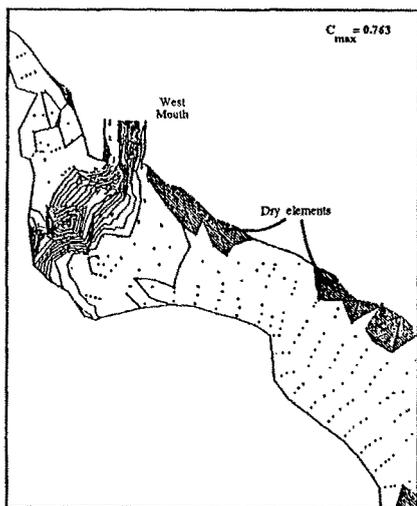


Fig. 4c : Barbamarco Lagoon on Delta Po :
representation of isoconcentration lines for a
instantaneous source of solute released near West
Mouth since 8 [h] from the beginning of simulation

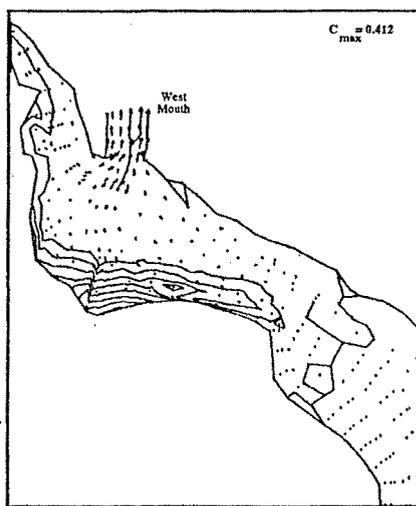


Fig. 4d : Barbamarco Lagoon on Delta Po :
representation of isoconcentration lines for a
instantaneous source of solute released near West
Mouth since 14 [h] from the beginning of simulation

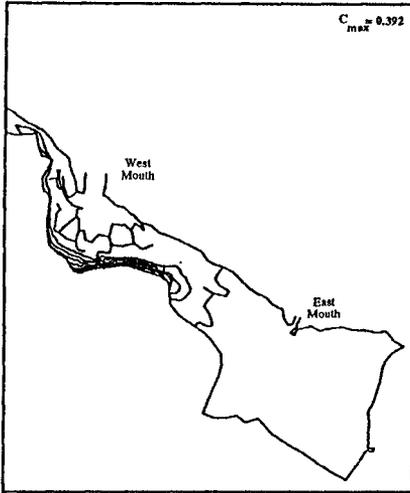


Fig. 5a : Barbamarco Lagoon on Delta Po : representation of isoconcentration lines for a instantaneous source of solute released near West Mouth since 1 [d] from the beginning of simulation

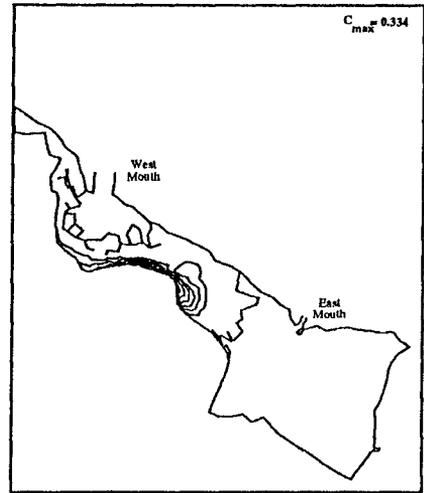


Fig. 5b : Barbamarco Lagoon on Delta Po : representation of isoconcentration lines for a instantaneous source of solute released near West Mouth since 2 [d] from the beginning of simulation

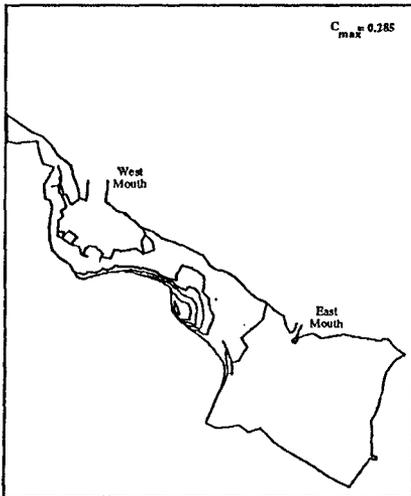


Fig. 5c : Barbamarco Lagoon on Delta Po : representation of isoconcentration lines for a instantaneous source of solute released near West Mouth since 3 [d] from the beginning of simulation

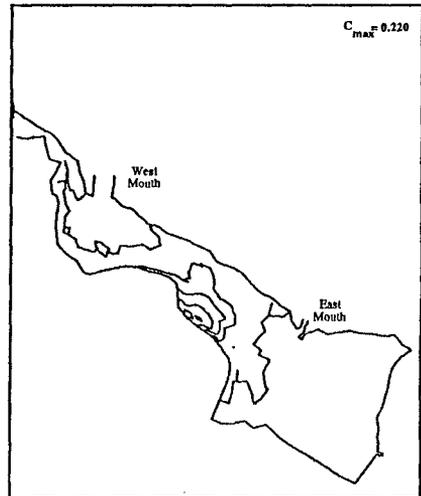


Fig. 5d : Barbamarco Lagoon on Delta Po : representation of isoconcentration lines for a instantaneous source of solute released near West Mouth since 4 [d] from the beginning of simulation