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Estuary Scale

Abstract

The MOHID 2000 system was implemented in the Tagus estuary in the framework of the EUROSAM project. Interactions between hydrodynamic, cohesive-sediments and water quality were studied. The system was calibrated comparing with field data. The model was able to reproduce the main features of the system. The hydrodynamic model was calibrated comparing model results with tidal gauges located along the estuary in the framework of other project (OPCOM and SANEST). The cohesive-sediments and the water quality models were compared with campaigns done between the years 1981-84. After calibration the system was used to simulate scenarios as an example of how models can help decision makers. A formulation to simulate arsenic processes in the Tagus estuary was added to the system (task 8).

Numerical tool description (MOHID 2000)

MOHID2000 is a full 3D-baroclinic model and has been developed using an object oriented programming philosophy and using all the FORTRAN 95 potential. The system has two main classes: the first one manages the hydrodynamic properties (e.g. velocity, elevation, water fluxes, turbulent viscosity) and the second one the water properties (e.g. salinity, temperature, density, SPM, nutrients, phytoplankton, coliforms).

The model is based on a finite volume concept. In this approach the discrete form of the governing equations are applied macroscopically to the cell control volume in the form of flux divergence. As a consequence this method automatically guarantees the conservation of transported properties (Adcroft et al., 1997).

The hydrodynamic properties evolution is computed solving the three-dimensional primitive equations in rectangular co-ordinates for incompressible flows. Hydrostatic equilibrium is assumed as well as Boussinesq approximation. The turbulent viscosity can be computed using several models. In the horizontal the options are constant value or Smagorinsky models. In the vertical the models that can be used are: a constant value, a mixing length model (Nihoul, 1984), a one-equation (K) model or a two-equations (K-L) model (Gaspar, 1990). The water properties evolution is computed solving the advection diffusion equation explicitly in the horizontal and implicitly in the vertical. The sinks are computed forward in time and the sources are computed backwards to avoid negative values of mass.

The system can make use of five different types of boundary conditions: free surface, bottom, lateral closed boundary, moving boundary and lateral opened boundary (Santos and Neves, 1991). Moving boundaries are closed boundaries whose position varies with time. For the lateral and moving boundaries the conditions are always null flux. Any exchange between land and the sea is computed as a discharge (for example a river or an outfall). The discharge class can compute the discharges of hydrodynamic properties (ex: momentum) and also of water properties (ex: SPM, salinity). For each of the other three boundary conditions: bottom, surface and open boundary, there are specific classes. The bottom class is responsible for the fluxes between the bottom and the water column (*e.g.,* shear friction, erosion/deposition of sediments). The surface class is responsible for the fluxes between the atmosphere and the water column (*e.g.,* wind forcing, gas emission, solar radiation).

A model is more than a program that uses a set of algorithms to solve a set of equations. A model with only good equations and good algorithms is not able to grow in orderly way. To avoid chaotic growth it is necessary to implement program techniques that ensure reliability and maintainability. The object-oriented programming is the most powerful technique to achieve these goals. This issue is especially important for large software systems like the MOHID 2000. These systems are usually developed by several collaborators separated in space and in time and for this reason a model must be able to incorporate new contributions always with a smiling face.

Another very important issue is the input data (pre-processing) of complex models like this one. It's necessary to develop graphical interfaces to help users to give the necessary data in a systematic way to the model. If the user does not belong to the development team the probability of introducing input data mistakes is high if the input data methodology is for example Ascii files. Output data (post-processing) analysis is also an important issue especially when you are talking of a 4D numerical tool (3 spatial dimension plus time) that is able of computing the evolution of almost 30 properties. If the users do not have access to tools that allows them of seeing the output data in an intuitively way this task can lead to madness. A graphical interface was developed to allow the user to explore the data using 2D images (3D slices) animated in time.

This chapter is divided in four main points: equations, algorithms, program development and management, finally pre/pos-processing.

Equations

Hydrodynamic class

The hydrodynamic class solves the three-dimensional primitive equations in Cartesian coordinates for incompressible flows. Hydrostatic equilibrium is assumed as well as Boussinesq approximation. The mass and momentum evolution equations are:

$$\frac{\partial u_i}{\partial x_i} = 0 \qquad (1)$$

$$\frac{\partial u_1}{\partial t}+\frac{\partial\left(u_j u_1\right)}{\partial x_j}=-fu_2-g\frac{\rho_\eta}{\rho_0}\frac{\partial\eta}{\partial x_1}-\frac{1}{\rho_0}\frac{\partial p_s}{\partial x_1}-\frac{g}{\rho_0}\int_z^\eta\frac{\partial\rho'}{\partial x_1}dx_3+\frac{\partial}{\partial x_j}\left(A_j\frac{\partial u_1}{\partial x_j}\right) \tag{2}$$

$$\frac{\partial u_2}{\partial t}+\frac{\partial\left(u_j u_2\right)}{\partial x_j}=fu_1-g\frac{\rho_\eta}{\rho_0}\frac{\partial\eta}{\partial x_2}-\frac{1}{\rho_0}\frac{\partial p_s}{\partial x_2}-\frac{g}{\rho_0}\int_z^\eta\frac{\partial\rho'}{\partial x_2}dx_3+\frac{\partial}{\partial x_j}\left(A_j\frac{\partial u_2}{\partial x_j}\right) \tag{3}$$

$$\frac{\partial p}{\partial x_3}=-\rho g \tag{4}$$

Where u_i are the velocity vector components in the Cartesian x_i directions, η is the free surface elevation, f the Coriolis parameter, A_i the turbulent viscosity and p_s is the atmospheric pressure. ρ is the density and ρ' its anomaly.

Water Properties Class

The flow field computed by the Hydrodynamic class is used to compute advection-diffusion equation (5).

$$\frac{\partial P}{\partial t}+u_i\frac{\partial P}{\partial x_i}=\frac{\partial}{\partial x_i}\left(K_i\frac{\partial P}{\partial x_i}\right)+Sources-Sinks \tag{5}$$

The density is calculated as a function of temperature and salinity by the equation of state (6):

$$\rho=\left(5890+38T-0.375T^2+3S\right)/\left(\left(1779.5+11.25T-0.0745T^2\right)-\left(3.8+0.01T\right)S+0.698\left(5890+38T-0.375T^2+3S\right)\right) \tag{6}$$

Water Quality (or Pelagic) Class

The Water Quality (or Pelagic) class uses the formulations proposed by (EPA, 1985) and developed to the MOHID System by (Miranda, 1997) and (Rodrigues, 1997). In (EPA, 1985), (Valiela, 1995) (Jorgensen *et al*, 1991) the authors gather a very complete list of rates and parameters and (Portela, 1996), (Grillot and Ferreira, 1996) and (Rodrigues, 1997), developed water quality applications in the Tagus Estuary.

The Water Quality class computes sinks and sources terms associate with the Carbon, Nitrogen and Phosphorous cycle. The properties that are change by this class are: phytoplankton, zooplankton and Nitrogen (Ammonia, Nitrate Nitrite, particulate organic nitrogen, dissolved refractory and non-refractory organic nitrogen), Phosphorus inorganic and organic, Dissolved Oxygen and BOD (Biochemical Demand of Oxygen). In this simplified approach only the Nitrogen and Phosphorus are found a limiting factor to the primary production, which is true to most coastal areas. Zooplankton is included in this model, enabling it to simulate accurately phenomena such as the spring bloom.

Cohesive sediments processes

The erosion algorithm is based on the classical approach of Partheniades (1965). Vertical sediment transport between layers is a function of vertical diffusion, vertical flow and sediment settling. The hydrodynamic model computes the former two factors. Settling velocity depends on flocculation processes and is calculated as a function of the concentration (Dyer, 1986). Deposition is modelled as proposed by Krone (1962). The bed properties are assumed to be constant (e.g. consolidation is ignored). The sediment properties used by the model are those of fine (or cohesive) sediments (particle diameter less than 64 μm), found by calibrating the model, starting with values from the literature.

Algorithms

Hydrodynamic Class

The class uses a semi-implicit ADI algorithm with two time levels per iteration. Two numerical schemes are currently implemented: the 4 equations S21 scheme (Abbott et al., 1973) and the 6 equations Leendertse scheme (Leendertse, 1967). The free surface elevation is computed through integration of equation (1) over the water column. The two components of the horizontal velocity are globally centered in $t+1/2$ leading to a second order time accuracy (Martins et al., 1998). Vertical fluxes are also computed by continuity (hydrostatic approach), integrating over each cell volume. Since the mesh is allowed to move along the vertical direction the computation of the vertical fluxes and the redefinition of the geometry are calculated in conjunction.

Water Properties Class

The water properties evolution is computed solving the advection diffusion equation explicitly in the horizontal and implicitly in the vertical in the same grid used by the hydrodynamic class. The sinks are compute forward in time and the sources are computed backwards to avoid negative values of mass.

Water Quality (or Pelagic) Class

This Water Quality class has been developed in terms of sinks and sources. Such an approach is convenient to give these models the desired flexibility, providing it with the capability of being coupled to either a Lagrangian or an Eulerian resolution method. Because of the properties interdependency a linear equation system is computed for each control volume and this system can be compute forward or backward in time.

Cohesive sediments processes

The simulation of cohesive sediment transport is performed solving the 3D-advection-diffusion equation in the same grid used by the hydrodynamic model. The sediments processes are computed using fluid velocities, shear stress and eddy diffusivities calculated by the hydrodynamic model. Numerically, horizontal transport is solved explicitly, while the vertical transport (including settling) is solved implicitly for numerical stability reasons.

Program development and management

FORTRAN is one of the most used scientific and engineering programming languages. On one hand it enables the use of reliable, tested and 'already written' software and, on the other hand, the handicap of learning a new language does not exist (Nyhoff and Leestma, 1997). Nevertheless from some years on several limitations were becoming more and more clear. Those limitations reflected themselves in an increasing difficulty to design, develop and maintain, clear, reusable and robust scientific software. Some of the most important draw backs of FORTRAN 77 were the lack of dynamic storage, the inexistence of user-defined types and the lack of polymorphism.

FORTRAN 90, and later FORTRAN 95, made possible the use of the Object-Oriented (OO) paradigm in FORTRAN software. Although FORTRAN 9x does not have all the features other OO languages have (*e.g.* inheritance), it is nevertheless possible to write good quality OO programs with it.

When developing OO software the gravitational centre of every object is information. To start thinking in terms of objects one must split the information (data) into elemental and natural pieces. One step forward would lead us to visualize an object as a physical memory area. The object that owns this information becomes from now on responsible for it and this object alone is authorized to modify it, *i.e.*; object data must be *encapsulated* (Rumbaugh et al, 1991). When it is necessary for other object to access that information it asks for it to the owner creating a *Client/Server* relationship (Duffy, 1995).

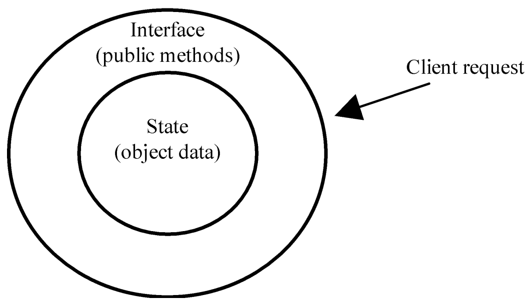


Figure 1 – Layer approach.

An object is at the same time the information that it owns and the methods that can operate or access it. Public methods form the interface that client objects use to communicate with the server. An object has well defined boundaries and a state. The *behavior* of an object is the way it reacts to an event, *i.e.*, a client request; the behavior depends on the state of the object (Duffy, 1995).

A class is an abstraction, it is the software code and it has no associated memory. An object is an instance of a class and it always has associated memory. MOHID 2000 system is OO software so it is possible to create several instances of the same class. One of the obvious advantages of this approach is simplification of nested models; the same code is run as many times as needed, creating the corresponding (nested) model implementation in a straightforward manner.

Objects are dynamically created in run time; it is no longer necessary to compile the program each time it is applied to a new site.

MOHID 2000 uses a layered approach (Figure 1). The use of a layered approach ensures that client/server relationship is maintained. A hierarchy is set where lower level subsystems (layers) are servers to upper level systems (Duffy, 1995).

Most MOHID 2000 applications use four main objects; most of its objects are internal classes that act as 'glue' between application objects (Duffy, 1995) (*e.g.*, object Model). The most obvious object is Hydrodynamic; there are also WaterProperties, Bathymetry and Time objects.

The Hydrodynamic class is responsible by the water surface elevation and water fluxes between cells (velocities). Using this class it is possible to choose if computations are to be made (there are several algorithms) or a file to be read from.

The WaterProperties class is responsible for every intensive property, e.g., salinity, heat (temperature), sediments, phytoplankton, etc. Advection-Diffusion processes and sinks and sources are controlled here.

The Bathymetry class is responsible by for the bathymetry and thus provides essential information concerning the grid formation.

Time is the class that keeps information about the execution instant. This class is the core of the synchronism system.

Reliability and maintainability are the most important features of a well-engineered software system. There is always a trade-off between efficiency and reliability. Inefficiency is predictable and measurable; reliability is not. It is possible to improve the program efficiency hence it should not be the main concern during the development phase. On the other hand, if a program proves unreliable, it is not easy (it may even prove virtually impossible) to enhance it. The best way to assert software quality is reliability rather than efficiency.

The use of OO paradigm to develop large software systems like MOHID 2000 is the most powerful software-engineering available techniques to ensure reliability. Encapsulation, responsibility and client/server relationships between objects prove to be important features assuring that unpredicted software behaviour is both minimized and, whenever present, easily located. When an object is found not to function properly, the problematic functionality is either replaced or repaired without interfering with the rest of the program.

Pre/Post-Processing

The use of computer models can be divided in three main tasks:

- Acquisition and supply of the input data for the model (Pre-processing)
- Execution of the model
- Exploration and interpretation of the model results (Post-processing)

Numerical models, with origin inside universities, usually have a very limited number of users. Basically they are not build considering the user point of view that is why data supply and result analysis are so complex and just a restricted number of persons, usually the scientists which developed the model, are able to produce results . The object oriented strategy used during the development of MOHID 2000 permitted to create easily a graphical user interface (GUI). This interface is able to supply input data and analyse results produced by the model. The main goal of this GUI is to make the model accessible to users that are not members of the development team.

MOHID 2000 is written in Fortran 95 ANSI standard. This is very important for platform independence (Nyhoff, and Leestma, 1997). User friendly pre and post processing software cannot be written in Fortran 95 standard, so it was necessary to use additional libraries. To build a window based GUI the development team of MOHID 2000 used the libraries from the Windows Platform SDK. These libraries are nowadays easily transported to Unix based systems. For the graphical post processing part, the base library is the widely used OpenGL package, which is also platform independent.

Pre-processing

There are several tasks, which the pre-processing GUI must handle. One task is to organize the whole project by itself. Every project consists of several simulations and every simulation consists of one or more runs. For every run there are several data files needed, e.g. hydrodynamic, turbulence, water properties, to name a few, depending on the compute options chosen by the user. Such complexity easily results in huge amount of data files. Figure 2 shows an example of the MOHID 2000 pre-processor main window.

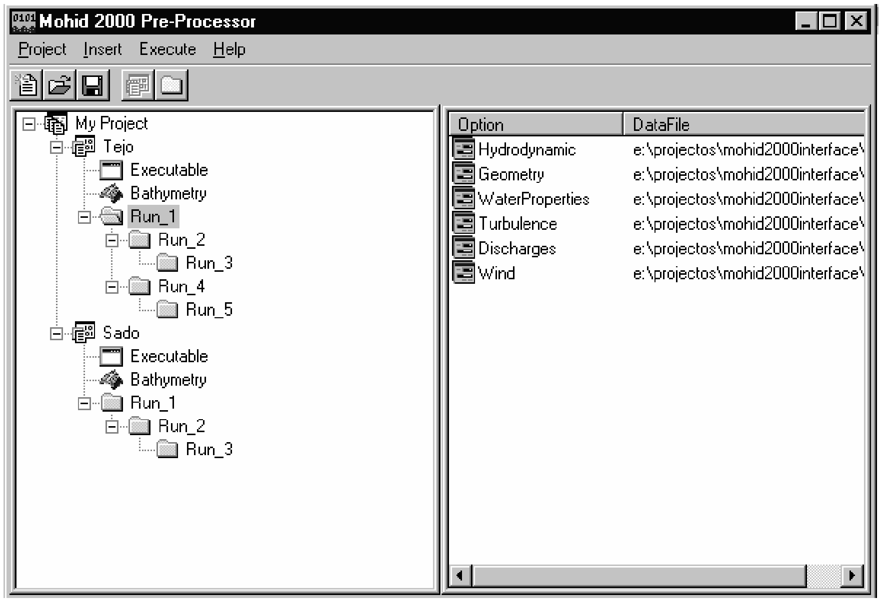


Figure 2: The MOHID 2000 Graphical User Interface

Another task is to receive numerical data input from the user. In the GUI written for MOHID 2000, that numerical data input can be supplied in window based dialog boxes. After successful numerical data input the data is written to ASCII files, which is intended(understood) by MOHID 2000. In these files, every numeric data field is preceded by a keyword, allowing these files being organized in a random order and easily understood. Figure 3 shows a sample dialog box, where it is possible to supply data for the hydrodynamic class.

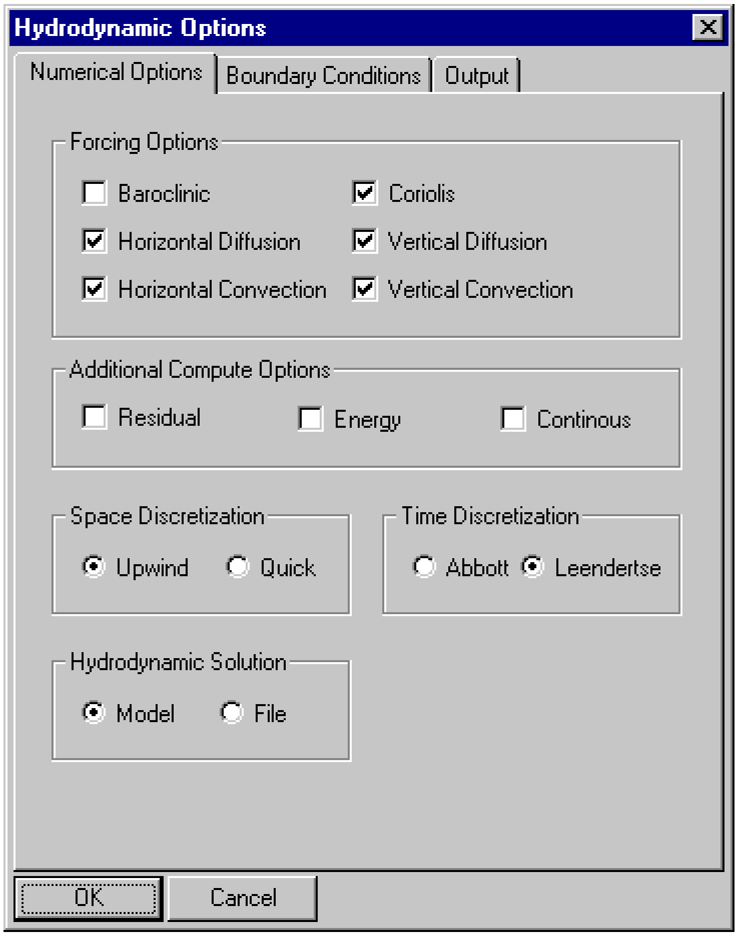


Figure 3: Dialog based numerical data input

Another task is to let the user a possibility to define points graphically (e.g. time series location, discharge places, particle emission points, etc.) or regions (e.g. water quality monitoring boxes). Figure 4 shows an example of the Tagus estuary.

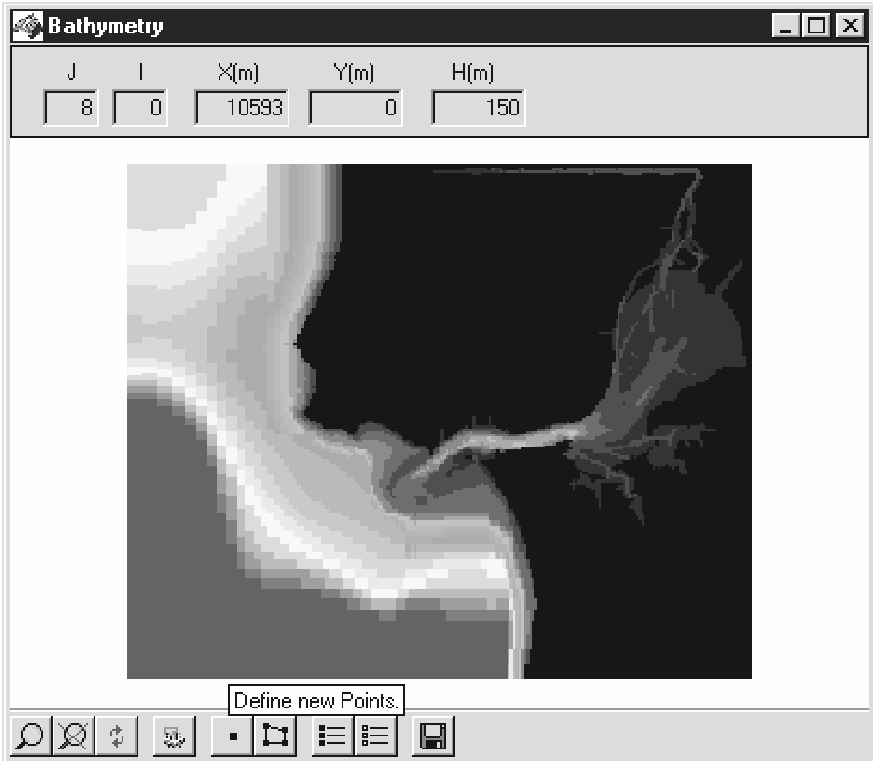


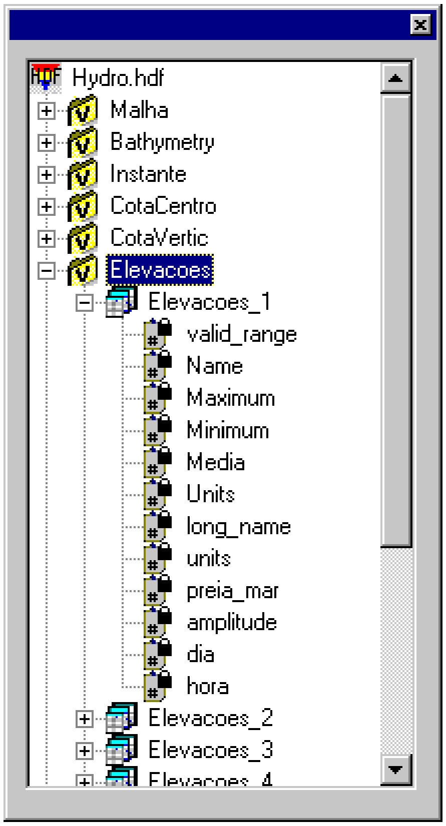
Figure 4: Graphical pre-processing

Post-processing

Like the pre processing, the post processing of the results produced by large computer programs should be, as much as possible, user friendly. The results produced by MOHID 2000, are principally two: results stored as column data (e.g. time series) and results stored in matrix format (e.g. velocity fields). The first ones are stored in ASCII files, allowing these results to be portable and easy to use by spreadsheet applications, like MS Excel. In the case of matrix data the amount of data to store is much bigger and the organization of matrixes inside of ASCII files is complex. For example, a typical discretization for the Tagus estuary is 146*188*10 grid points, simulating hydrodynamics (6 properties) and all possible water properties supported by the model (about 18) and writing output data in 10 different time instants, the total amount of data (single precision) is about 146*188*10*24*10*4 = 264Mb.

To organize the huge amount of data MOHID 2000 uses another standard to write matrix data, which is the widely used Hierarchical Data Format (HDF). The HDF software is developed and supported by the National Centre for Supercomputing Applications (NCSA) and is freely available. The advantages of using HDF are, among others, that the HDF files are self-describing, very efficient in storage, and platform independent (Folk, 1998). Many visualization tools are available to browse HDF files and the MOHID 2000 development team developed a post-processor, which turns the exploration of the results produced by the model simple. The tasks of post-processing are three: selecting the information to represent, choose how to represent this information and finally represent the information graphically. In the first task the fact that the data produced by the model is stored in an HDF data file is very useful, so its possible to select the data from an HDF tree view, like shown in Figure 5.

Actually there are three ways to represent the data: in form of color, contour lines or vector data. The user has the possibility to define additional parameters, before displaying the final image. In the case of 3 dimensional models it is very important to have in mind that the user would like to define any kind of vertical or horizontal plane to represent a final 2 dimensional image (the possibility of representing 3 dimensional graphics is not implemented yet). Figure 6 shows the interface of the second tasks of the MOHID 2000 post-processing tool: choosing the type of graphic.



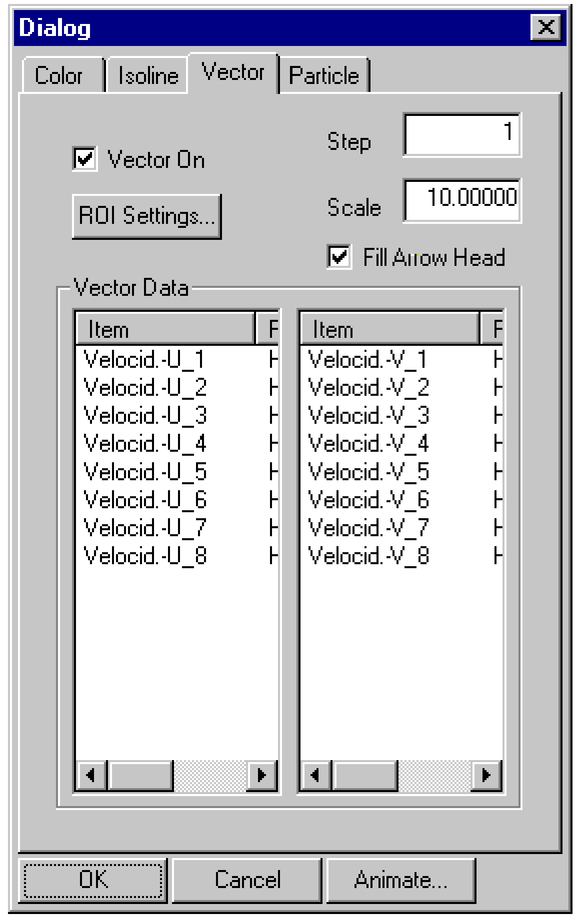


Figure 5: Selecting the information to represent

Figure 6: Choosing how to represent the selected information

The final image, like referred above, is rendered using the OpenGL graphic package (Segal and Akeley, 1994). A typical final image looks like the one represented in Figure 7. This last task is the main goal of a Post-Processing tool to access the information generate by a model in an intuitively way in this case 2D images. Using the “Animate” command its possible to access to one more dimension (time).

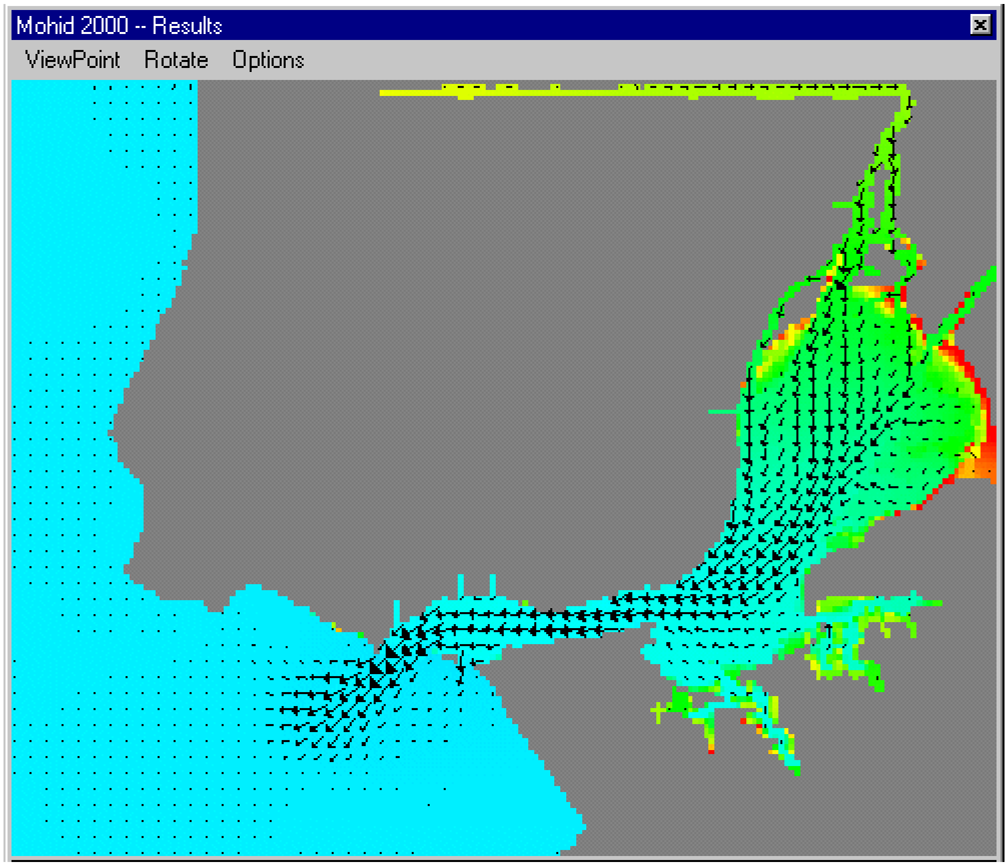


Figure 7: The final representation of the data.

Implementing MOHID 2000 at the estuary scale

The Tagus estuary is one of the widest estuaries in the West Coast of Europe and the larger in Portugal, covering almost a 320-km2 area (Vale, 1990, Vale and Sundby, 1987). The Portuguese capital, Lisbon is the most important city built on its margins. The metropolitan area has nowadays around 2 million inhabitants, an important harbour and big industrial complexes around the estuary.

The estuary is a mixing place of river and oceanic waters. The salinity distribution depends mostly on the river flow and on the mixing imposed by the tidal regime, which is the main mechanism controlling the distribution of aquatic organisms and suspended particulate matter in the estuary. In ecological terms, it works as a nursery for several species.

Hydrodynamic can be seen as the first driving mechanism of a cascade of complex processes. The water flow is responsible for transporting chemical (e.g. Ammonia), biological (e.g. phytoplankton) and geological (e.g. sediments) in the water column. It is also responsible for the sediments fluxes between the bottom and the water column. The hydrodynamic model was forced only with tide because the main goal of this project is the study of salt marshes and inter-tidal areas where tide is the main forcing mechanism. The cohesive-sediment model use shear stress compute by the hydrodynamic model to quantify bottom fluxes. The sediments concentration deeply interacts with the water quality processes. The light extinction factor that regulates the amount of light that primary producer receives, is sensible to sediment concentration, causing low growth rates in high turbidity areas (Portela, 1996).

The simulation of the water quality processes was developed considering that the autotrophic producers consume inorganic nutrients and depend on both their availability and sunlight as a source of energy for photosynthesis. Nitrate and ammonia are the inorganic nitrogen forms that primary producers consume. The primary and secondary producer's excretions are considered, acting as source for the nitrogen cycle. Primary producers are consumed by secondary producers, which in turn are consumed by higher trophic levels.

Hydrodynamic Processes

The Tagus estuary hydrodynamic calibration has been done in the framework of other projects (OPCOM and SANEST) and was been the subject of a PhD. thesis. In this report only some results to illustrate the main features of the Tagus estuary hydrodynamic are presented.

Residual velocities presented in Figure 8 (surface values) were obtained through time integration of transient velocities. Residual velocities do not usually provide much direct information but they can be helpful to understand long-term phenomena with time scales much larger than the tidal period. There is a jet outward the estuary associated with a strong anticyclone off Costa do Estoril; a cyclone and an anticyclone inside the channel reveals a very complex hydrodynamic system coupled with the topography.

Figure 9 shows instantaneous surface velocities during ebb (5h 44m after high water, tide amplitude 3m). The maximum velocity occurs in the channel. This figure shows the Cascais' bay periodic anticyclone (it appears during ebb time) and the outward jet. These features, also visible in the residual velocity (Figure 8) have a strong influence in the bathing coastal area of Cascais; because of this gyre the estuarine ebb water weakly affects the area. Model results (and other field studies) strongly suggest that water quality in this area depends first of all on the proper control of local pollution sources.

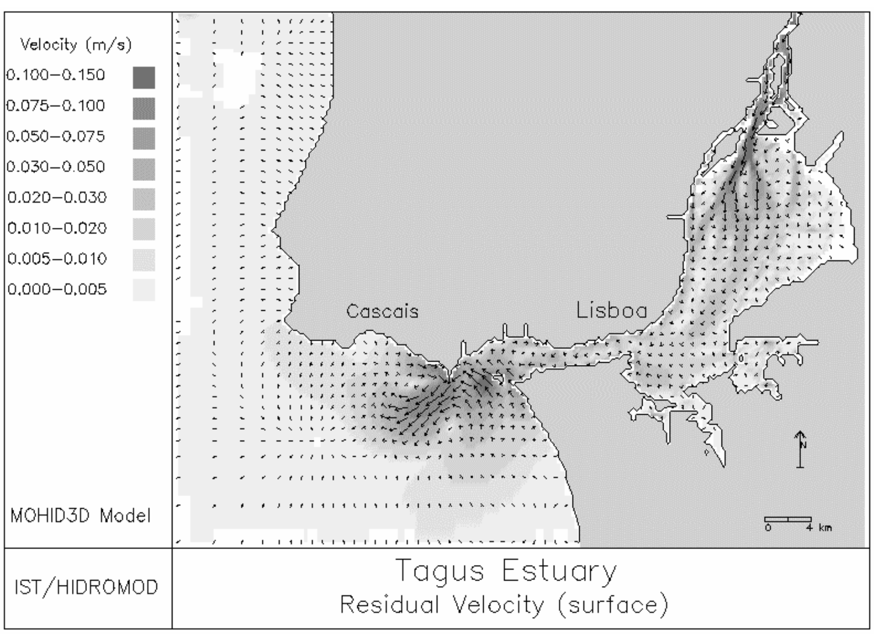


Figure 8 - Tagus Estuary surface residual velocity field.

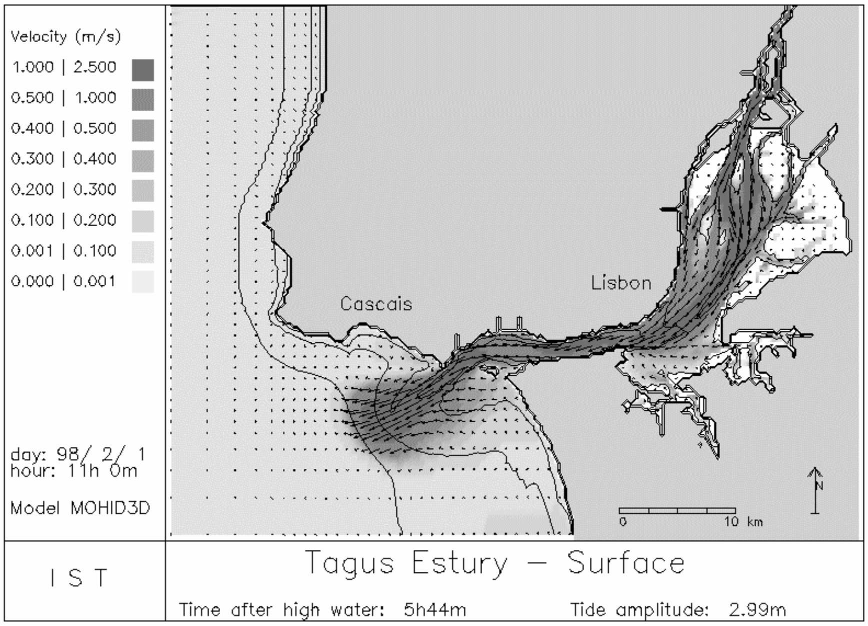


Figure 9 - Transient velocity field.

Cohesive sediments Processes

The 3D cohesive-sediments model calibration was presented in the EUROSAM progress report only some conclusions of this work are where presented.

The main transport mechanisms are well simulated by the model, since spatial (longitudinal and lateral) suspended sediment distributions follow observed patterns, and semi-diurnal as well as spring-neap tide fluctuations are about the same magnitude as field data indicate.

A finer grid might eliminate small scale differences, especially apparent in the time series of Castanheiro and Crespo (1983), arising because of the special locations chosen for the sampling stations. The use of a more realist flocculation algorithm will probably improve the results in the upstream end of the estuary, although computational cost should be weighed against the limited extent of this phenomenon in the Tagus estuary. A further improvement would be the simulation of consolidation processes. These improvements are being made in the framework of a Ph. D thesis. The model calibration was the subject of two masters thesis (Clipper, 1998 and Pina, 1998).

Water Quality processes

The calibration of the water quality model offers a serious challenge duo to the number of variables and processes involved. These parameters and rate values are specific to each case study, so they should be gathered threw bibliographic review and by local measurements, or if that's not possible, the modeller should know their variation limits in order to study the model sensitivity to those limits. In conclusion sensitivity analysis should be tested for model parameters. This analysis is not exhaustive for two main reasons. First, the number of variables and processes involved would make it unreasonable. Second, each process is controlled by rates and parameters that in some cases are generally established by several authors including for specific applications in the Tagus estuary (Portela, 1996).

Tank application

In order to diminish the time spend in each test, a tank simulation was developed. In this tank with a much smaller compute domain, the forcing functions are very similar to the ones in the actual Tagus model.

The model sensitivity analysis for the nitrogen semi-saturation constant (kN) is presented as an example. The choice of this parameter happens because of its profound influence in all the properties of the water quality model allowing demonstrating the model behaviour.

The nitrogen semi-saturation constant (kN) affects the primary producers behaviour for two reasons: First, it will affect the preference factor between ammonia and nitrate. In Figure 10 it's clear that for constant ammonia and nitrate concentrations with and increasing kN the preference of phytoplankton will shift from ammonia (preference factor equal to 1) to nitrate (preference factor equal to 0).

Second, it will affect phytoplankton growth rate, by influencing the growth limiting function for nutrients. This function varies from 0 for no nutrients available to 1 for nutrient saturation. In Figure 11 it's clear that for constant ammonia and nitrate concentrations with and increasing kN the growth limiting function for nutrients will diminish. This means that for the same simulation if we choose a higher Kn, phytoplankton will growth less. Figure 3 shows that in a 4-year simulation the phytoplankton concentration is higher for the smallest kN value and lower for the higher kN value. Nitrate concentration in the tank diminishes in time because there is no source of this nutrient and there is a sink duo to denitrification. Because of this fact, in the 4-year simulation, in the last two years we have low nutrients concentration. For the lower kN values, no problem is caused to phytoplankton growth because this low nutrients concentration is steel "enough" to maintain the growth limiting function for nutrients with high values (near 1). By the other hand with higher kN values, the nutrients concentration steps away from saturation, showned by the near zero values of the growth limiting function and phytoplankton tends to extinction.

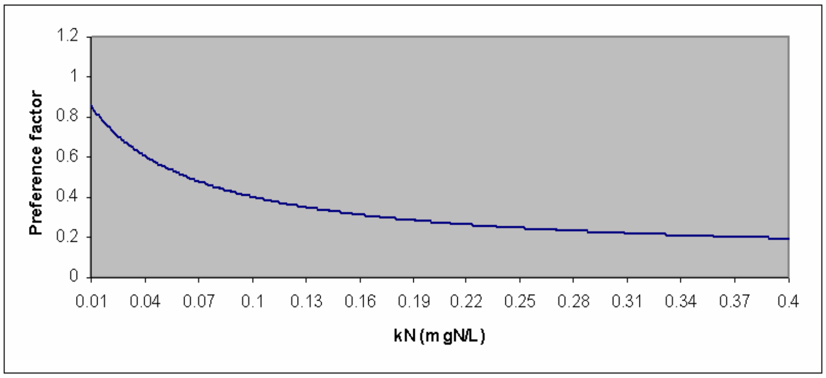


Figure 10 – Phytoplankton preference factor variation with increasing kN.

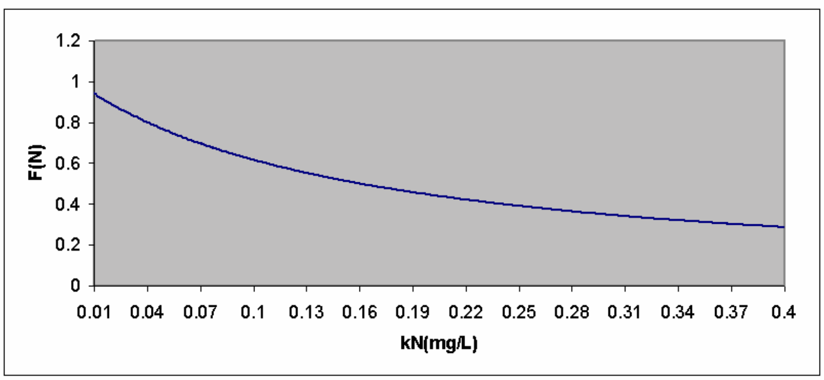


Figure 11 Phytoplankton growth limiting function for nutrients variation with increasing kN.

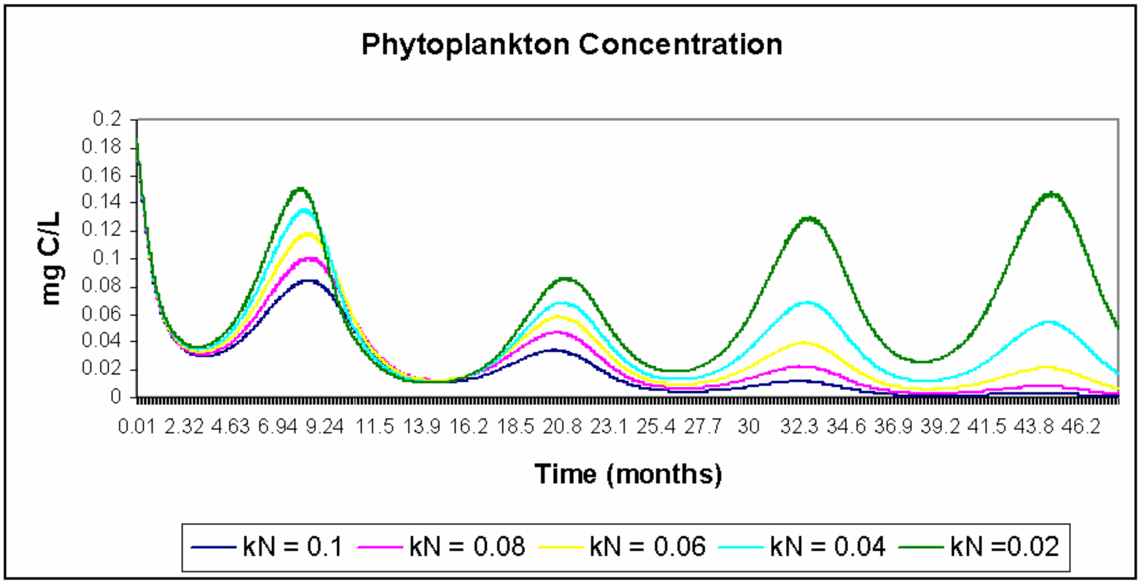


Figure 12- Phytoplankton variation for different kN values over a 4 year time period.

The tank simulations were carried out, for computing speed reasons, a 4-year simulation with the tank domain takes about 6 min, instead of the 12 hour spent in a one year run in the Tagus domain. The tank simulations are useful to understand the rates and parameters influence over the water quality properties but the Tagus runs are indispensable to confront the water quality with the physical dynamics. One of the several test runs performed had the objective to understand the influence of the zooplankton growth rate in the overall system. Figure 4 shows phytoplankton and zooplankton total mass evolution over a year. The results were integrated spatially using the integration boxes tool already described. This result shows that for the simulation carried out with the higher zooplankton growth rate (test A) the peak value for phytoplankton is lower then in test A (with a lower zooplankton growth rate). The zooplankton peak is about the same value in both cases but occur with a small time delay between tests duo to the faster zooplankton growth accomplished in test A. This fact is the cause of the lower peak for phytoplankton in test A.

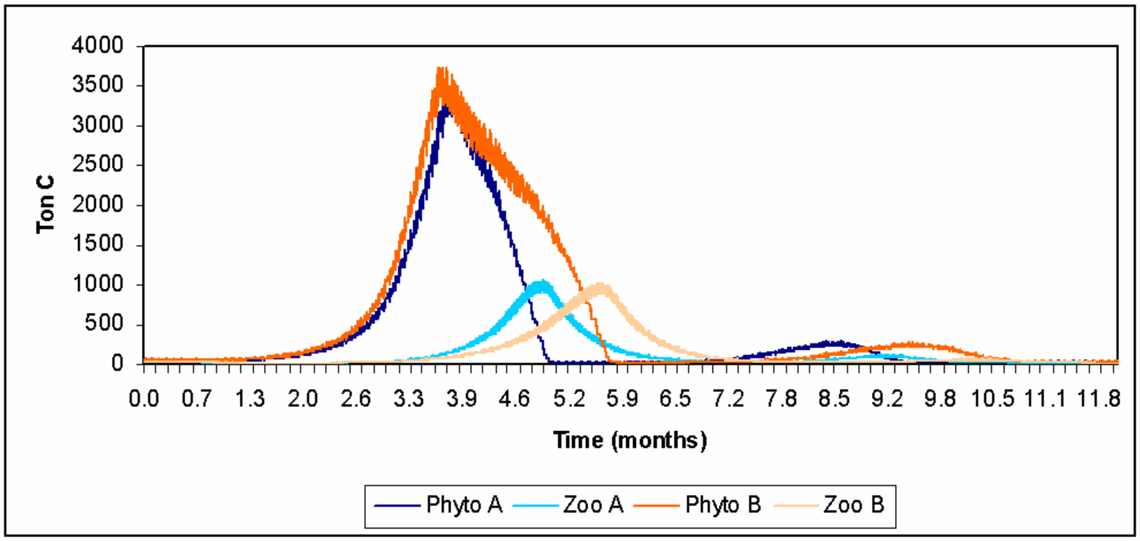


Figure 13 – Mass of Phytoplankton and Zooplankton variation for different ZooPlankton maximum growth rates (Test A = 0.16 1/day ; Test B =0.14 1/day), in the Tagus estuary over a year.

Tagus estuary application

At modeler's heaven, one should manage to find perfect parameterization to use on a total-process-descriptive model with the most complete set of field data to compare model results with environment behavior. In real world the models aren't able to simulate the full processes involved, the parameterization is very difficult to achieve and the available field data is often scarce and inappropriate. However, often it's possible to reach a commitment solution with these adversities and produce not perfect, but good results.

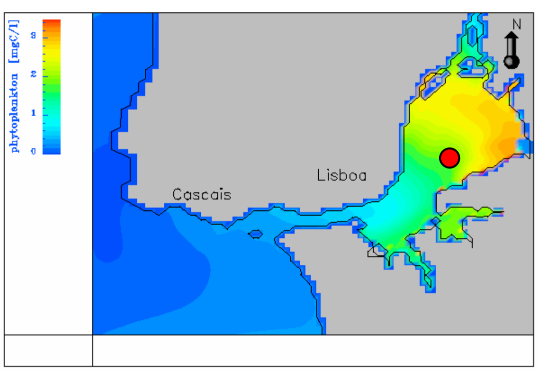


Figure 14 - Field station 3.5 location

The following results show time series comparisons between model and field data from the Tagus Field Station 3.5 (Figure 14) after Martins & Dufner (1982), Martins *et al*. (1983a, 1983b) and Silva *et al.* (1986a), for four consecutive years: 1980, 1981, 1982 e 1983

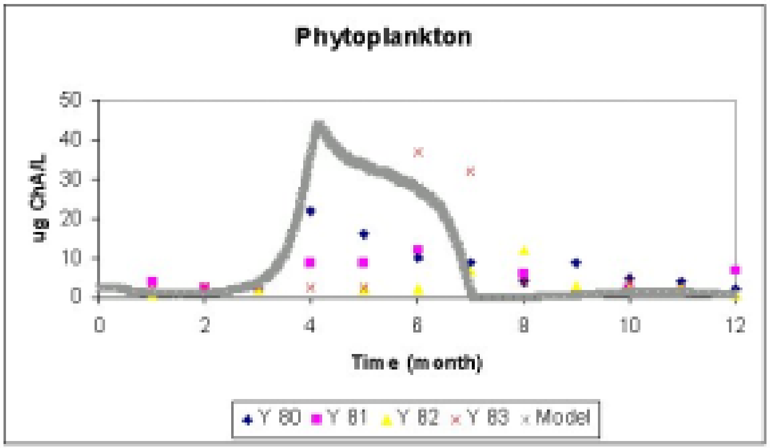


Figure 15 – Phytoplankton variation over a year

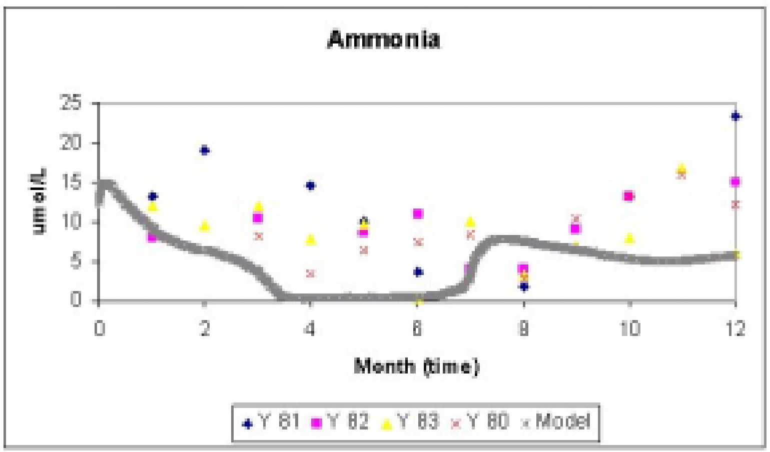


Figure 16 - Ammonia variation over a year

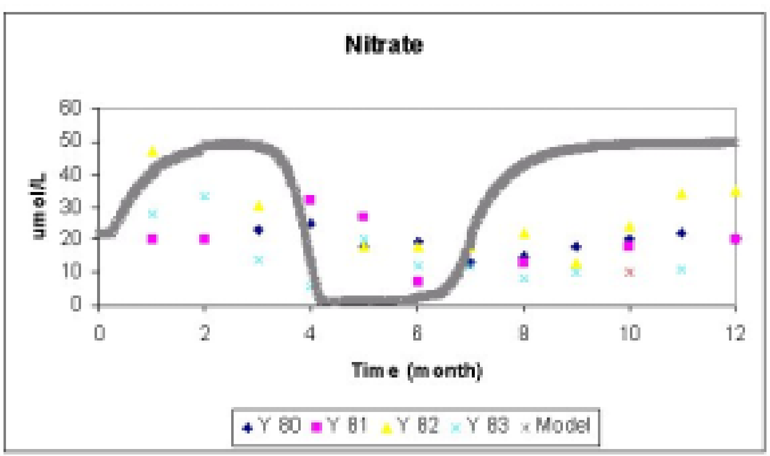


Figure 17 - Nitrate variation over a year

The model results show a pronounce phytoplankton bloom in May (Figure 15), caused by the nutrients availability and increased sun radiation. After the bloom the phytoplankton concentration is controlled by the zooplankton strong growth (not represented) and lower nutrients concentration. Nitrate (Figure 17) and Ammonia (Figure 16) suffer heavy grazing during the phytoplankton peak. Afterwards Ammonia increases duo to zoo and phytoplankton respiration and excretion loses and Nitrate increases duo to nitrification processes.

The next results show the spatial distribution of Phytoplankton, Nitrate and Ammonia in two distinct situations: during winter with low phytoplankton concentrations and high nutrients concentration and during the Spring/Summer phytoplankton bloom with low nutrients concentration.

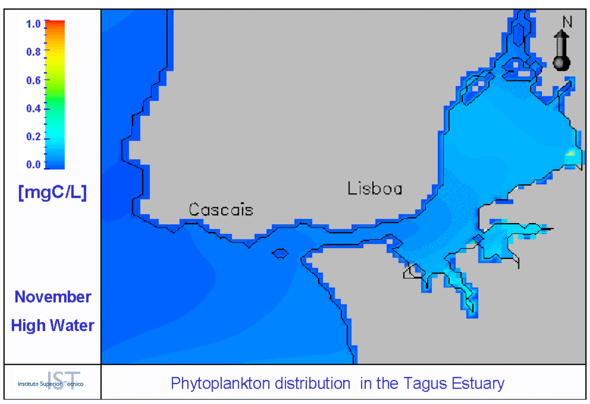


Figure 18 – Phytoplankton distribution at the Tagus Estuary, in a winter simulation.

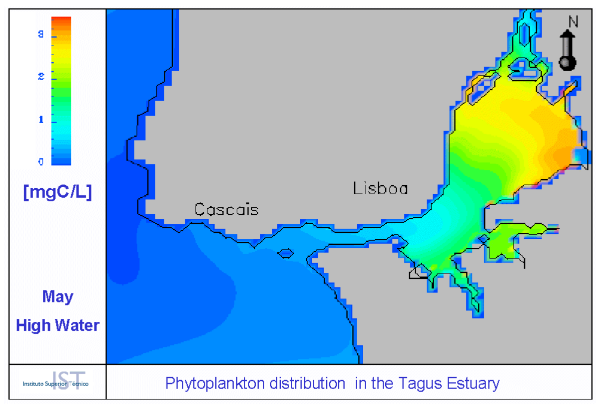


Figure 19 – Phytoplankton distribution at the Tagus Estuary, in a spring simulation.

Both Figure 18 and Figure 19 show high concentration of phytoplankton in the upper part of the estuary especially in the salt marsh region. Due to the low water level (more light available) and high nutrient concentration this region will have an intense production. The next pictures confirm the nutrients distribution near the salt marsh reason of the estuary and show the differences between seasons due to the phytoplankton consumption.

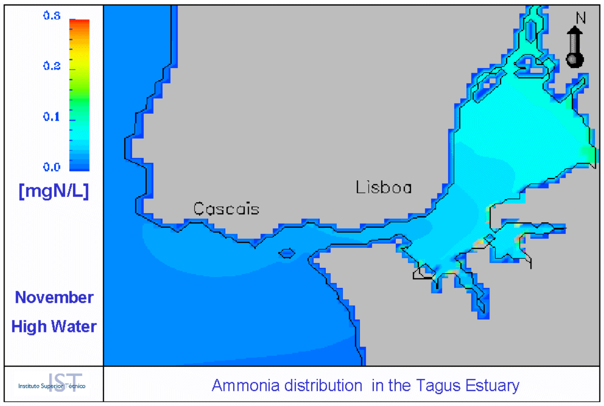


Figure 20 – Ammonia distribution at the Tagus Estuary, in a winter simulation.

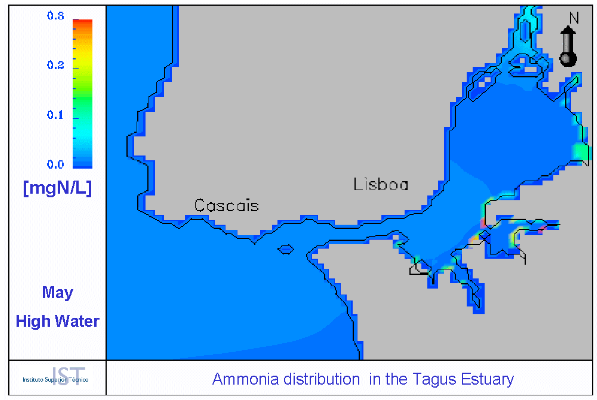


Figure 21 – Ammonia distribution at the Tagus Estuary, in a spring simulation.

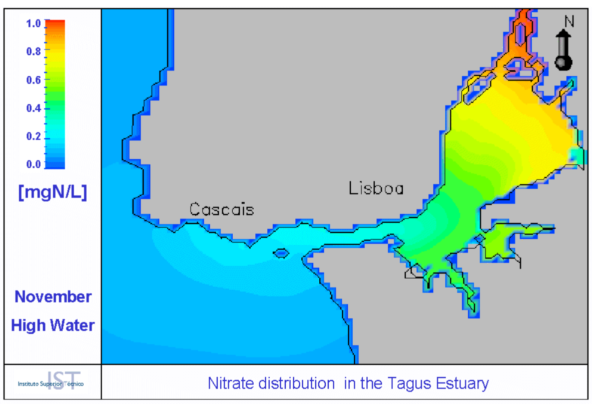


Figure 22– Nitrate distribution at the Tagus Estuary, in a winter simulation.

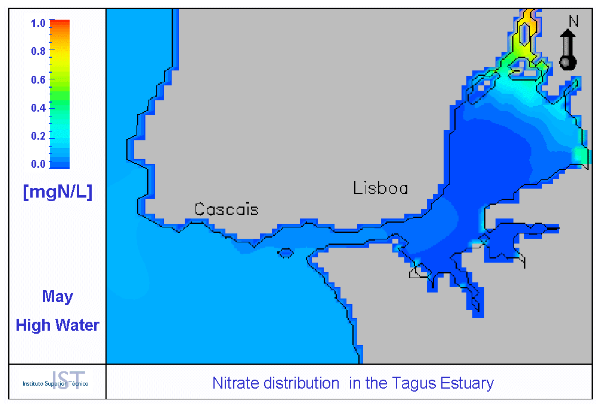


Figure 23– Nitrate distribution at the Tagus Estuary, in a spring simulation.

The next pictures show the time and spatial integrated fluxes of phytoplankton, nitrate and ammonia over a year in the Tagus estuary. In every case the estuary is exporting to the ocean. With Phytoplankton all the production occur inside the estuary so the river input it's almost null and a large part of this production is exported to the ocean. With ammonia (Figure 25), although phytoplankton preference to this nutrient instead of nitrate, the estuary exports more then it receives from river input because of respiration and excretion loses. With nitrate (Figure 26) the estuary exports to the ocean less then it receives from the river input duo to denitrification process and assimilation by phytoplankton.

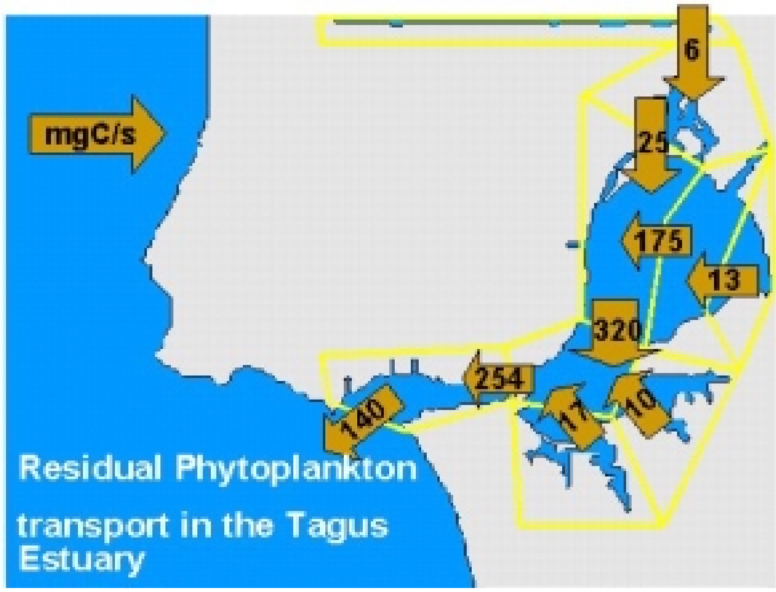


Figure 24 – Residual phytoplankton transport.

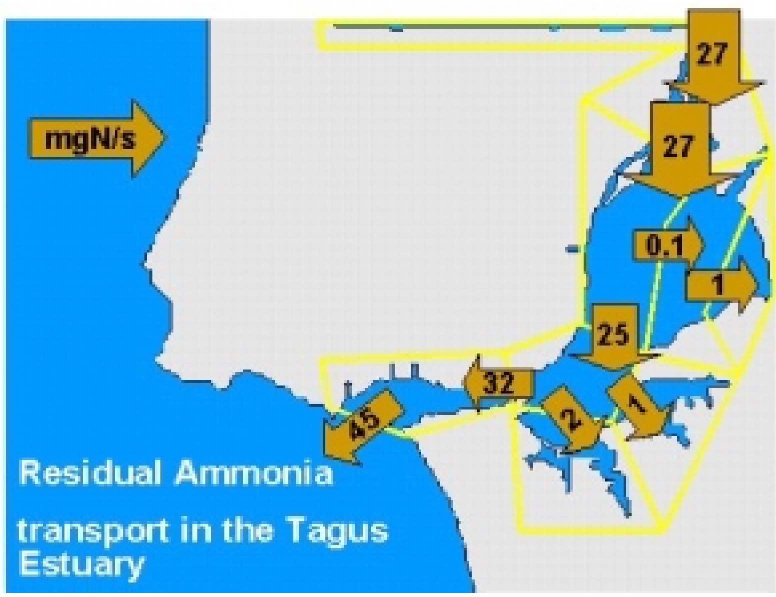


Figure 25 – Residual ammonia transport.

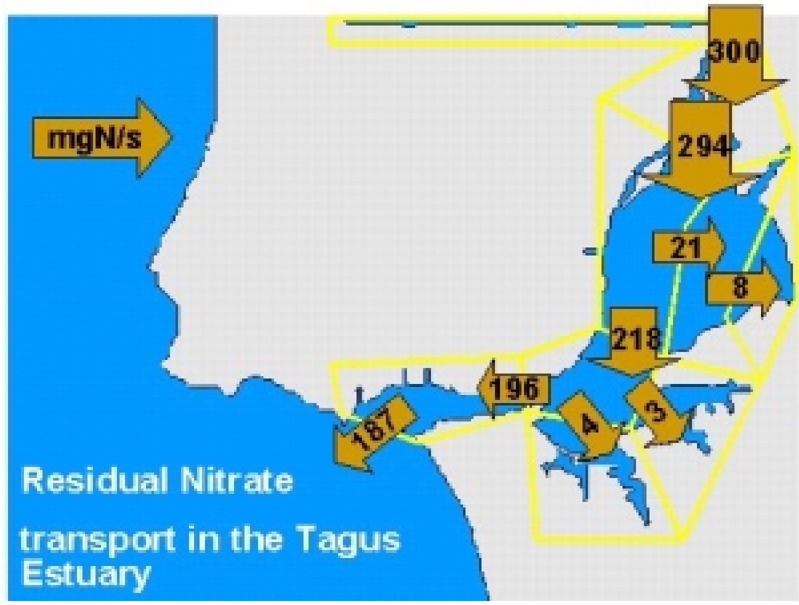


Figure 26– Residual nitrate transport.

Support Decision Makers

Coastal zones are the most heavily populated and ecologically vulnerable areas worldwide. Here many different and often contradictory interests exist which have to be carefully managed. For this purpose it is absolutely necessary to enhance the forecast capacity regarding the medium to long-term evolution of the coastal marine system in view of human activities and natural changes.

Forecast models for coastal waters, complemented by continuous monitoring systems and supported by efficient databases, can provide this kind of assistance, helping in the development of management concepts compatible with sustainable growing and with the preservation of ecosystems integrity. These integrated systems, if used in a regular basis by local authorities, can help them to achieve important improvements in coastal management practice (including risk assessment).

In the framework of different projects presently running in Tagus estuary (e.g. OPCOM, EUROSAM) a modelling system driven by field data from monitoring sites and larger scale forecast models is being applied. The results and information from the modelling system are used to integrate the local measurements, understand the system behaviour and help the local users to efficiently manage the system.

In the case of EUROSAM the aim is to investigate the interaction between the different ecological components of muddy coastal ecosystems, salt marshes and mud flats. To achieve these objectives an ecological model, supported by field measurements, was implemented in Tagus estuary.

Regarding the specific needs in terms of data, it is important to remember the important development achieved in what concerns the field instrumentation technologies, which led to a fast growing of the capacity to produce information. This capacity is making possible the implementation of monitoring plans with lower costs and a better coverage of the areas of interest but it also implies the necessity of making available efficient data analysis and visualisation tools capable of exploring all this information.

Directly or indirectly the Tagus estuary is the final disposal place of the region-produced effluents. Some of these are subjected to land-treatment while others are simply disposed in the estuary margins without any kind of treatment, or dispersion mechanism.

Besides all the domestic and industrial effluents produced in the estuary margins, we also have to consider high organic matter and nutrient inputs from the affluent rivers Tagus, Trancão and Sorraia, resulting from the farming activity in their respective hydrographic basins. The coastal zone near the estuary's mouth is an important recreational and leisure zone.

All those factors contribute for the need of efficient managing tools that allow the local authorities to make decisions based in the better knowledge that they may have available in each moment. To achieve this knowledge it is necessary to collect information about the different parameters that play an important role in the ecosystem, integrate this information in order to make it representative of the whole estuary and, finally, make it available in a comprehensive way to the decision makers.

If the existence of some kind of operational or pre-operational system has proved to be useful to manage the functioning of an engineering work, it can be shown also that such a system is equally useful in what concerns the management of the whole estuary ecosystem.

In the case of the Tagus estuary, those concepts are also used to understand and to forecast the system behaviour in what concerns the water quality and sediment transport problems. The MOHID 2000 is being used to characterise the reference situation and to evaluate the possible consequences of different scenarios (e.g. sea level rise, reduction of fresh water input, increase of nutrients).

This data is nowadays essential to support the decision making process in what concerns the needs of future actions or the licensing of a new industry for instance.

The simulation of the reference situation must be done for two reasons: (a) to complement our understanding of the system functioning and (b) because model results always have some errors that reduce the absolute meaning of the obtained results. This is especially important in long-term simulations where errors on boundary conditions can become important, as well as minor processes not considered in the model. The comparison of results of several scenarios with a reference situation allows not only to compare different solutions, but also to identify where and when strong modifications are expected.

Also the simulations should be carried on for periods large enough to allow the system to forget the initial conditions and to give meaning to the average values. In the case of the Tagus Estuary, the residence time is of the order of 3 weeks and the flow is mainly tidally forced. Three-month simulations were performed to eliminate errors in the initial conditions. After that, one-month simulations were performed and average values were calculated.

Two example cases are presented to illustrate the kind of results obtained: the evaluation of the importance of the seasonal river variability and the potential consequences of sea-level rise.

In what concerns the first case, it must be considered that the river input depends essentially on the policy of management of the river basin. An increase of the agriculture activity, without any modification of the agricultural techniques, increases, in general, soil erosion and, therefore, sediment input to the estuary. Climate changes are expected to increase storm strength and, consequently, erosion. On the contrary, a forestry increase is expected to reduce the sediment discharge.

In Figure 27a one can see strong modifications of the residual fluxes and sediment concentration, mainly in the upper part of the estuary due to a strong reduction of the river input. These results confirm the observations made by Vale and Sundby (1987) and Vale et al. (1993), about the importance of the river input in the dynamical process of sediment transport at the Tagus estuary. Those kinds of results may help the local authorities to better manage the system, at least in what concerns the parameters that depend on the human activity.

The other aspect presented is the effect of the sea level rise. This problem is being object of a great concern mainly along the last decade. Accordingly to most climate change models, a rise of mean sea level is expected in the future. Some predictions point to differences of one meter in certain locations. This value is probably too pessimistic, but it was chosen for our simulation. Being an extreme value it also gives a clear insight of its importance.

Results show that the effects in the estuary will be different according to the regions but, for instance, one of the consequences will be an increase of the erosion processes with direct impacts in the salt marshes areas (e.g. Figure 27b).

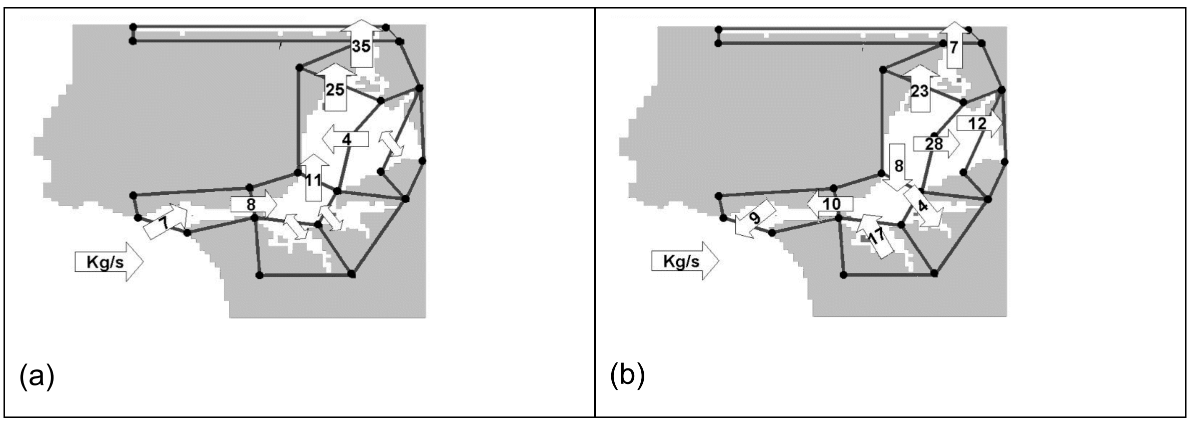


Figure 27: Residual sediment fluxes. Differences between the reference situation and a situation with no river input (a) and a scenario considering a sea level rise of 1 m (b)

Contribution to other research activities

It was already explain that the MOHID 2000 modelling tool is a net of classes that are controlled by two main classes, “Water Properties” and “Hydrodynamic Properties”. The “Water Properties” class is responsible for the evolution of a list of water properties. This class for each property sees the classes that can have some effect in the property evolution and interrogates them. For the property phytoplankton the class “Water Properties” would interrogate the classes: “Advection+Diffusion” (transport), “Water Quality” (water quality reactions), “Free Vertical movement” (settling velocity) and “Surface” (solar radiation) to quantify the effect of each process in the phytoplankton evolution (Figure 28).

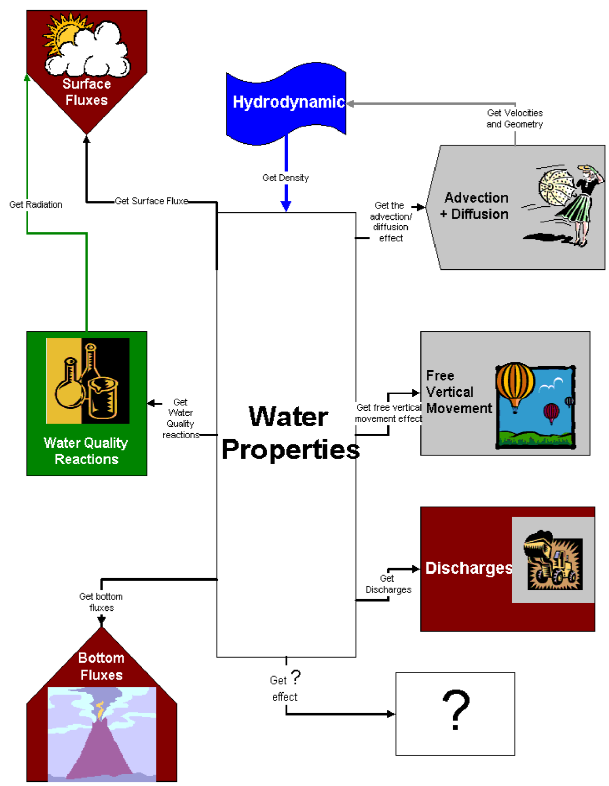


Figure 28 – Diagram showing the information flux between the class “water Properties” and other classes.

This methodology opens a very wide door to partnership. Small models simulating specific processes can be easily coupled and developers do not have to know how the other classes work . Following this philosophy, arsenic dynamics was introduced in the numerical tool with very few changes. To simulate the arsenic processes two new properties were introduced in the system, particulate and dissolved arsenic. Dissolved arsenic change in time due to advection-diffusion processes ("Advection/Diffusion" class) plus the sinks and sources reactions. Particulate arsenic change in time due to the same processes of the dissolved form plus settling velocity ("Free Vertical Movement" class) and bottom fluxes processes ("Bottom" class). These two processes were assumed equal to the ones implemented in cohesive-sediments dynamics. The sinks and source terms are compute backwards in time.

For the arsenic Sinks/Sources a simple formulation was used (7) to compute the fluxes between the particulate (A_{SP}) form of arsenic and the dissolved (A_{SD}) one.

$$\frac{\partial As_D}{\partial t} = k_{DP}\left((D\% \times As_P - P\% \times As_D\right)$$
$$\frac{\partial As_P}{\partial t} = k_{DP}\left((P\% \times As_D - D\% \times As_P\right) \qquad (7)$$

K_{DP} – transfer rate [s^{-1}];

D% and P% - partition coefficients of the dissolved and particulate forms of arsenic respectively [%].

Preliminary results of concentration values in the water column and in the bottom sediment are presented in Task 8.

Conclusions

The main conclusion of task 14 is that the processes at the estuary scale like the primary production cannot be dissociated from hydrodynamic in the Tagus estuary. The variability of a water quality property induced by the horizontal transport (tidal period) can be of the order of magnitude of the seasonal variability. The study of primary production in the Tagus estuary cannot also be dissociated from cohesive-sediments transport, because light penetration in the water column is mainly controlled by sediments concentration. Portela, 1996 proposed a correlation between the light extinction factor and sediments concentration. Water quality results also show that the spring bloom is mainly conditioned by zooplankton activity and not by nutrients depletion as observed in the deep ocean.

The main deliverables of task 14 are a calibrated interdisciplinary tool that is able to analyse relations between hydrodynamic, cohesive-sediments and water quality. The numerical system can easily incorporate new specific processes (e.g. arsenic dynamics) and can also be used to support management decisions (Table 1). The work done in this project was the support of 3 masters thesis. The main dissemination activities are 2 papers already finished to be present in the international conference Hydrosoft 2000. A paper to be published in an international journal with the water quality modelling results is also being prepared.

Table 1 – Final deliverables of Task 14 to the EU.

Deliverables	**Final user**	**Objective**
Calibrated Model	Scientific Community Decision makers	Study of hydrodynamic, of sediments and of water quality processes at the estuary scale Simulate management scenarios (e.g. no river input, sea level rise)
3 Master thesis	Scientific Community Decision makers	Calibration results presented in a systematic way Instruct specialise technicians able to work with modelling tools
2 papers presented in an international conference	Scientific Community	Results dissemination

Future work

Interest in tools able to give specific answers in the marine environment is growing. Environmental agencies need to now how a new bridge or salt marshes reclamation or outfall input can affect the marine environment. Numerical models associated to well designed data bases and to good monitoring networks are becoming the tool of the future to answer this complex questions. In our days the main challenge is not creation of knowledge but the access and integration of it. Numerical models are the best tools to integrate knowledge, while databases using WWW are the best tools to access it. Monitoring networks are needed to accumulate systematic information that can be used to generate knowledge in an efficient way. These networks are also needed to calibrate our integration tools (models). Similar systems are being implemented in fast transport boats that need to minimize time travels and avoid collisions with sand banks.

In the framework of OPCOM (EU project) a pre-operational modelling system is being implemented in Tagus estuary. The MOHID 2000 is being "coupled" with a data base that is able to store and access field data and models results via WWW. The MOHID 2000 system is also being used to study the impact of outfalls along the Portuguese coast. The study of Matozinhos and Lisbon outfalls are underway, the Aveiro and Funchal outfalls impact study will be done in the future.

Due to the development philosophy of the MOHID 2000 it will be easy in the future to study more and more complex processes. In the next year the system will be able to do the first simulations of fish dynamics in the Tagus estuary. At the moment a master student is implementing fish growth and in the future movement will also be simulated. A project has been submitted to Portuguese authorities with the main goal of simulating fish dynamics in the Tagus estuary.

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