8. NUMERICAL MODELS AS DECISION SUPPORT TOOLS IN COASTAL AREAS

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8.1. Decision Support Tools

Whenever policy decisions are to be made affecting the natural resource Water—arguably the most precious natural resource—an implacable scrutiny is to be expected. Legal demands are huge as the large number of EU directives targeting water testifies, from which stand out the Nitrates Directive, the Urban Wastewater Directive, the Drinking Water Directive, the Bathing Water Directive and the Water Framework Directive. Media and public opinion at large are continuously exerting a strong pressure over these policies. Decisions need to be thoroughly supported and documented and this is where computers come into play. Modelling tools, in the form of Decision Support Tools, are extensively used both to detect and select the "best" solution and to prove that the best solution was chosen.

Nowadays modelling tools are used as Decision Support Tools. In fact models' results are acceptable justification to major decisions, e.g. the location and configuration of ports, sewage systems and ecological reserves.

Increasingly, computer models are the corner stone in ecological impact studies, being the single most important factor to support policy decisions.

For a model to qualify as a Decision Support Tool it must be able to produce results that describe a reference situation—usually representing conditions for a generic year—and hypothetical scenarios. Most often it is the comparison among a set of results that enables decision makers to make good decisions.

What is a decision support tool?

- It is a model or set of models;
- It produces quantified results;
- The results must be available in time for decisions to be made;
- There is a trend to be run by non-specialists in numerical methods. The operator should be able to pre-process and post-process using a GUI (Graphical User Interface). Usually it is operated by someone that, in one hand, has a deep knowledge of the processes being modelled but, on the other hand, does not know how to build a model;

I. E. Gonenc et al. (eds.), Assessment of the Fate and Effects of Toxic Agents on Water Resources, 171–195.

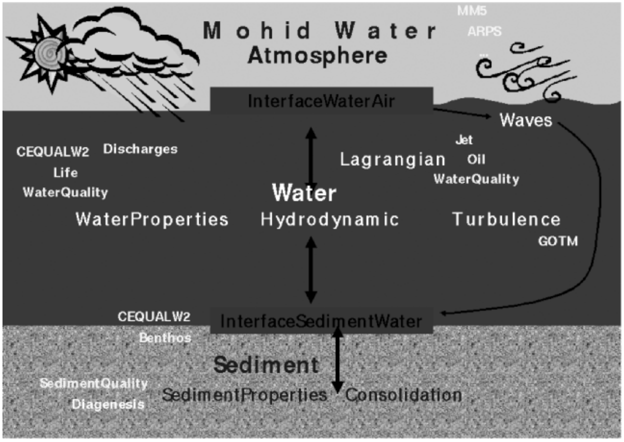

Figure 1. MOHID graphical representation

- A Decision Support Tool integrates several domains covering hydrodynamics, transport and diffusion phenomena and some chemical and biochemical cycles;
- The results are not the decisions in themselves. A decision maker is mandatory.

MOHID Water grew from a 2D hydrodynamic modelling tool in the nineteen eighties to the Decision Support Tool it is today. Figure 1 shows a graphical representation of MOHID's structure. The hydrodynamic module (component model) is the foundation of the entire modelling system. Hydrodynamic fields are used by other components as inputs, e.g., pollutants drift and dilute due to water currents, density, temperature, etc.

Lets suppose that a deep water sewage system is to be built. Inevitably a Decision Support Tool will be used, first of all to provide an accurate characterization of the ecosystem prior to the intended intervention—reference situation. Afterwards several locations and configurations might be simulated, covering as wide a range of natural conditions and ecological stress as possible—scenarios. Some sensitivity analysis should be expected. The comparison between each scenario and the reference situation illustrates the respective technical solution's impact on the ecosystem.

This set of ecological impacts must be evaluated against quantified and objective criteria.

8.2. Brief History of Modelling Tools

Hydrodynamic modelling was initiated in the early 1960s, with the birth of computation, a decade where the first temporal discretization methods for flows with hydrostatic pressure were published (Leendertse, 1967; Heaps, 1969) and developed for two-dimensional vertically integrated models. In the 1970s, the number of applications was multiplied and extensive research on numerical methods was carried out, namely on forms to minimize numerical diffusion introduced from solving advection terms (e.g. Spalding, 1972; Leonard, 1979). Three-dimensional models necessary to simulate oceanic circulation had a high development in the 1980s, benefiting from the increase in computing capacity and in the breakthroughs in turbulence modelling based on work since the 1970s which had in Rodi (1972) one of its main pioneers. In the 1990s, hydrodynamic models were consolidated and several models with great visibility started to emerge, e.g. POM (Blumberg and Mellor, 1987), MOM (Pacanowskid et al., 1991) but also from European schools, e.g. GHER model (Nihould et al., 1989). Benefiting from technological advances, including both hardware and software (e.g. compilers, data management, graphical computation), from the second half of the 1990s, the dawn of integrated models, coupling modules developed by several authors, was witnessed. Turbulence modelling packages like GOTM (Burchard et al., 1999) constitute one of the first examples of this integration, but coupling GOTM to other models constitutes a second level integration example.

Together with the development of hydrodynamic models, ecological models were also developed. Among the pioneer models one can mention WASP developed at EPA (Di Toro et al., 1983) and BOEDE model developed at NIOZ (Ruardij and Baretta, 1982). These models were developed in boxes and in former times used a time step of one day, being the short term variability of flow (e.g. tidal) accounted using diffusion coefficients. Ecological models have improved a lot during the 1980s and 1990s, benefiting from the scientific and technological progress and have been coupled to physical (hydrodynamic) models thus generating the present integrated models.

Current research on modelling is oriented towards operational modelling, integrating different disciplines and assimilating as much field data as possible, with especial emphasis for remote sensing.

Modelling at UTL followed the world trends and benefited from high investments on computing systems in the 1980s. The development of MOHID system (http://www.MOHID.com) was initiated at that time (Neves, 19855) as a 2D hydrodynamic model and was subsequently developed for becoming an integrated modelling system for tidal flow in estuaries and progressively generalized to waves (Silva, 1991), water quality (Portela, 1996), three-dimensional flows (Santos, 1995), new numerical methods (Martins, 2000), extended set of different open boundary conditions (Leitão, 2003) and finally to be reorganized in an integrated perspective in order to accommodate alternative modules for different processes (Braunschweig et al., 2004). The model evolution enabled to couple alternative modules to compute biogeochemical and water quality processes (Trancoso et al., 2005; Saraiva et al., 2006; Mateus, 2006), the broadening to flow through porous media (Galvão et al., 2004), model water flow in a river basin (Braunschweig and Nevas, 2006), and ocean circulation (Leitão et al., 2006).

This model is a working tool of the environmental modelling group of MARETEC research centre, having been used in more than 30 research projects, 50% of which with European funds and currently has around 500 registered users in its online website.

8.3. MOHID

With the growing model complexity, it was necessary to reorganize the MOHID model. In 1998 the whole code was submitted to a complete rearrangement, using new FORTRAN features and also the capacities of modern computers. The main goal of this rearrangement was to make the MOHID more robust, reliable, protect it against involuntary programming errors and make it scalable. An object oriented philosophy based on Decyk's framework was put to in place (Decyk et al., 1997). The whole model is programmed in ANSI FORTRAN 95.

The philosophy of this new version of MOHID (Miranda et al., 2000) allows it to be applied to one-, two- or three-dimensional problems. MOHID makes intensive use of FORTRAN modules, corresponding as far as possible to logical entities, being it:

- physical domains, e.g. water column, benthos, air;
- interfaces, e.g. air/water, water/sediments, domain/sub-domain;
- phenomena, e.g. turbulence;
- numerical methods, e.g. Lagrangian and Eulerian approaches;
- models that make an intensive use of hydrodynamic results, e.g. pollutants dispersion, oil spills, biogeochemical cycles.

Presently MOHID is composed of more than 40 modules which complete over 150 thousand code lines. Each module is responsible to manage a certain kind of information. The main modules are the modules listed in Table 1.

Another important feature of MOHID is the possibility to run nested models. This feature enables the user to study local areas, obtaining the boundary conditions from the parent model. Computer power is the unique limitation to the number of nested models.

TABLE 1. MOHID's main modules

Module name	Module description
Model	Manages the information flux between the hydrodynamic module and the two transport modules and the communication between nested models.
Hydrodynamic	Full 3D dimensional baroclinic hydrodynamic free surface model. Computes the water level, velocities and water fluxes.
Water Properties (Eulerian Transport)	Eulerian transport model. Manages the evolution of the water properties (temperature, salinity, oxygen, etc) using an Eulerian approach.
Lagrangian	Lagrangian transport model. Manages the evolution of the same properties as the water properties module using a Lagrangian approach. Can also be used to simulate oil dispersion.
Water Quality	Zero-dimensional water quality model. Simulates the oxygen, nitrogen and phosphorus cycle. Used by the Eulerian and the Lagrangian transport modules. Based on a model initially developed by EPA (Bowie et al.,1985).
Oil Dispersion	Oil dispersion module. Simulates the oil spreading due thickness gradients and internal oil processes like evaporation, emulsification, dispersion, dissolution and sedimentation.
Turbulence	One-dimensional turbulence model. Uses the formulation from the GOTM model.
Geometry	Stores and updates the information about the finite volumes.
Surface	Boundary conditions at the top of the water column.
Bottom	Boundary conditions at the bottom of the water column.
Open Boundary	Boundary conditions at the frontier with the open sea.
Discharges	River or Anthropogenic Water Discharges
Hydrodynamic File	Auxiliary module to store the hydrodynamic solution in an external file for posterior usage.

8.4. MOHID: A Modular System

8.4.1. MODEL MODULE

8.4.1.1. *Introduction*

Module Model is MOHID's topmost module and has two main responsibilities:

- Hydrodynamic and the transport modules execution coordination and; Figure 2 illustrates these relations.
- Parent-son communication management (nested models).

8.4.1.2. *Single Model*

A single model execution coordination consists of the global model time actualization and hydrodynamic and transport modules update. Transport

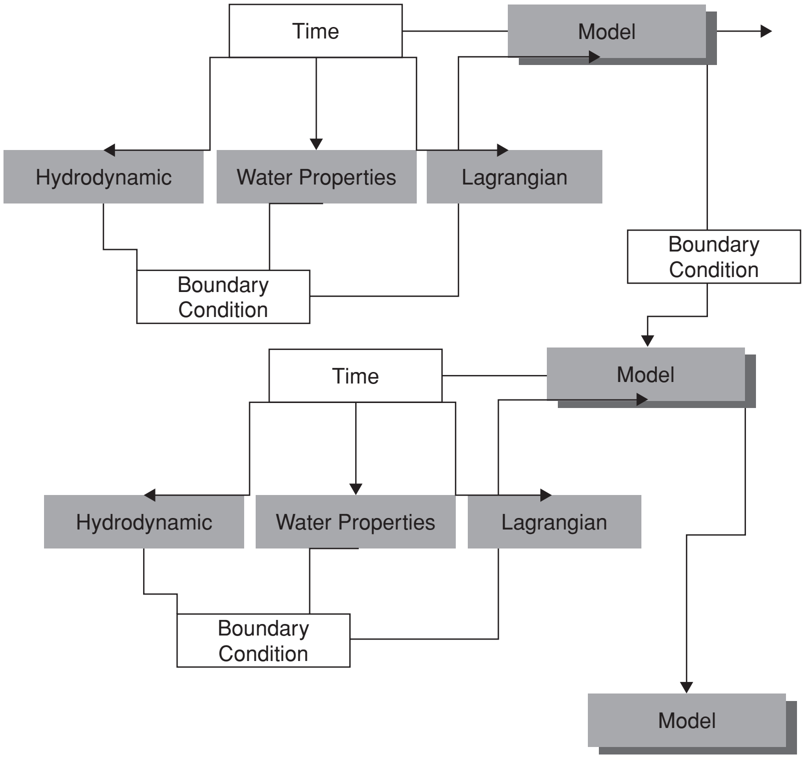

Figure 2. Information flux among nested models

modules' time steps may differ from hydrodynamic module's time step (it is mandatory that transport modules' time steps are multiples of hydrodynamic's time step).

8.4.1.3. *Nested Models*

Information flux coordination among nested models includes their synchronization because nested models may run with different time steps. Nested models coordination is done in a hierarchical way. Every model can have one or more nested child models which, recursively, can have one or more child models. Information flow is one way, consisting on boundary conditions being passed from parent to son(s).

8.4.2. BATHYMETRY MODULE

The Bathymetry module is one of the bottom modules of the MOHID water modelling system. It reads bathymetry data from the input file and publishes this data to all client modules. Bathymetric data can be stored in any regular

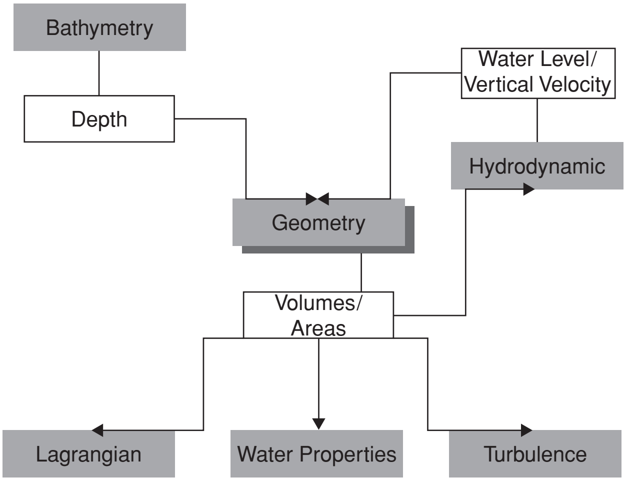

Figure 3. Information flux among the Geometry Module and other modules

grid, with independent variable spacing along the X and Y directions. For every grid point the depth of this point must be given. The horizontal coordinates can be supplied in variety of coordinates systems; the most commonly used are metric and geographic coordinates.

8.4.3. GEOMETRY MODULE

The Geometry Module computes finite volume's lateral areas and volumes, based upon surface elevation and bathymetric data. This information is updated as needed, and made available to other modules. Figure 4 represents the information flux among geometry module and other modules.

8.4.3.1. *Finite Volume*

MOHID uses a finite volume approach (Chippada et al., 1998; Martins et al., 1999, 2000) to discretize equations. In this approach the discrete form of the governing equations is applied macroscopically to a cell control volume. A general conservation law for a scalar U, with sources Q in a control volume Ω is then written as

$$\partial_t \int_{\Omega} U \, \mathrm{d}\Omega + \oint_{S} \vec{F} \, \mathrm{d}\, \vec{S} = \int_{\Omega} Q \, \mathrm{d}\Omega,$$

where F are the fluxes of the scalar through the surface S embedding the volume. After discretizing this expression in a cell control volume Ω_j where

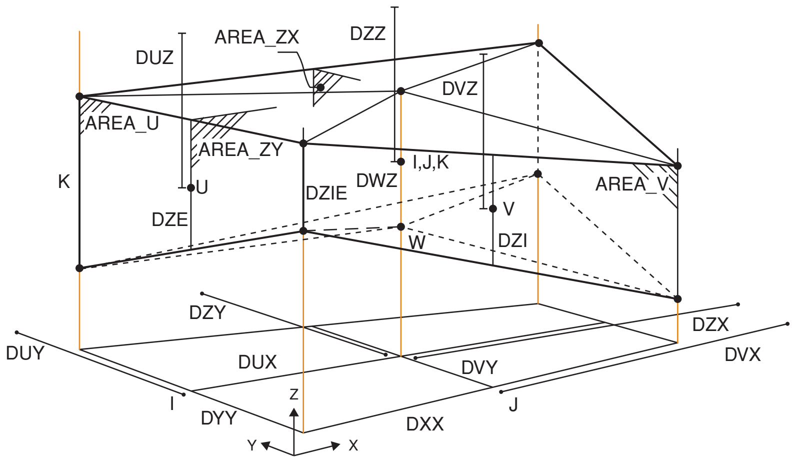

Figure 4. Finite volume element of MOHID model

U_j is defined:

$$\partial_t(U_j \Omega_j) + \sum_{\text{faces}} \vec{F} \cdot \vec{S} = Q_j \Omega_j.$$

This way the procedure for solving the equations is independent of cell geometry. Cells can have any shape with only some constraints—the computational mesh must be regular—because only fluxes among cell faces are required (see Montero (1999) or Martins (2000)). Therefore, a complete separation between physical variables and geometry is achieved (Hirsch, 1988). As volumes can vary during a run, geometry is updated in every time step after computing flow properties. Moreover, spatial coordinates are independent, meaning that different geometry types can be chosen for each dimension, e.g., Cartesian or curvilinear coordinates can be used in the horizontal dimensions and a generic vertical coordinate with several sub-domains can be used in the vertical. This general vertical coordinate allows minimizing errors if compared with some classical vertical coordinates (Cartesian, sigma, isopycnal) as pointed in (Martins et al., 2000).

8.4.3.2. *Vertical Coordinates*

The Geometry module can divide the water column in different vertical coordinates: Sigma, Cartesian, Lagrangian (based on Sigma or based on Cartesian), “Fixed Spacing” and Harmonic. A water column subdivision into different domains is also possible. Sigma and Cartesian sub-domains are often used. The Cartesian coordinate can be used with or without “shaved cells”. Lagrangian coordinates move both top and bottom faces with the vertical flow velocity.

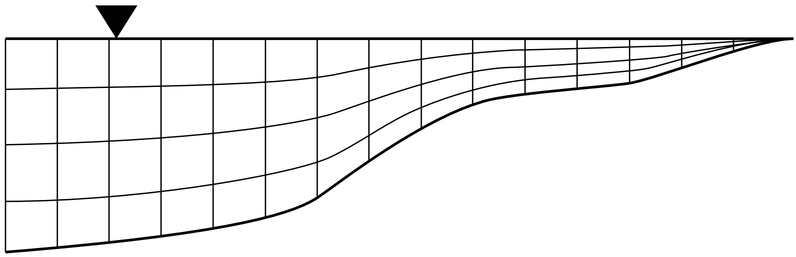

Figure 5. Sigma domain with 4 Layers

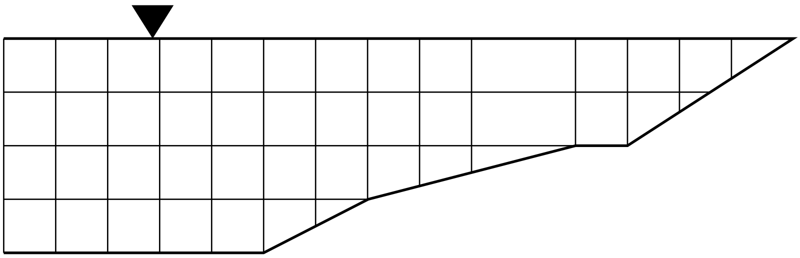

Figure 6. Cartesian domain with 4 Layers (shaved cells)

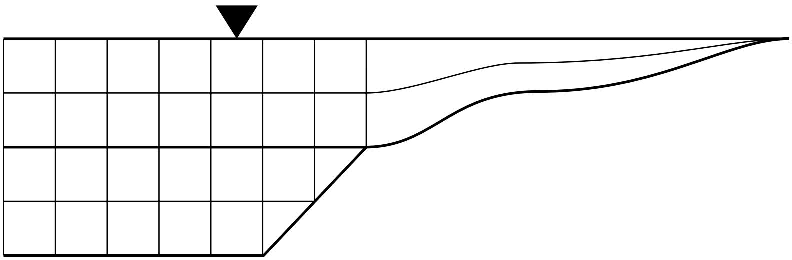

Figure 7. Water column sub-division in a Cartesian domain (inferior) and a Sigma domain (superior)

"Fixed Spacing" coordinates allow the user to study flows close to the domain bottom and Harmonic coordinates work like Cartesian coordinates, just that the horizontal faces close to the surface expand and collapse depending on the variation of the surface elevation. This Harmonic coordinates system was implemented to simulate reservoirs.

8.4.4. HYDRODYNAMIC MODULE

In this section MOHID's hydrodynamic module is described. The information flux of the hydrodynamic module, relative to the other modules of MOHID, is shown in Figure 10.

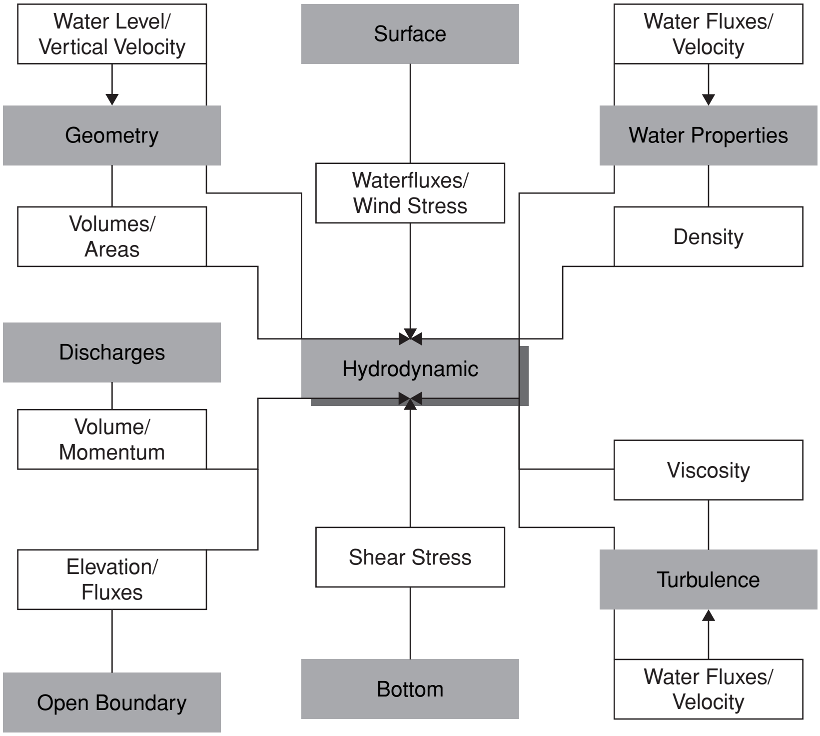

Figure 8. Information flux among the Hydrodynamic Module and other modules

The model solves the three-dimensional incompressible flow primitive equations. Hydrostatic equilibrium is assumed as well as Boussinesq and Reynolds approximations. The density is obtained from salinity and temperature fields, which are transported by the water properties module.

8.4.4.1. *Open Boundary Conditions*

Open boundaries arise from the necessity of confining the domain to the study area. Variables values must be introduced in such a way that information about what is happening outside the domain is guaranteed to enter the domain, so that the solution inside the domain is not corrupted. Waves generated inside the domain should be allowed to go out. There exists no perfect open boundary condition and the most suitable would depend on the domain and the phenomena being modelled. A recent review paper comparing open boundary conditions in test cases can be found in Palma and Matano (1999) and in Blayo (2005). Some different open boundaries are already introduced in MOHID 3D (Santos, 1995; Montero, 1999) and some others like FRS (Flow Relaxation Scheme), radiation processes (Flather, 1987; Orlansky, 1991) and the viscosity sponge layer.

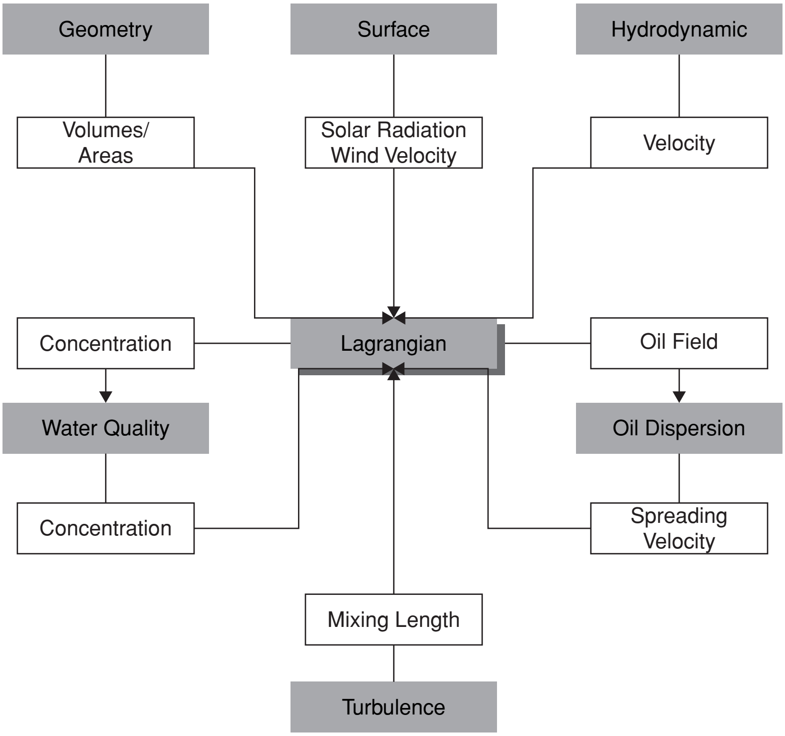

Figure 9. Information flux among the Lagrangian module and other modules

8.4.4.2. *Moving Boundaries*

Moving boundaries are closed boundaries that change position in time. If there are intertidal areas in the domain some points are periodically covered and uncovered, depending on tidal elevation. A stable algorithm is required for modelling these zones and their effect on hydrodynamics of estuaries. A detailed exposition of the algorithms used in MOHID can be found in Martins et al. (1999) and Martins (1999).

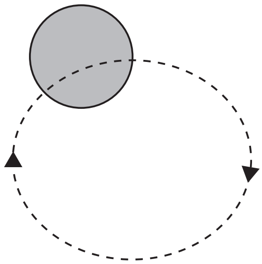

Figure 10. Random movement forced by an eddy larger than the particle

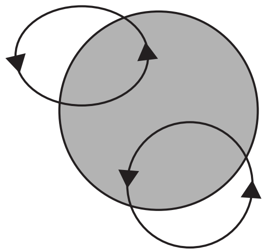

Figure 11. Random movement forced by an eddy smaller than the particle

8.4.5. LAGRANGIAN MODULE

Lagrangian transport models are very useful to simulate localized processes with sharp gradients (submarine outfalls, sediment erosion due to dredging works, hydrodynamic calibration, oil dispersion, etc).

MOHID's Lagrangian module uses the concept of tracer. The most important property of a tracer is its position (x, y, z). For a physicist a tracer can be a water mass, for a geologist it can be a sediment particle or a group of sediment particles and for a chemist it can be a molecule or a group of molecules. A biologist can spot phytoplankton cells in a tracer (at the bottom of the food chain) as well as a shark (at the top of the food chain), which means that a model of this kind can simulate a wide spectrum of processes.

Tracers movement can be influenced by the velocity field from the hydrodynamic module, by the wind from the surface module, by the spreading velocity from oil dispersion module and by random velocity.

At the present stage the model is able to simulate oil dispersion, water quality evolution and sediment transport. To simulate oil dispersion the Lagrangian module interacts with the oil dispersion module. To simulate water quality evolution in time the Lagrangian module is a client of the water quality module. Sediment transport can be associated directly to the tracers using the concept of settling velocity.

Figure 12 represents the information flux among the Lagrangian module and other modules of MOHID.

Another feature of the Lagrangian transport model is its ability to calculate residence times. This can be very useful when studying the exchange of water masses in bays or estuaries.

8.4.5.1. *Tracer Concept*

Like referred above, the MOHID's Lagrangian module uses the concept of tracer. Tracers are characterized by three spatial coordinates, volume and a list of properties (each with a given concentration). Properties can be the same ones described in the water properties module or coliform bacteria. Each tracer has associated a time to perform the random movement.

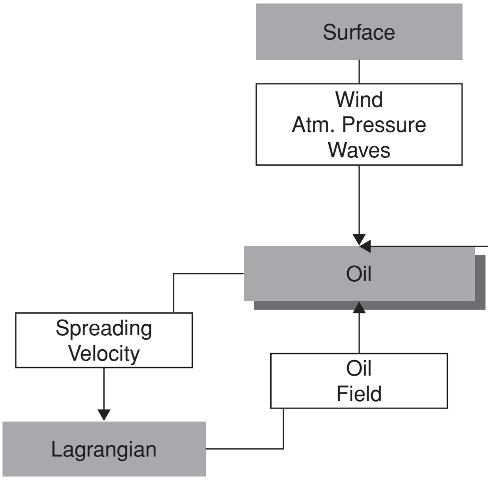

Figure 12. Information flux between the oil module and other modules

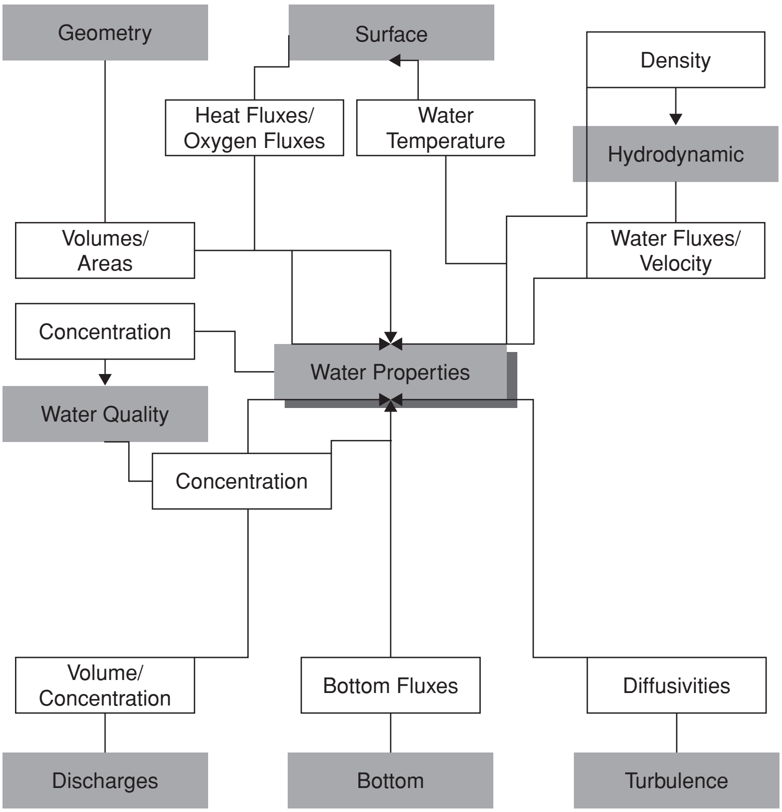

Figure 13. Information flux among the Water Properties Module and other modules

The tracers are “born” at origins. Tracers which belong to the same origin have the same list of properties and use the same parameters for random walk, coliform decay, etc. Origins can differ in the way they emit tracers. There are three different ways to define origins in space:

- a “Point Origins” emits tracers at a given point;
- a “Box Origins” emits tracers over a given area.

There are two different ways in which origins can emit tracers in time:

- a “Accident Origins” emit tracers in a circular area around a point;
- a “Continuous Origins” emits tracers during a period of time;
- a “Instantaneous Origins” emits tracers at one instant.

Origins can be grouped together in Groups. Origins which belong to the same group are grouped together in the output file, so it is easier to analyse results.

8.4.5.2. *Tracer Movement*
Usually the mean velocity is the major factor influencing particles movement. Spatial coordinates are given by the definition of velocity:

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = u_i(x_i, t)$$

where u stands for mean velocity and x for particle position.

The Lagrangian module allows several tracers trajectory computations for each hydrodynamic time step.

8.4.5.3. *Turbulent Diffusion*
Turbulent transport is responsible for dispersion. The effect of eddies over particles depends on the ratio between eddies and particle size. Eddies bigger than the particles make them move at random as explained in Figure 14. Eddies smaller than the particles cause entrainment of matter into the particle, increasing its volume and its mass according to the environment concentration, as shown in Figure 16.

Mass decay rate. The decay rate of coliform bacteria, which are can associated to tracers, is computed by the following equation:

$$\frac{\mathrm{d}C}{\mathrm{d}t} = -\frac{\ln 10}{T_{90}}C$$

where C represents the concentration, and T_{90} the time interval for 90% of the coliform bacteria to die.

A backward in time method is used to solve the above equation numerically, preventing a negative number of coliform bacteria.

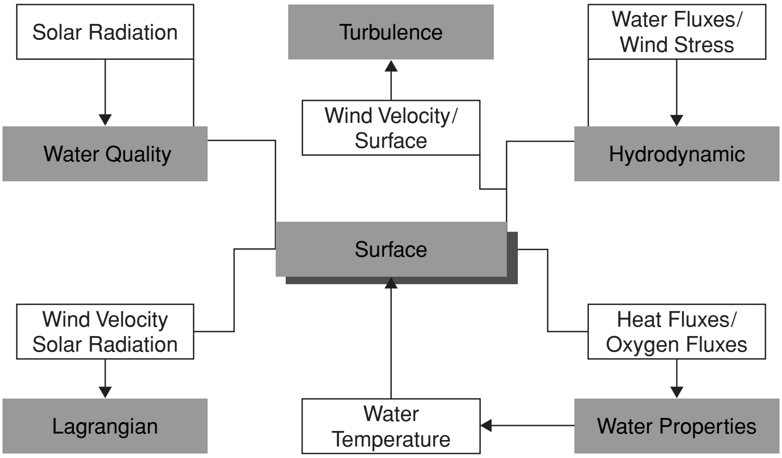

Figure 14. Information flux among the Surface Module and other modules

8.4.5.4. *Monitoring Boxes*

The Lagrangian module permits to monitor particles distribution inside "monitoring boxes". This feature is very useful to compute the residence time of water inside these monitoring boxes and the origins of the water present inside each box at each moment. The Lagrangian module "monitors" the boxes the following way:

- In every instant the volume of each box b, InstBoxVol(b) is calculated:

$$\mathrm{InstBoxVol(b)} = \int (h + Z)\,\mathrm{d}x\,\mathrm{d}y.$$

- In every instant the water origin "o" inside each monitoring box "b" is identified and the water volume from each origin is stored in the variable InstVolumeByOrigin(b, o):

$$\mathrm{InstVolumeByOrigin}(b, \mathrm{o}) = \sum_{o} \mathrm{Vol}_j^b.$$

- *In the case of instantaneous emissions in boxes*, these contributions are integrated over time, given the integrated contribution over time, IntgVolumeByOrigin(b, o)

$$\mathrm{IntgVolumeByOrigin}(b, o) = \int \mathrm{InstVolumeByOrigin}(b, o)\,\mathrm{d}t.$$

A residence time measure for tracers emitted in box "o" in monitoring box "b" is given by

$$\mathrm{ResidenceTimePerBox}(b, o) = \mathrm{IntgVolumeByOrigin}(b, o)/\mathrm{IntialVol(o)}.$$

Adding the values for all monitoring boxes inside the estuary one gets the residence time inside the whole system of the water emitted into box "o":

$$\text{ResidenceTime}(o) = \sum_b \text{ResidenceTimePerBox}(b, o).$$

These values also permit to compute how each monitoring box is influenced by each emitting box:

$$\text{InfluenceOverBox}(b, o) = \text{IntgVolumeByOrigin}(b, o)/\text{InitialVol}(b).$$

In case of a continuous emission, the residence time can be computed as:

$$\text{ResidenceTimePerBox}(b, o) = \text{InstVolumeByOrigin}(b, o)/\text{DischargeRate}(o).$$

8.4.6. OIL MODULE

The prediction and simulation of oil spills trajectory and weathering are essential to the development of pollution response and contingency plans, as well as to the evaluation of environmental impact assessments.

In order to predict the behaviour of oil spilled in coastal zones, an oil weathering model was developed, which predicts the evolution and behaviour of processes (transport, spreading and behaviour) and properties. Some pollution response methods are also integrated in the model.

8.4.6.1. *Implementation*

Oil density and viscosity, and many different processes are included in oil module, such as oil spreading, evaporation, dispersion, sedimentation, dissolution, emulsification, oil beaching and removal techniques.

Different alternative methods were coded for the prediction of some processes like oil spreading, evaporation, dispersion, sedimentation and emulsification. Therefore, when using the model, there is more than one way of simulating the same process, depending, for example, on the characteristics of the computational mesh or on the magnitude of the spill.

The oil weathering module (OWM) uses mainly the 3D hydrodynamics and 3D Lagrangian transport modules. The hydrodynamic module simulates the velocity field necessary for the Lagrangian module to calculate oil trajectories. These oil trajectories are computed assuming that oil can be idealized as a large number of particles that independently move in water. Water properties and atmospheric conditions are introduced in the Lagrangian module and used by the oil module for determination of oil processes and properties. Excepting spreading and oil-beaching, all weathering processes and properties are assumed uniform for all tracers, like water properties and atmospheric conditions, which are considered equal to these environmental conditions determined in accident origin.

As it was already mentioned, the movement of oil tracers can be influenced by the velocity field from the hydrodynamic module, by the wind from the surface module, by the spreading velocity from the oil module and by random velocity.

Oil temperature is assumed equal to water temperature, neglecting solar radiation or any other energy transfer process that may influence oil temperature.

8.4.6.2. *Oil-Beaching*

When oil reaches a coastal zone, it might become beached. This model estimates the amount of beached oil when the model user predefines a beaching probability (or different beaching probabilities for different coastal zones).

8.4.6.3. *Removal Techniques*

Some removal techniques like chemical dispersion or mechanical cleanup are also included in model.

8.4.7. WATER PROPERTIES MODULE

The water properties module coordinates the evolution of the water properties in the water column, using an Eulerian approach. This coordination includes the transport due to advective and diffusive fluxes, water discharges from rivers or anthropogenic sources, exchange with the bottom (sediment fluxes) and the surface (heat fluxes and oxygen fluxes), sedimentation of particulated matter and internal sinks and sources (water quality).

In its present state MOHID can simulate 24 different water properties: temperature, salinity, phytoplankton, zooplankton, particulate organic phosphorus, refractory dissolved organic phosphorus, non-refractory dissolved organic phosphorus, inorganic phosphorus, particulate organic nitrogen, refractory organic nitrogen, non-refractory organic nitrogen, ammonia, nitrate, nitrite, biological oxygen demand, oxygen, cohesive sediments, ciliate bacteria, particulate arsenic, dissolved arsenic, larvae and fecal coliforms. Any new property can be easily added, due to the object-orientated programming used within the MOHID model.

In the water quality module, nitrogen, oxygen and phosphorus cycle can simulate the terms of sink and sources. Figure 19 represents the information flux of the water properties module.

8.4.8. WATER QUALITY MODULE

Efforts towards ecological modelling are being made in most countries where water quality management is a major concern. Fransz et al. (1991) notices that most new generation models tend to become much more biologically and chemically diversified than earlier models, as it is now largely recognized that there is no way to simulate in sufficient detail the ecosystem behaviour without an in-depth treatment of the full cycle of organic matter.

These processes are not strange to the preoccupations caused by the eutrophication and its various manifestations. Although there is general consensus that the inputs of nutrients to the sea must be reduced there is so far no firm scientific basis to decide upon the extent of such reductions.

An appropriate way of addressing the problem of eutrophication and of testing nutrient reduction scenarios is to simulate the phenomenon with numerical models. It is probably correct to assume that any ecological model with a sufficiently complex internal structure and the multiple relationships that are found at the lower trophic levels will come close to an answer, provided the right time scale is applied.

The ecological model included in MOHID is adapted from EPA (1985) and pertain to the category of ecosystem simulations models, i.e., sets of conservation equations describing as adequately as possible the working and the interrelationships of real ecosystem components. It is not correct to say that the model describes the lower trophic levels with great accuracy. In fact the microbial loop that plays a determinant role in water systems in the recycling processes of organic waste is very simplified in MOHID.

Lower trophic levels appear in nearly all marine ecosystem simulation models since there is at least a compartment "phytoplankton" required to compute the organic matter cycle. Some early models applied in the North Sea were one-compartment models, especially endeavouring to simulate phytoplankton growth, in relation with the physical environment and with grazing pressure (treated as a forcing variable). Both the influence of the Lotka-Volterra equations—developed in the 1920s—and that of findings in the field of plant physiology (photosynthesis-light relationship) were discernible. It was not long before limiting nutrient and herbivorous zooplankton were incorporated as well, as state variables in simulation models (Fransz et al., 1991)

8.4.9. SURFACE MODULE

The surface module stores boundary conditions at the water column surface. These boundary conditions can be divided in two types. One type of boundary conditions which are given directly by the user, usually meteorological data (wind velocity, air temperature, dew point, evaporation, cloud cover) and boundary conditions calculated by the model from the meteorological data/conditions of the water column (wind stress, solar radiation, latent heat, infra-red radiation, sensible heat, oxygen flux). The information flux between the surface module and other modules is shown in Figure 21.

8.4.9.1. *Wind*
Wind stress is calculated according to a quadratic friction law:

$$\vec{\tau w} = C_D \rho_a \vec{W} \left| \vec{W} \right|$$

where C_D is a drag coefficient that is function of the wind speed, ρ_a is air density and W is the wind speed at a height of 10 m over the sea surface.

The drag coefficient is computed according to Large and Pond (1981):

$$(W < 10\,\mathrm{m/s})$$

$$C_D = 4.4\,\mathrm{e}^{-4} + 6.5\,\mathrm{e}^{-5} \vec{W} \left| \vec{W} \right| (10\,\mathrm{m/s} < W < 26\,\mathrm{m/s}).$$

8.4.9.2. *Heat Fluxes*
Heat fluxes at the surface can be separated into five distinctive fluxes: solar short-wave radiation, atmospheric long-wave radiation, water long-wave radiation, sensible heat flux and latent heat flux. These fluxes can be grouped into two ways: in (i) radiative fluxes (first three fluxes) and (ii) non-radiative fluxes (last two fluxes) or in (iii) fluxes independent of the water temperature (first two fluxes) and in (iv) fluxes dependent of the water temperature (last three fluxes).

8.4.9.3. *Solar Radiation*
Solar radiation is an important ecological parameter, and is often the key driving force in ecological processes (Brock, 1981). The solar radiation flux of short wavelength is computed by:

$$Q = Q_0 At(1 - 0.65C_n^2)(1 - R_s)$$

where Q_0 is the solar radiation flux on top atmosphere (W m^2), A_t the coefficient for atmospheric transmission, C_n the cloud cover percentage and R_s stands for albedo (0.055). The solar radiation flux on top atmosphere can be expressed as

$$Q_0 = \frac{I_0}{r^2} \mathrm{senz}$$

where I_0 stands for the solar constant which is the energy received per unit time, at Earth's mean distance from the Sun, outside the atmosphere, a standard value is 1353 W m^{-2} (Brock, 1981), r stands for the radius vector and z stands for the solar high.

8.4.10. BOTTOM MODULE

The bottom module computes boundary conditions at the bottom of the water column. It computes shear stress as a boundary condition to the hydrodynamic and turbulence modules. It is also responsible for computing fluxes at the water-sediment interface, managing boundary conditions to both the water column properties and the sediment column properties.

Both in the water column or in the sediment column, properties can be either dissolved or particulate. The evolution of dissolved properties depends greatly on the water fluxes, both in the water column and in the sediment interstitial water. Particulate properties evolution in the water column depends also on the water fluxes and on settling velocity. Once deposited in the bottom they can either stay there or be resuspended back to the water column. If they stay there for a determined period of time, they can become part of the sediment compartment by consolidation.

8.4.11. FREE VERTICAL MOVEMENT MODULE

The free vertical movement module computes particulate properties vertical fluxes. It is normally used to compute settling velocity for cohesive sediment or particulate organic matter transport.

8.4.12. HYDRODYNAMIC FILE MODULE

In this section the hydrodynamic file module of the model MOHID is described. This module can be seen as an auxiliary module, which permits the MOHID user to integrate the hydrodynamic solution in space and time and store this solution in a file. This file can be later used to simulate longer periods, like water quality simulation which needs simulation times for at least one year.

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