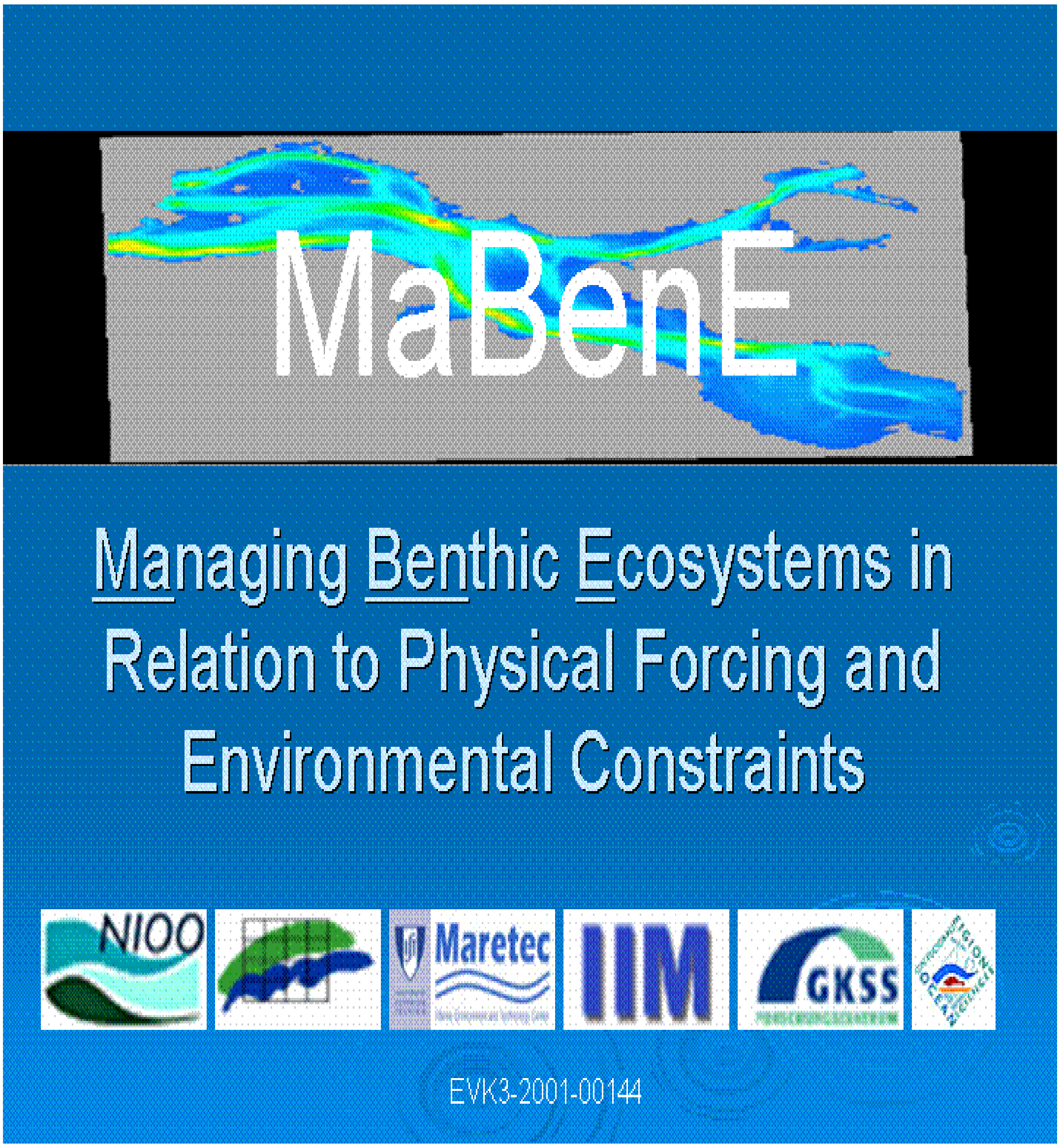
MARETEC / IST Progress report on MaBenE



Lisbon, November 2003

Introduction

This report aims to describe the work done so far by the Instituto Superior Técnico (IST) team in the framework of MaBenE project. The following text will include a description of IST tasks, current milestones and deliverables. It will also perform an overview on the field data gathered and its availability as well as on the preliminary results obtained for the Oosterschelde and Ria de Vigo with the current model version and the methodologies used in both applications.

A description of the model is made including the used methodology to couple hydrodynamics and transport with biogeochemical models.

Tasks, milestones and deliverables

IST contributes its hydrodynamical model MOHID to the system-wide application for Ria de Vigo, and also (in a comparison exercise with BBH's model GETM) for the Oosterschelde. IST must also co-ordinate the application of the 3D models in Ria de Vigo and Oosterschelde and is co-operating with BBH in the specification of the technical standards for module set-up and exchange. It will lead the development of the suspended matter module and the benthic biogeochemical module, and will co-operate with other partners to the detailed 1D applications of the coupled modelling tool.

Tasks

Exception made to MaBenE's Work Package 1 (WP1), these is a summary of the IST tasks:

Work package	Description
WP 4.1	Cooperation in the specification of the technical standards for interfacing modules for the integrating modelling environment of MaBenE
WP 4.2	3D hydrodynamic modelling applications for Ria de Vigo and the Oosterschelde
WP 4.5	Development of a suspended matter module
WP 4.6	Development of a benthic biogeochemical module
WP 4.8	Development and testing of 1D coupled model application

Milestones

In the Lisbon meeting, November 2003, the following milestones are achieved:

Milestone	Month	Description
M4.1	6	technical interfacing standards
M1.2	12	
M4.2	12	coding of integrating modelling environment

Deliverables

First deliverables by IST, are to be made only in Month 24; that is in November 2004.

Modelling applications I: Oosterschelde

Field data

Summary

Table 1 contains a summary of field data availability for the Oosterschelde, including a small description on its origin and status.

Field data	Available	Description
Bathymetry	Yes	20x20m resolution bathymetric data
Water elevation	Yes	Very complete
Currents	No	-
Wind	Yes	Very complete
Waves	Yes	Known availability
Water properties	Yes	Known availability
Discharges	No	-

Table 1 – Summary of field data availability for the Oosterschelde

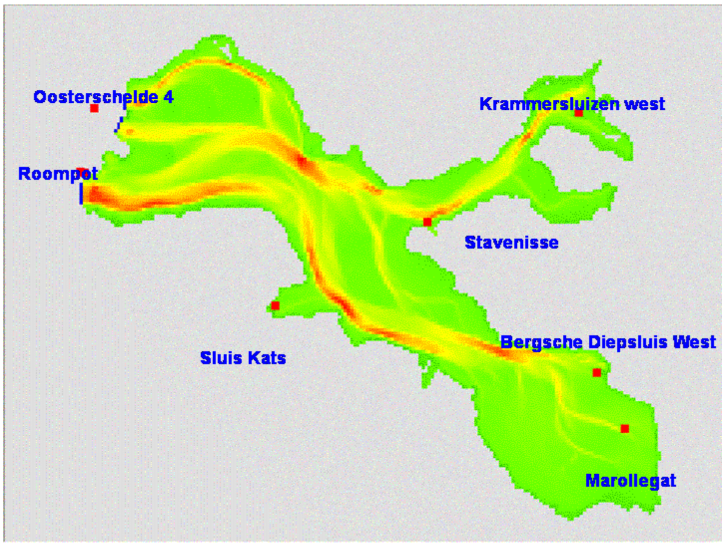


Figure 1- Location on some of the stations used to gather field data

Bathymetry

Bathymetries were generated using 20x20m raw data provided by project partners at NIOO.

Tide and water elevation

Time series covering several years in various field stations are available online in database websites. These time series are in some stations very complete (e.g. elevation values for the past 4 years in 10 minutes time interval with little or no gaps). The used websites were www.waterbase.nl and www.hmcz.nl.

More information is, however needed, relatively to how the storm surge barrier works, namely the gates mechanism, regulation and dimension, in order to improve modelling methodology in that particular aspect.

Currents, wind and waves

There is currently no available data on currents (water velocity and direction) for the Oosterschelde. On the other hand the availability on wind and waves is very complete. All the data was collected at www.hmcz.nl.

Regarding the wind data, four meteorological stations were chosen to represent the wind patterns (intensity and direction) on the Oosterschelde region. Time series (10 minutes time interval) were gathered between 2000 and 2003 for the following stations: Marollegat, Stavenisse, Oosterschelde 4 (sea station) and Sluis Katz (except 2000).

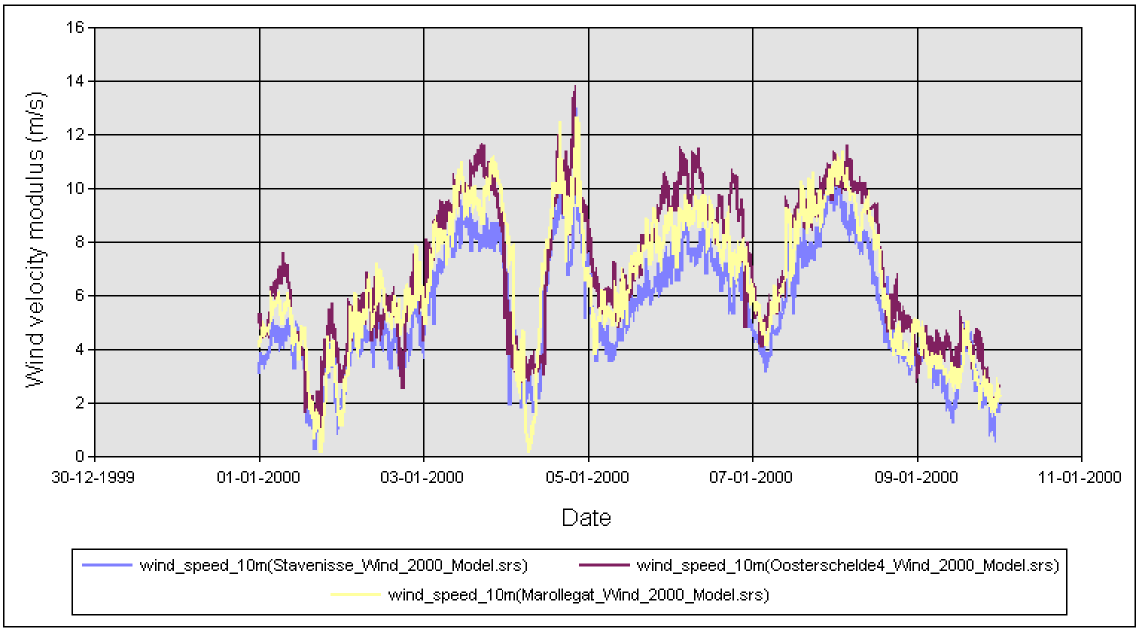


Figure 2 – Wind velocity between January 1st 2000 and January 10th 2000 in Stavenisse, Oosterschelde 4 and Marollegat meteorological stations.

Relatively to the field data on waves, its availability is known (namely through the www.hmcz.nl website), but the information was not yet gathered nor treated.

Water properties

Water properties relate to temperature, salinity or to substances concentration in the water. Field data is available extensively in the above cited websites. Note is made for the high number of parameters available on www.waterbase.nl and to the completeness of the temperature and salinity data in some stations on www.hmcz.nl.

Discharges

Discharges relate to river/fresh water inflow and respective water properties concentrations. More information will be needed relating how and where these discharges into Oosterschelde, take place, once they are controlled by dams and barriers separating the estuary from the channels and the rivers. This information is imperative to impose boundary conditions to the model, in order to validate the transport model.

Methodology

In order to simulate the hydrodynamics and transport in the Oosterschelde estuary, a 3D hydrodynamic and transport model Mohid (http://www.mohid.com), developed at MARETEC of the Instituto Superior Técnico, Lisbon, was used. The model was set up as described below.

Grid and bathymetry

Two horizontal discretizations were assumed: 100x100 m and 200x200m. As field data had a 20x20m resolution, a simple interpolation method was applied to generate the two bathymetry grids. Specific software developed by the IST team was used in this operation.

Vertical discretization

Two vertical discretizations were assumed: 2D (1 layer) and 3D double sigma (5 + 1 layers) domains.

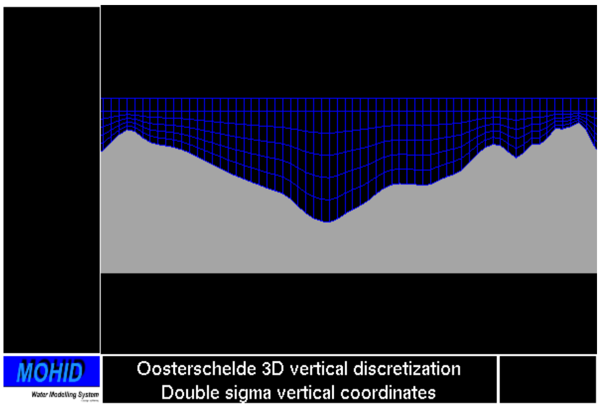


Figure 3 – Double sigma vertical coordinates used for 3D simulations in the Oosterschelde

Tide

Tide was imposed at the storm surge barrier by directly imposing the water level with measured values at the Roompot binnen station.

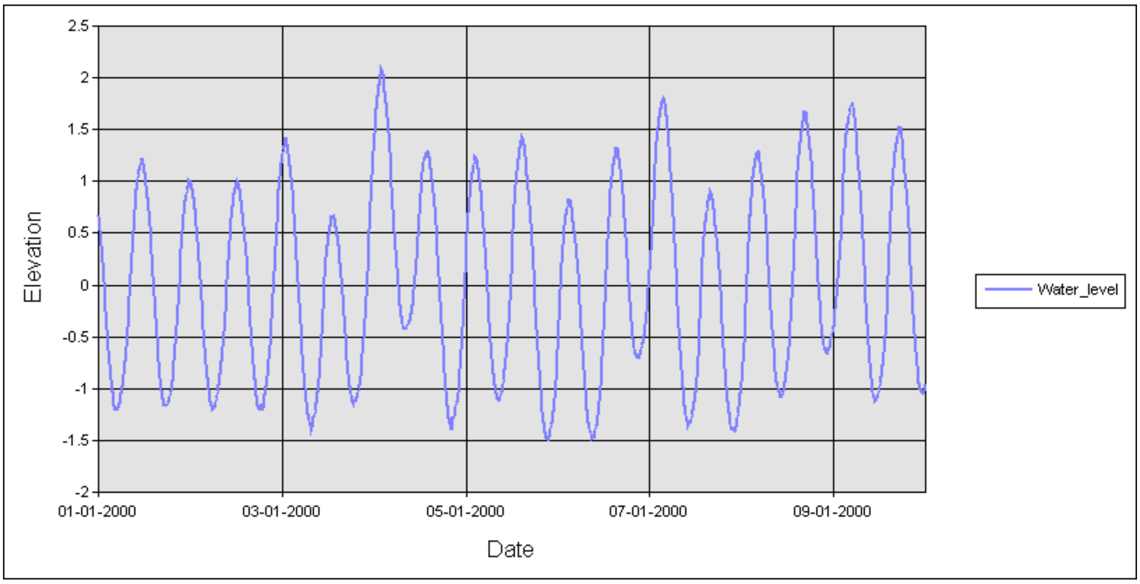


Figure 4 – Elevation measured at Roompot binnen station used to impose the water level at the storm surge barrier.

Wind

Wind was imposed using the Stavenisse station wind time series values as it had almost complete data series since 2000 till the present day, and it is located in the middle of the estuary. This way, Stavenisse meteorological station is assumed to be represent the wind over the Oosterschelde.

Discharges

No discharges were considered by now and will be included as soon as fresh water inflow values are gathered.

Results

As referred above, two horizontal grids were created for the Oosterschelde. However, results are only presented for the 200x200m resolution.

In the following pages some illustrating results are shown for the 2D and 3D applications.

Elevations

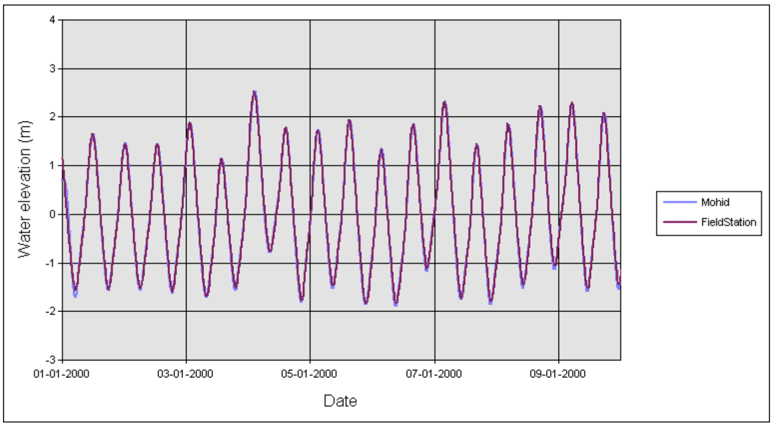


Figure 5 - Water level comparison for Bergse Diepsluis west field station with model result

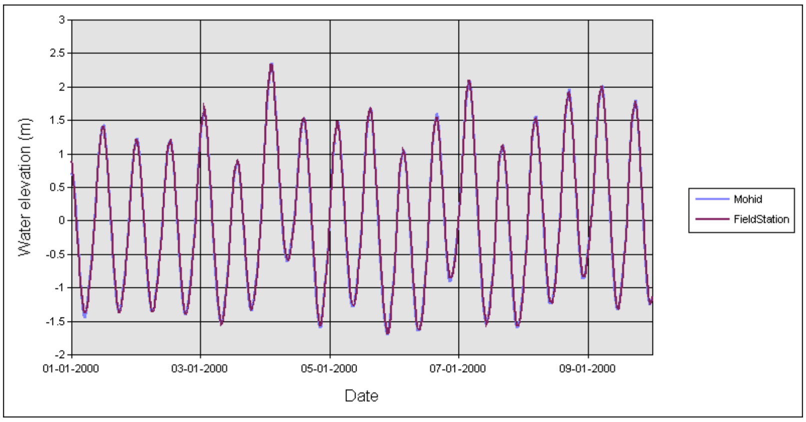


Figure 6 - Water level comparison for Stavenisse field station with model result

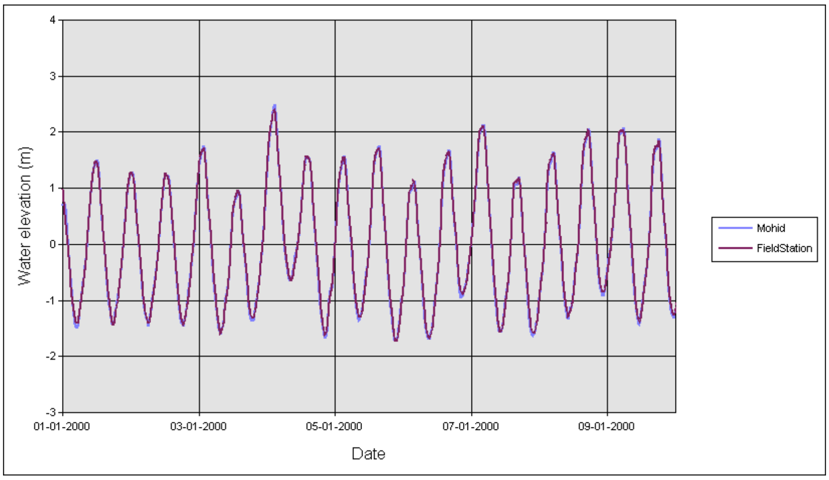


Figure 7 - Water level comparison for Krammersluizen west field station with model result

Currents

Some typical results on water velocity and direction field are presented below in high and low tide and during flood and during ebb. Note that, as these results were not compared with field data, some caution must be taken in interpreting them as accurate.

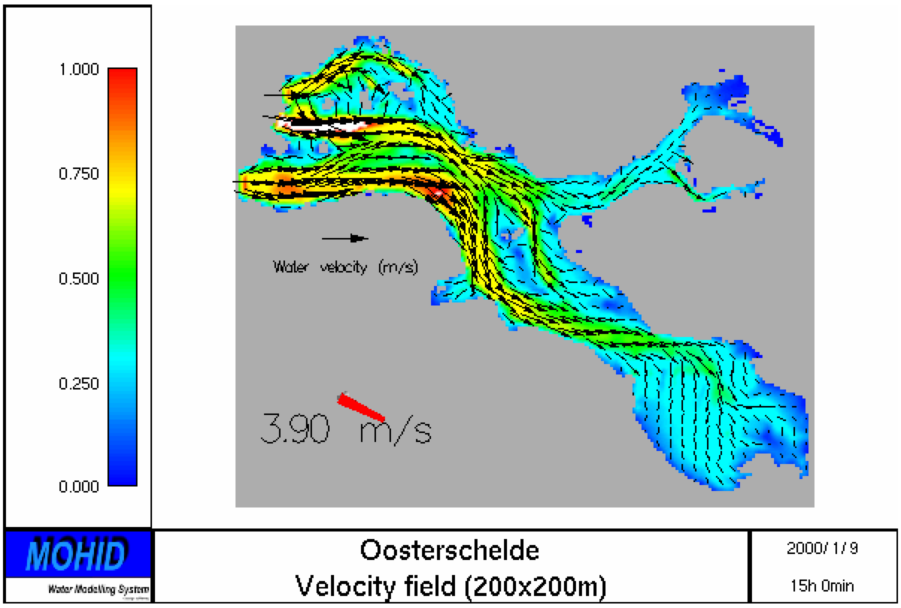


Figure 8 - Velocity field during flood

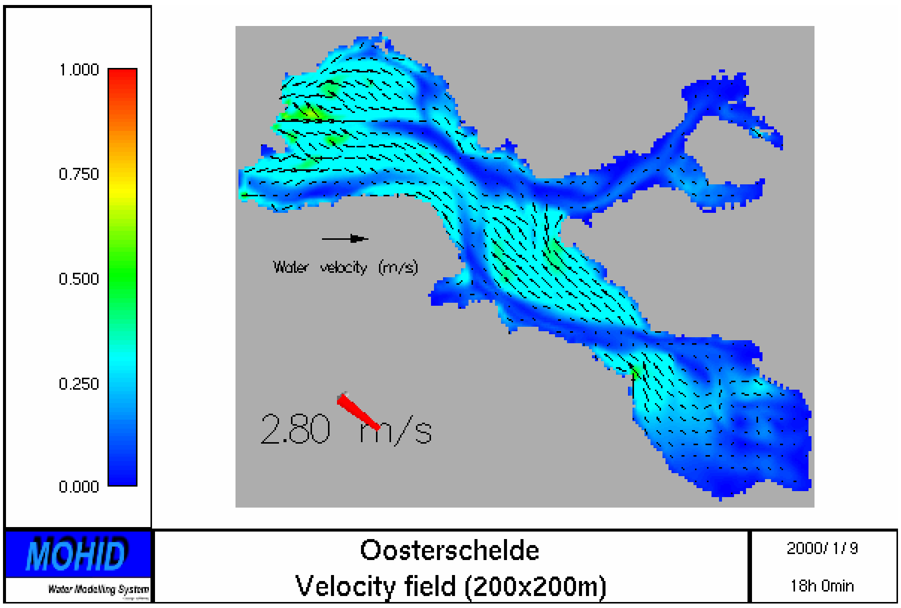


Figure 9 - Velocity field during high tide

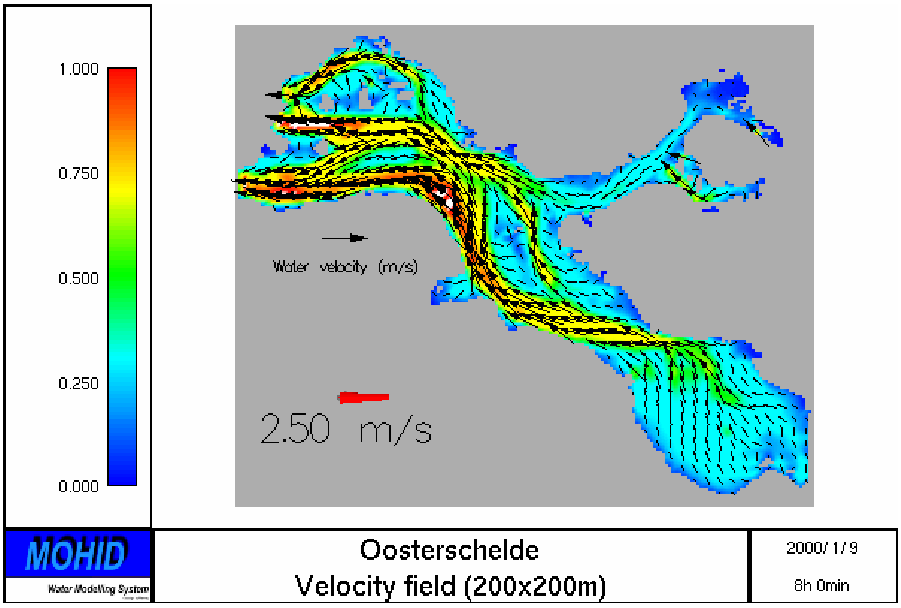


Figure 10 - Velocity field during ebb

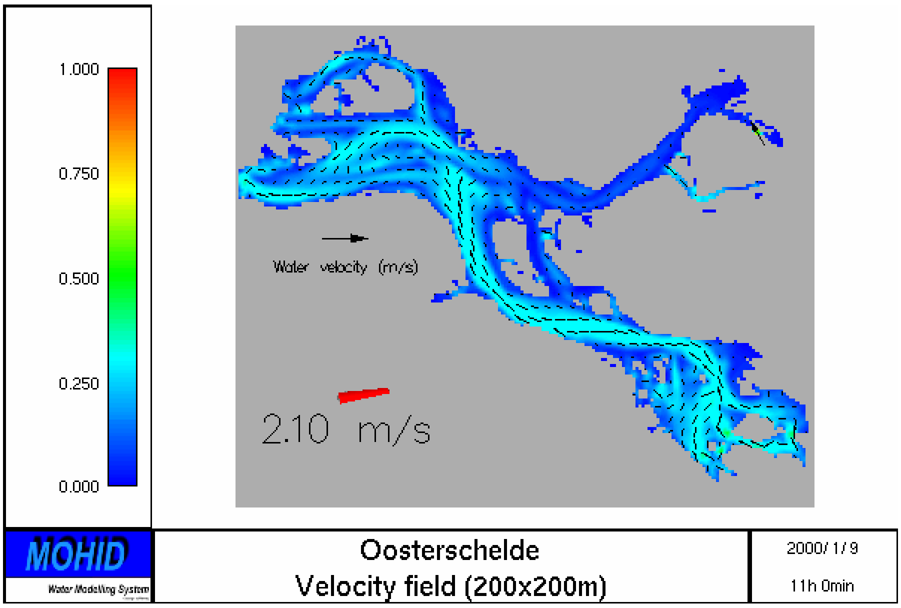


Figure 11 - Velocity field at low tide

Cohesive sediments

Two experimental simulations were performed with cohesive sediments aiming to test the suspended particulate matter module in the Oosterschelde and also to determine the influence of waves induced bottom shear stress. An initial constant concentration of 10mg/l in the water column and a constant distribution of initially deposited sediments in the bottom were considered. Both simulations had equal initial conditions, but in one of them it was considered a constant wave field with a 3 seconds period and 25 cm height.

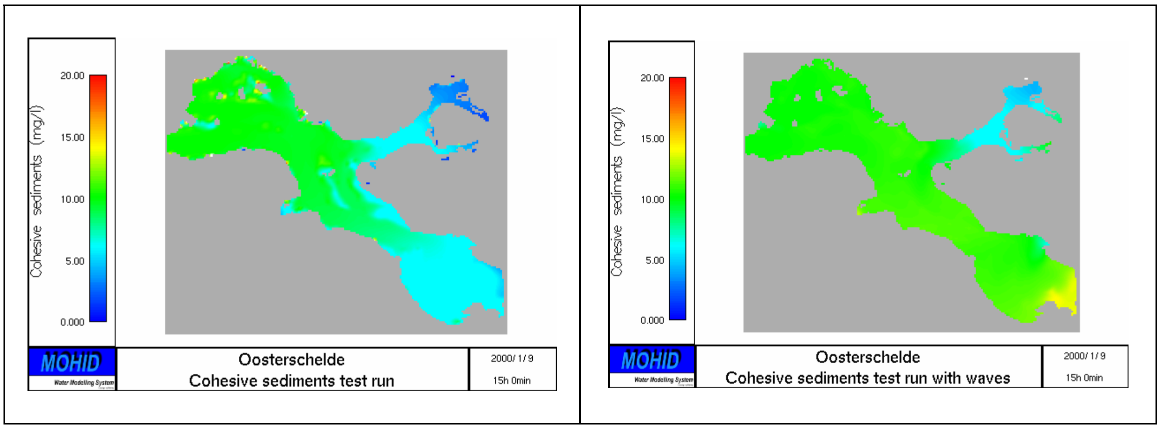


Figure 12 - Comparison between cohesive sediments concentration in performed test runs with and without waves induced shear stress (flood)

As Figure 12 shows, and as it was expected, cohesive sediment concentration in the water column is higher in the simulation with waves, especially in the shallow areas, where waves induced shear stress penetrates till the bottom.

Modelling applications II: Ria de Vigo

Field data

Summary

Table 1 contains a summary of field data availability for Ria de Vigo, including a small description on its origin and status.

Field data	Available	Description
Bathymetry	**Yes**	Etopo, digitalisation of nautical charts – Univ.Santiago
Water elevation	**Yes**	Various stations inside the Ria
Currents	**Partially**	Some currentmeters inside the Ria; little data available on the oceanic zones
Wind	**Partially**	3 meteorological stations in Ria de Vigo zone. No information in oceanic zones
Water properties	**Partially**	CTD data inside the Ria and in coastal zones
Discharges	**No**	-

Table 2 – Summary of field data availability for the Oosterschelde

Bathymetry

Bathymetric data was already available for the Galicia zone as the model has been applied to that area before, both in local and regional applications. The source of this data was Etopo and nautical charts digitalisation performed by the Santiago de Compostela University.

Tide and water elevation

Using tidal components computed by global tide solution software FES5.2 (Le Provost et al., 1998) astronomical tidal elevations can be achieved. However, this information is an estimative, has it does not include other processes (wind, atmospheric pressure, etc).

Some information is available for the Galician West coast provided campaigns performed by Univ. Sant. Compostela, Univ. of Vigo and by the OMEX project data set. This data is mostly relative to the years of 1994, 1996, 1997, 1998 and 1999.

Currents, wind and waves

It is available wind data on 3 meteorological stations in Ria de Vigo zone for some periods in the year of 1997. No information in oceanic zones was encountered.

Regarding currents, little and scattered data is available, having the same sources has reported to tidal elevations.

Water properties

There is some availability for profile data on temperature, salinity and chlorophyll. However this is also scattered and is very low on any other type of measured parameters.

Methodology

Model nesting

In order to study and model the Ria de Vigo, known to be a complex coastal upwelling system, a structure of 3 nested models was constructed. Each model is defined by a different bathymetry, each representing a level of scaling. The "father" model provides boundary conditions to the "son" and this one to its "son", and so on. The first level (0.1º spacing) corresponds to the Galician coast (Northwest of Iberian Peninsula); the second (maximum spacing of 0.04º) to the West coast of Galiza, including Rias de Vigo, Pontevedra, Arousa and Muros; the third level (maximum spacing of 0.02º and maximum resolution of 0.003º inside Ria de Vigo) includes only Ria de Vigo and Ria de Pontevedra.

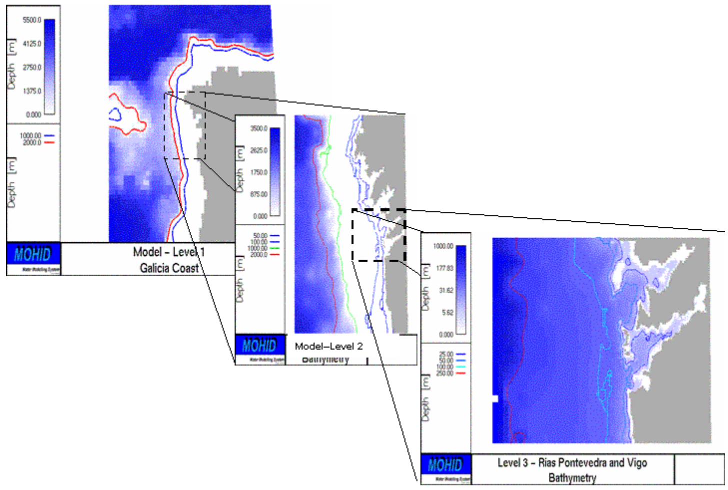


Figure 13 - 3 levels model nesting application for Ria de Vigo

Vertical discretization

First level: 1 layer (simplified 2D application)

Second level: 10 layers (cartesian vertical coordinates)

Third level: 10 layers (cartesian vertical coordinates)

Tide

Tide was explicitly imposed only in first level model (Galiza scale) using tidal components computed by global tide solution software FES5.2 (Le Provost et al., 1998). Water level is imposed in the boundaries of the second and third levels sub-models.

Wind

As no representative data was available for the type and duration of the simulations, two scenarios were idealized: North constant wind and south constant wind. Both scenarios were accomplished by imposing directly at the water surface of 0.1 Pa in each respective direction and in each of the three model levels.

Temperature

A simplified stratified temperature profile was considered, with 18ºC at the surface layers and 13ºC in the bottom layers.

Results

Some results are shown below for each wind scenario.

North wind

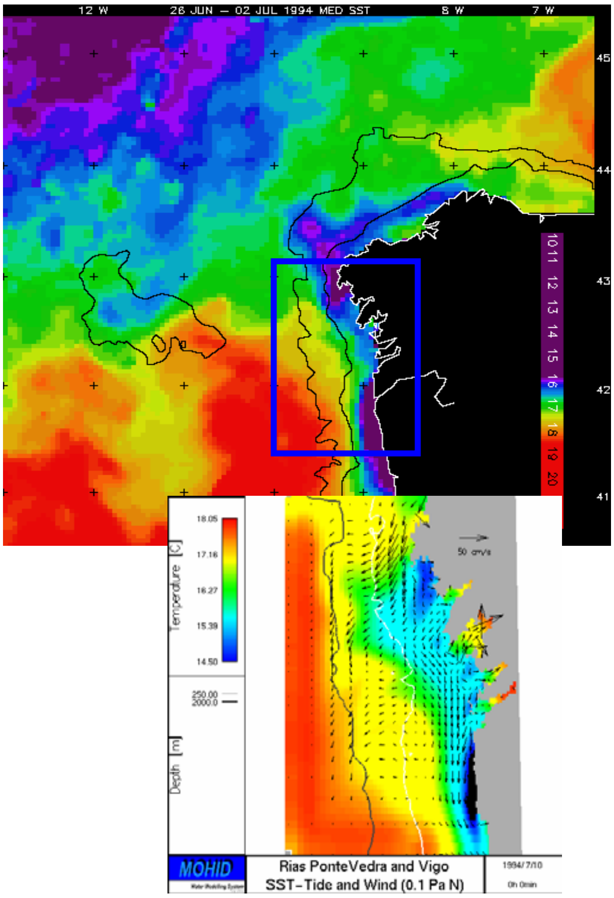


Figure 14 – Comparison between satellite image and model SST results for an upwelling event (1994)

In Figure 14, cold water reaches the coast by an upwelling, as a result of imposed North wind.

South wind

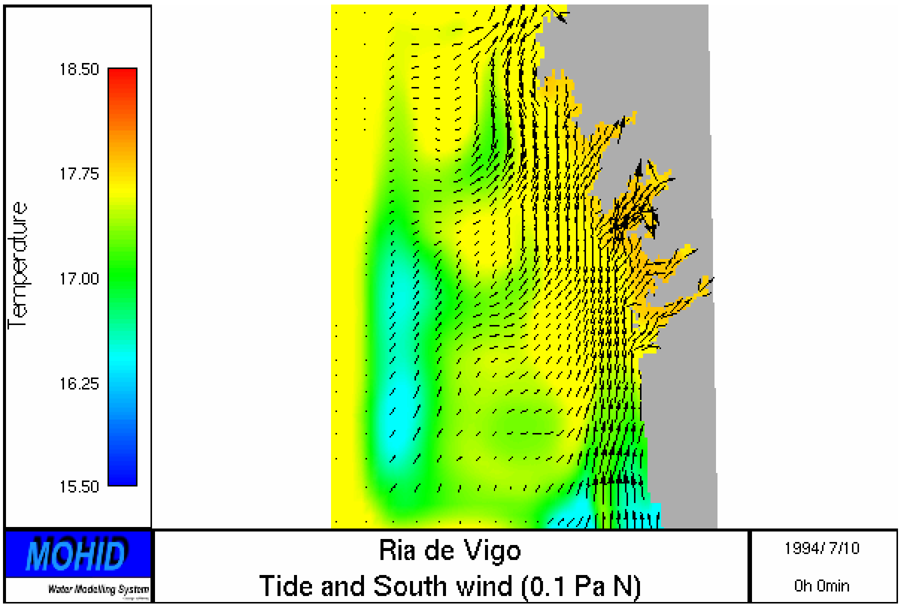


Figure 15 – SST after 10 day simulation with South wind (0.1 Pa wind stress)

In opposition to the North wind scenario, the surface water temperature is warmer near the coast as a result of the water accumulation inside the Rias.

Modelling tools: Mohid

Overview

MOHID is a modular finite volumes water modelling system written in ANSI FORTRAN 95 using an object oriented programming philosophy, integrating about a dozen programs written in FORTRAN95 and supported by graphical user interfaces both in FORTRAN (using OpenGL libraries) and Microsoft Visual Basic .NET. It is an integrated modelling tool able to simulate processes in a water column and in the sediments and the coupling between these two domains and the atmosphere.

The water column model is composed by a free surface three-dimensional baroclinic hydrodynamic module, a turbulence module (including GOTM), an eulerian transport module, a lagrangian transport module, an oil dispersion model and a three zero-dimensional biogeochemical modules. The sediments model is composed by a saturated one-dimensional consolidation, an eulerian transport model and by a zero-dimensional sediment quality/biogeochemical model. Atmospheric processes can be included by imposing atmospheric observed data or atmospheric model results.

Model applications

The model has been applied to several coastal and estuarine areas and it has showed its ability to simulate complex features of the flows. Several different coastal areas have been modelled with MOHID in the framework of research and consulting projects. Along the Portuguese coast, different environments have been studied, including the main estuaries (Minho, Lima, Douro, Mondego, Tejo, Sado, Mira, Arade and Guadiana) and coastal lagoons (Ria de Aveiro and Ria Formosa), INAG [2001]; Martins et al. (2000). The model has been also implemented in most Galician Rías: Ría de Vigo by Taboada *et al*., (1998), Montero, (1999) and Montero *et al*. [1999], Ría de Pontevedra by Taboada *et al.* [2000] and Villarreal *et al.* [2000] and in other Rías by Pérez Villar *et al* [1999].

Some North European estuaries have also been modelled - Western Scheldt , The Netherlands, Gironde, France by Cancino and Neves, [1999] and Carlingford, Ireland, by Leitão, [1997] - as well as some estuaries in Brasil (Santos SP and Fortaleza).

Regarding to open sea, MOHID has been applied to the North-East Atlantic region where some processes including the Portuguese coastal current, Coelho (2002), the slope current along the European Atlantic shelf break, Neves *et al*. (1998) and the generation of internal tides, Neves *et al*. (1998) have been studied and also to the Mediterranean Sea to simulate the seasonal cycle, Taboada, (1999) or the circulation in the Alboran Sea, Santos, (1995).

More recently MOHID has been applied to the several Portuguese fresh water reservoirs Monte Novo, Roxo and Alqueva, (Braunschweig, 2001), in order to study the flow and water quality.

Model structure

MOHID modular structure enables that each module can correspond to a different compartment (water column, sediments, atmosphere) or to a specific process or set of processes, that is, each module is responsible to manage a certain kind of information. For example module "WaterProperties" is responsible for computing the properties evolution in the water column, corresponding in this case to the water column domain. To do so, this module uses other modules, responsible for specific processes like module "AdvectionDiffusion" which computes properties transport, or module "WaterQuality" which computes properties biogeochemical reactions, and so on.

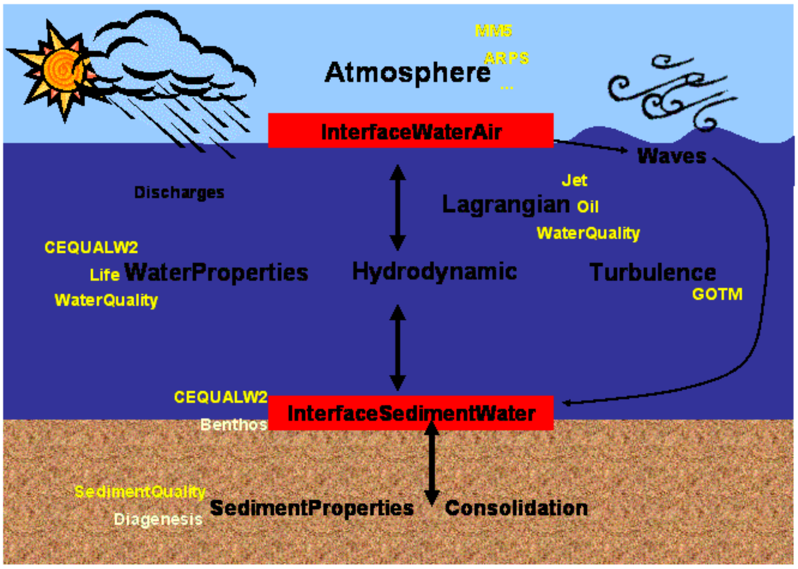


Figure 16 - Mohid modular structure (main modules)

In terms of global organization, MOHID can be divided in the water column (module "WaterProperties" and module "Hydrodynamic"), in the sediment compartment (module "SedimentProperties") and the atmosphere (module "Atmosphere"). Each compartment is separated by an interface, which controls the information and communications between two domains, namely the "InterfaceWaterAir" module and the "InterfaceSedimentWater" module. MOHID does not explicitly compute the atmosphere processes. Module "Atmosphere" works as a database module, in which this processes are given to the model as inputs, with origin in atmospheric observed data or in atmospheric model results.

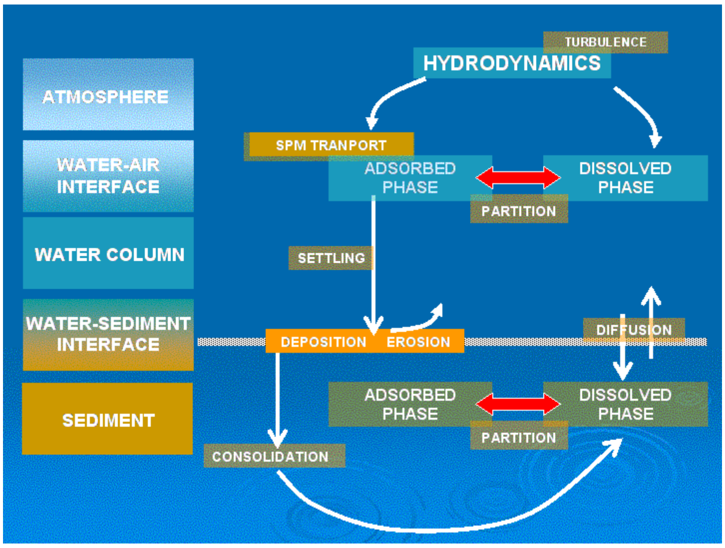


Figure 17 – Water-sediment interface processes in Mohid

The water column

The water column entity is, as said, module "WaterProperties". This module uses module "Hydrodynamic" to compute water fluxes that are then used to compute properties transport. MOHID is prepared to simulate properties such temperature, salinity, cohesive sediments, phytoplankton, nutrients, contaminants, etc. These properties can be considered as being dissolved in the water, therefore following the currents, or as being particulate or adsorbed on to particulate matter, thus being subjected to one more transport variable: the settling velocity. This causes particulate properties to deposit in the bottom and thus become a part of the sediments.

The ability to simulate different properties in both dissolved and particulate states is an important feature included in the model. But probably even more important, is the possibility of computing the distribution of a property between the solid and the dissolved phase, using a partition coefficient formulation. This is a very common modelling approach to simulate transport and fate of contaminants. In these cases the roll of particulate matter is very important, namely the through cohesive sediment transport, due to the important percentage of, not only, contaminants adsorbed on to its surface, but also due to the fraction of organic matter that is part of this kind of sediments and that influences the nutrient cycling in marine systems.

The water-sediment interface

Module “InterfaceSedimentWater”, the entity for water-sediment interface, controls the cohesive sediment fluxes between the water-column and the sediments, namely through computing erosion and through enabling deposition, both processes being determined by the flow intensity near the bottom, in the form of shear stress. The water-sediment interface is a zone with transient characteristics, and it can be seen as a thin high porous layer constituted of water and sediments. The processes that take place here depend on the processes taking place above, in the water column, and below in the “quiet” sediment. For example, once deposited in the bottom, particulate matter can either stay there or be resuspended back to the water column. If the tendency is to remain deposited, that is, if the deposition flux is higher than the erosion flux, then it becomes part of the sediment. This source to the sediment compartment is computed as a consolidation rate applied to the deposited particulate matter. This is true not only as a sediment source, as well as a source of adsorbed properties to the sediment compartment. On the other hand, if the erosion flux is very high, and the particulate matter deposited in the water-sediment interface is fully eroded, the upper sediment layers can be eroded, depending, in this case, on their characteristics.

Dissolved properties fluxes depend on water flow across the water-sediment interface and on concentration gradients between the water column’s lower layer concentration and the concentration on the interstitial water of the sediment’s upper layer. Therefore one can divide this boundary fluxes on an advective flux and a diffusive flux. For the latter, the rate at which the gradient tends to be eliminated depends on the water column flow, i.e. on the bottom shear stress. Therefore, it is considered a bottom shear stress dependent mass transfer coefficient.

Benthic filter-feeders, macro-algae and other benthic organisms interacting with the water column and the sediment are also managed (or to be managed) by the module “InterfaceSedimentWater”.

The sediment compartment

The model structure used for simulating sediments is very similar with the one used to simulate the water column. The most important modules are, in this case, module “Consolidation”, module “AdvectionDiffusion” and module “SedimentQuality.

The MOHID’s sediment compartment is seen as a media composed of sediment, water and in some cases air. Properties, in resemblance to the “WaterProperties” module, can either be dissolved in the interstitial water or adsorbed onto the sediment. They also can be specific of the sediment or they can interact with the water column. Module “Consolidation” is responsible for computing the water flow within the sediment layers and is a simple consolidation model that considers a consolidation rate, at which the sediment layers compact. This is achieved with an interstice volume decay rate, reducing water content in the sediments and leading to an upward movement of the interstitial water till it reaches the water column. These water fluxes can become important, as they are responsible for advective transport of dissolved properties to the water column. Saturated conditions are considered, resulting in a simple formulation to compute the water velocity. This module receives as initial inputs the water content, the consolidation rate parameters and in run-time it receives a sediment flux from the water column, through module “InterfaceSedimentWater”, due to particulate matter settling.

Module “AdvectionDiffusion” solves the mass transport equations using the water fluxes computed by the interface module “SedimentHydrodynamic”.

Module “SedimentQuality” is a biogeochemical model, based on RZWQM/OMNI, for carbon and nitrogen cycling in soils (unsaturated porous media), presently being prepared to be adapted to estuarine and marine saturated sediments, as it includes already bacterial (autotrophic, heterotrophic and anaerobic) growth/organic matter mineralization with oxygen balance.

Coupling hydrodynamic and biogeochemical models

Overview

Biochemical processes can be added directly to the transport models equations in the form of sink and source terms. This approach is traditionally used in the definition of model equations, and is also followed when programming the algorithms. Thus, the biogeochemical module becomes coupled to only one transport model and vice-versa. This approach can be very limiting, especially if different groups plan to share biochemical formulation between them in order to use it in different transport models. In the MOHID system it is possible to use the same biochemical module to run 3D or 1D Eulerian transport modules or a 3D Lagrangian module. There are currently 4 biogeochemical modules connected 3D transport modules:

WaterQuality - Pelagic water quality module based on EPA model WASP
CEQUALW2 - Adapted pelagic and benthic module from CEQUALW2 (3.1)
Life - Pelagic multi-parameter ecological model with microbial loop and variable stoichiometry
SedimentQuality - Carbon-Nitrogen unsaturated biogeochemical cycle model with microbial loop and variable stoichiometry based on RZWQM/OMNI

The paradigm behind the MOHID system was inspired by Prof. DiToro's (member of HydroQual) words: "Phytoplankton does not have GPS", meaning that biochemical processes are 0D and do not depend on the referential and dimensions considered to quantify transport. In the MOHID case, the methodology consists in building a biogeochemical module, where the external forcing conditions are given (ex: light, temperature, salinity) and mass fluxes between state variables (ex: nitrate, phytoplankton and zooplankton) are computed for each control volume. This is an efficient way to guarantee a high level of robustness in the code and to maintain it. This approach is also followed by DHI's MIKE system, which like MOHID, has several transport models.

The goal in MABENE is to share a biogeochemical pelagic module with three eulerian transport models (GETM, MOHID – 3D and GOTM – 1D). One way to accomplish this coupling is to build a biochemical module that computes the reactions for one control volume. Consequently, the biochemical subroutines have to be called inside the loops, a method proved to be computational time consuming. The alternative is to build a module that solves the biochemical processes for a 1D array of control volumes. The MOHID system has an interface called ModuleInterface, responsible for transferring information (forcing conditions and state variables) from 1D, 2D or 3D structured grids to a 1D array and for calling the 0D biochemical module subroutines. MOHID system was developed following an object-oriented programming philosophy. This interface is a class (or module) currently used to transfer information from the module responsible for the transport processes in the bottom sediments to the module responsible for the biochemical process in the sediment. The same happens between the water column transport module to the water quality and water biochemical processes modules.

Constructing the interface

The interface construction phase consists on the memory allocation and options consistency to couple the transport model to the biochemical model. Thus, the variables needed to initialize the interface are:

- Name of the biochemical model to be executed;
- An array with the names of the state variables (properties) being modeled by the transport model which have been defined to have sinks and sources terms using the defined biochemical equations; this is important, so that properties are defined coherently in both models and the properties indexing task can be performed straightforwardly;
- A mapping matrix (WaterPointsxD, being x the number of dimensions) that takes the value of 0 for land points and 1 for water points; this is used to define the size of the 1D arrays where most information will be stored and then given to the biochemical module.
- A size variable (SizexD, being x the number of dimensions), used to translate (loop through) 2D and 3D matrixes to 1D arrays.

Interfacing during the run

ModuleInterface first task is to gather information on state variables needed by the biochemical models. So, the transport model must loop through all properties, sending its concentration as an argument. Optionally, other variables can also be sent, like

radiation at the top of the control volume, control volume thickness and the light extinction coefficient field. Mapping arrays (WaterPointsxD and OpenPointsxD) must be given so that biochemical processes can be computed, if desired, for example, only in covered cells. OpenPointsxD is a variable, which takes the value of 0 if the cell is uncovered and 1 if it is covered with water.
State variables information (i.e. concentration of properties which have sinks and sources defined by the biochemical module) is stored in a bi-dimensional array with size equal to the number of properties versus the number of control volumes, with each property properly indexed in this array. The indexing is done in the constructing phase in agreement with the two models. On the other hand, properties like temperature and salinity as well as light and mapping variables, are stored in specific 1D arrays.

The loop through all the properties continues until all information is gathered. This is achieved by creating a logical array with the indexed properties, defining the ones that have already been added to the state variables array. When everything is ready, the biochemical model is then called, looping through the number of control volumes, changing the state variables values.

The biochemical model time step can be, and often is, different from the transport model time step. The latter needs, due to numerical reasons, smaller time steps than the biochemical models. Thus, in each biochemical time step the state variables values are previously stored in another array, allowing to compute the concentration variation during this time step. This flux is then available to the transport model to actualize the properties concentration in its own time step.

Conclusions and future work

The IST team has applied Mohid numerical model to the Oosterschelde and to Ria de Vigo. Model applications will be improved with more field data provided by project partners and with the increasing knowledge of the two systems.

Future developments to be taken in the framework of MaBenE include:

- the improvement of the existing suspended particulate matter module;
- the development of a benthic biogeochemical module;

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