MOBYDICS

Integrating bioturbation and biodeposition processes in hydrodynamic and transport models for contaminated sediments

Progress report

MARETEC - IST

January 2003

INDEX

Introduction

This report was developed in the framework of the MOBYDICS project, regarding MARETEC tasks progress.

Overview

In estuaries and coastal zones, great amounts of particulate matter can be found in the water column. Many of this matter will ultimately deposit in the bottom and if not resuspended back to the water column, can become a part of the sediment, as more deposition of particulate material occurs. This means that, although it is removed from the water column, it does not exit the system, keeping the ability to influence it or be influenced by it. Once particulate matter is constituted by a significant fraction of organic matter and carries most of the contaminants present in aquatic systems adsorbed onto it, it is important to understand the processes that influence these constituents transport and fate, namely through understanding how they can influence not only the pelagic but also the benthic systems.

Benthic biological activity, process is known as bioturbation, can play a significant roll in the fluxes of matter between sediments and the water column in estuaries. Benthic organisms can disturb and mix sediments by their constant burrowing and feeding, as they look for shelter and as a result of their physiological functions. Therefore this activity may influence the habitat structure and functioning, by altering the properties of the sediment, which, on the other hand, influences sediment transport processes, namely erosion and deposition. Bioturbation may also enhance sediment oxygenation, organic matter decomposition and change the distribution and nutrient cycling, as well as it can influence the transport and fate of contaminants.

Numerical models play, nowadays, an important role as scientific tools, once they can help to understand complex systems with high number of variables. This is the case of estuarine and coastal systems, where physical processes interact with biological and chemical processes in a complex way. Therefore, models can constitute a bridge between these scientific areas as multidisciplinary tool.

Hypothesis

MOHID water modelling system can simulate the water flow and cohesive sediment transport in an annular flume, representing the groundwork to improve the contaminant transport model by coupling the bioturbation processes.

Objectives

This project main objective is to understand the influence of bioturbation on the fluxes across the water-sediment interface, mainly through the sediment transport processes and consequently its roll on nutrients and organic matter transport and on fate of contaminants.

The laboratory experimental results, performed in an annular flume, will be used to support a sediment and contaminant transport and biogeochemical model, which in a first step will be applied to an annular flume simulation, so that experimental results will be reproduced. Afterwards, the model will be applied to estuarine and coastal systems, representing then an important step to better describe and understand the complex occurring processes.

Methodology

MOHID water modelling system

MOHID[1] is a modular finite volumes water modelling system written in ANSI FORTRAN 95 using an object oriented programming philosophy. 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, an eulerian transport module, a lagrangian transport module, an oil dispersion model and a zero-dimensional water quality module. The sediments model is composed by a saturated one-dimensional consolidation and a non-saturated media three-dimensional water flow model, an eulerian transport model and by a zero-dimensional sediment quality model.

MOHID can also run nested models. This feature enables the user to study local areas, obtaining the boundary conditions from the "father" model. The number of nested models is just limited by the available computer power.

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.*

[1] http://www.mohid.com

[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.

In terms of global organization (Figure 1), MOHID can be divided in the water column (module “WaterProperties”) and in the sediment compartment (module

“SedimentProperties”), separated by an interface, which controls the information and communications between the two domains (module “Bottom). Above the water column is the atmosphere, performed by module “Surface”. MOHID does not explicitly compute the atmosphere processes. This makes module “Surface” to work more like 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. Note that, if the water column disappears, due to tidal water level variation or due to infiltration, module “Surface” is then coupled to module “SedimentProperties”, enabling that for example evaporation takes place directly from the sediment upper layers.

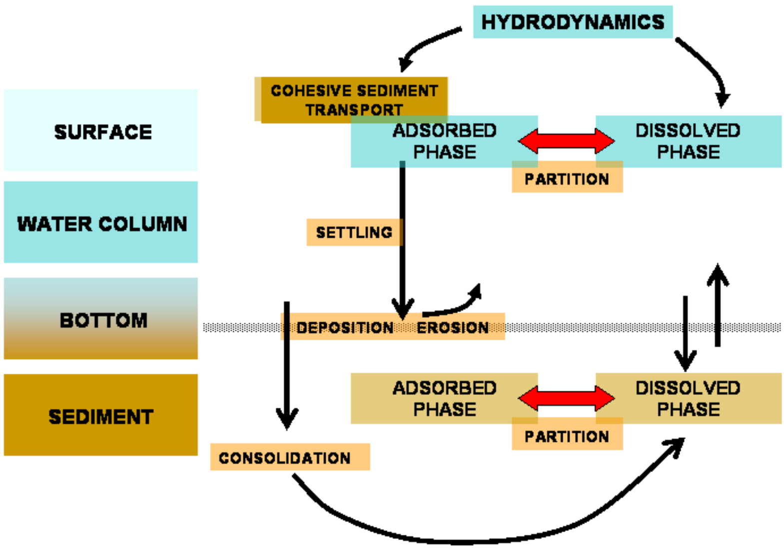

Figure 1- MOHID global organization

The modelling and coupling of the sediment compartment in MOHID is a relatively new feature. Therefore the description will relate more to the new modules added regarding this compartment.

Coupling sediments as a new compartment in the model can be seen not only as a possibility to study its specific processes but also as an improvement of the description of pelagic processes already included in the model. In that sense, a main goal is to describe and comprehend what is happening in the water-sediment interface. Other main objectives of module “SedimentProperties” are to compute water flow and property transport in consolidating sediments saturated media (e.g. estuarine sediment) or in non-saturated media (e.g. soil), as well as compute air-sediment exchange fluxes in case the water column is not present.

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 presently 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[2]. 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 “Bottom”, 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

[2] MOHID is presently being applied to the Tagus estuary to simulate the arsenic contamination problem, due to decades of discharges of this metalloid to estuarine waters.

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 more "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 (infiltration or exfiltration) 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, solved using a likewise *upwind* discretization, 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.

Filter-feeders, macro-algae and other benthic organisms interacting with the water column and the sediment are also managed by the module "Bottom".

The sediment compartment

The model structure used for simulating sediments is very similar with the one used to simulate the water column. Following MOHID's structure, module "SedimentProperties" uses other modules to compute specific processes and functions, presented in Table 1, along with a short description.

Module's name	Module's function
GlobalData	Handles the global variables, constants and parameters
Time	Handles the time
HDFOutput, HDF5	Handles HDF format input and output files
EnterData	Handles ASCII format input data files
TimeSerie	Handles ASCII time series format input and output files
Bathymetry	Handles the bathymetry / topography
HorizontalGrid	Computes the XY grid discretization
Geometry	Computes volumes, distances and vertical coordinates
HorizontalMap	Handles 2D horizontal compute points mapping
Map	Handles 3D horizontal compute points mapping
BoxDif	Handles variables integration within defined boxes
AdvectionDiffusion	Computes mass transport equations
SedimentHydrodynamic	Handles the sediment hydrodynamic modules: module Consolidation and module Soil, responsible for computing water fluxes in the sediment
SedimentQuality	Computes soil's carbon and nitrogen cycle

Table 1 - "SedimentProperties" server modules

The most important modules are, in this case, module "SedimentHydrodynamic", module "AdvectionDiffusion" and module "SedimentQuality", as all the other modules can be seen as auxiliary.

The MOHID's sediment compartment is seen as 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 "SedimentHydrodynamic" is responsible for computing the water flow within the sediment layers, taking two different approaches: the water flow in saturated media and in non-saturated media. This module functions as an interface using two modules, built on similar structures, that compute the water fluxes following those two approaches: module "Consolidation" and module "Soil".

Module "Consolidation" 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 "Bottom", due to particulate matter settling.

Module "Soil", considers non-saturated conditions that can normally be found in soils. This module solves the Richards equation, outputing water fluxes and water contents. This module requires as inputs the water contents and the hydraulic properties of the soil and during run-time it requires boundary conditions regarding the water pressure at the soil surface and atmospheric conditions.

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

Module "SedimentQuality" is a biogeochemical model for carbon and nitrogen cycling in soils, presently being prepared to be adapted to estuarine and marine sediments, as it includes already bacterial (autotrophic, heterotrophic and anaerobic) growth/organic matter mineralization with oxygen balance.

New developments in the project's framework

The first development in MOHID water modelling system, regarding the MOBYDICS project, was to prepare the model in order to simulate annular flumes. This development allows the validation of processes simulated by the MOHID system using the experimental data, enabling to validate the erosion and deposition processes, the transport of particulate and dissolved contaminants (e.g. copper) in the water column and in the sediment, and later the influence of macrofaunal bioturbation and biodeposition.

In order to adapt the model to such a small scale (1m), when compared with the normal scales (10, 100, 1000 km) used in the model, some artefacts had to be taken. The main developments performed in the model were:

- the introduction of the centrifugal acceleration in the inertial forces term when computing the hydrodynamic solution;
- the construction of a new type of horizontal discretization named CIRCULAR;
- the adaptation of the model to the new horizontal discretization.

All the other processes simulated were already included, having only to be provided to the model the necessary and correspondent data files and information.

Flume geometry

Geometry parameters are input data that the user provides to the model. This means that the dimensions of the annular flume can be different in different simulations, just by introducing a different geometry parameters file. Nevertheless, all the simulations performed to test the model were applied with the dimensions of the annular flume operated in the laboratory (Tabel 2).

Water column height	40-50 cm
Exterior diameter	60 cm
Interior diameter	30 cm
Channel width	15 cm

Tabel 2 - Annular flume geometry parameters

Various discretizations were used, combining fine resolution with time step, having in mind the type of flow generated in this kind of domain. Due to time computational reasons, a simplified horizontal discretization of 10x36 cells was used (Figure 2), plus a 10 layers vertical discretization using a sigma coordinate type (Figure 3).

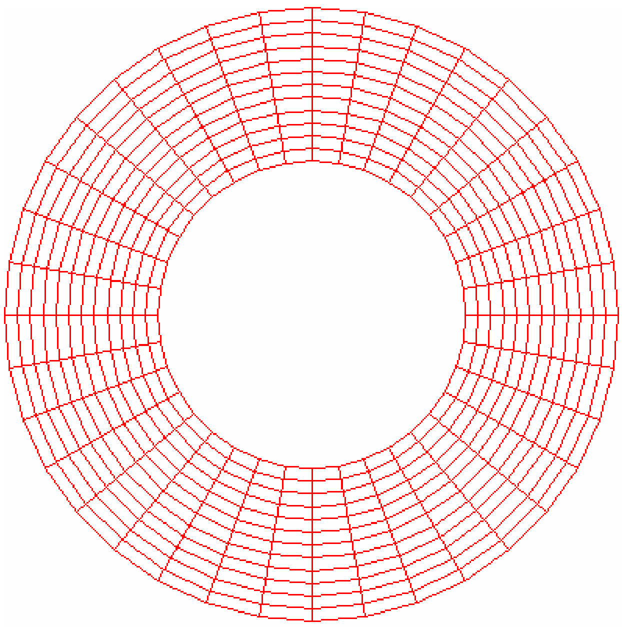

Figure 2- Horizontal grid discretization

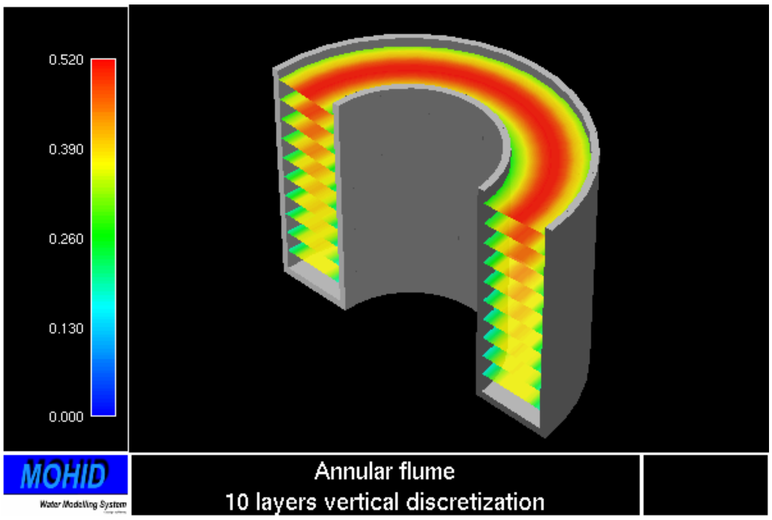

Figure 3 - 10 layers vertical discrezation

Hydrodynamics

As referred before, one of the processes that had to be introduced and developed in the hydrodynamic module was the centrifugal acceleration, due to the flow circular characteristics.

Forcing

Hydrodynamics was forced by applying a shear stress at the surface of the water column, increasing linearly with the flume radius. This approach pretends to simulate the actual mechanism that forces water to flow in the annular flume operated in the lab. This surface forcing provides momentum to the upper layer of the water column that by turbulent diffusion is transported to the lower layers and enables the water to speed up. The shear stress is imposed gradually in the beginning of the simulations, after what it remains constant enabling a steady state flow conditions to form. Shear values were applied so that maximum water velocity obtained, in the upper layer obviously, was about 50 cm/s.

Shear

A non-slipping condition was considered to both the bottom and lateral boundaries, having the latter the most important contribution to the shear forces.

Cycle boundary conditions

Cycle boundary conditions are considered to assure continuous flow. That is, if the domain is considered to be divided into to *1 to i* (*XX* direction) and *1 to j* (*radial* direction) then the boundary condition for example applied to *cell 1,1* is given by the hydrodynamics properties of *cell 1, j*. In the same way, boundary condition of *cell i, 1* is given by the hydrodynamics properties of *cell i, j*.

Cycle boundary conditions are also applied to the mass transport solution, similarly to the momentum transport.

Applications and results

Hydrodynamics simulations

The first test case applications were performed in the annular flume, attempting to run the model just by obtaining the hydrodynamic velocity fields. In the next figures, various kinds of results can be seen, representing flow velocity in the XYZ directions.

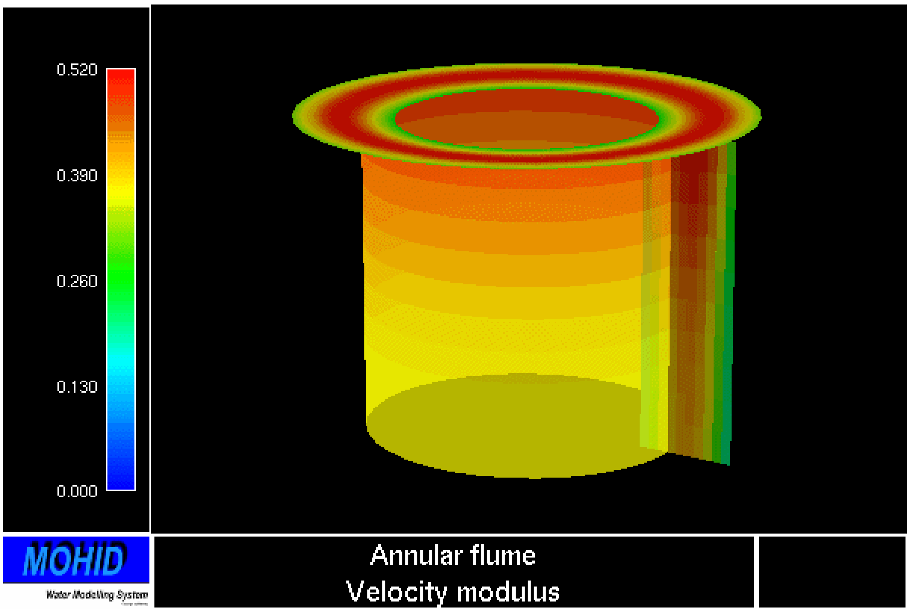

Figure 4 - Velocity modulus (3D view)

Figure 4 shows the velocity modulus field in a 3D perspective. The velocity is higher in the top layers, due to the shear stress applied at the surface. Velocity diminishes with depth (Figure 6 and Figure 7) due to viscous forces and bottom shear stress and with wall proximity (Figure 5) due to wall shear stress.

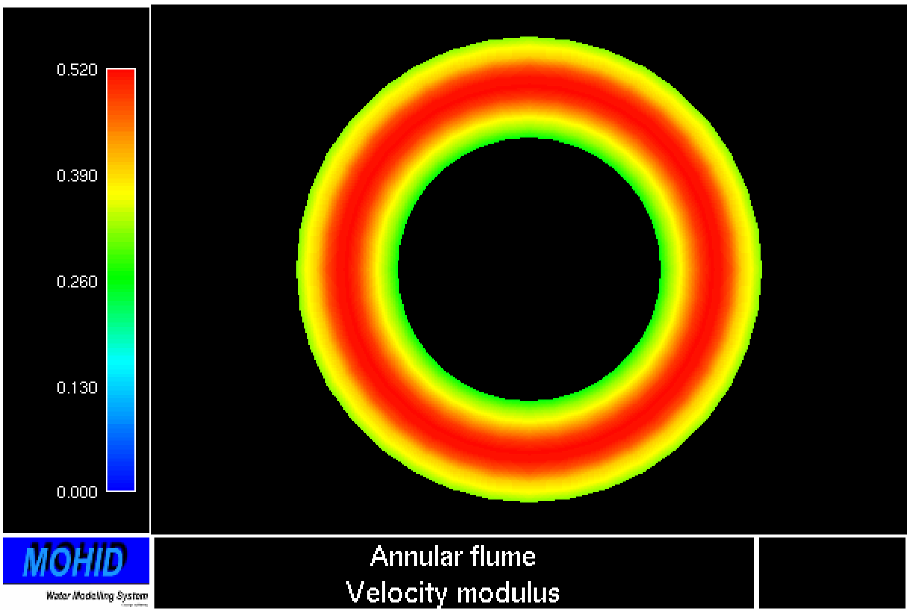

Figure 5 - Velocity modulus (top layer top view)

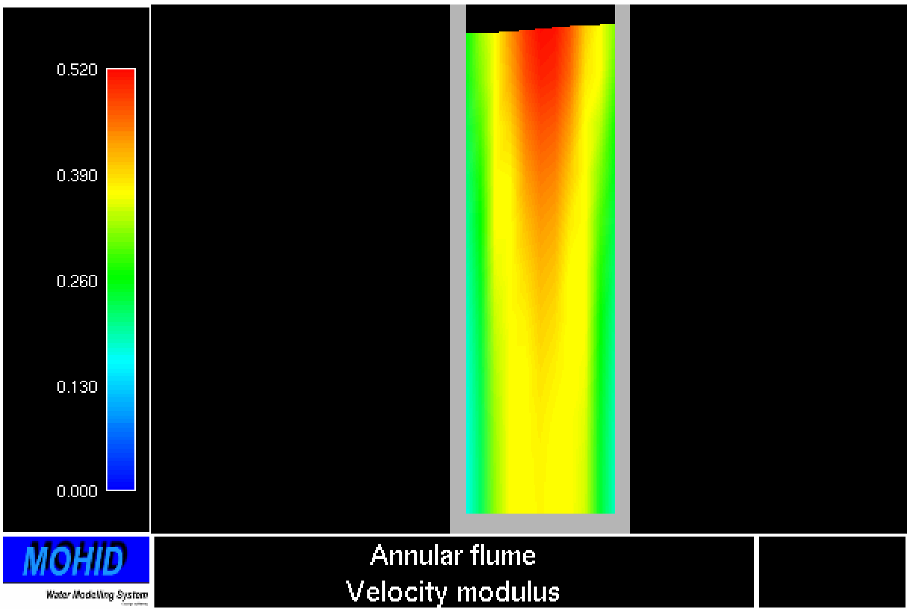

Figure 6 - Velocity modulus (XZ cut)

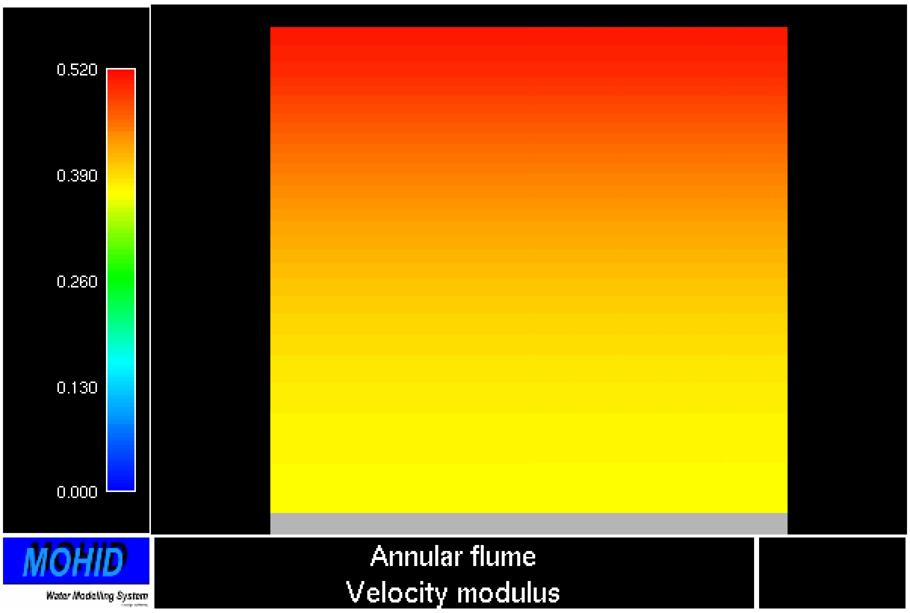

Figure 7 - Velocity modulus (YZ cut)

The flume's circular geometry and the flow's circular characteristics generates secondary flows that can be observed in the velocity intensity in the radial direction and in the vertical direction, correspondently represented by Figure 8 and Figure 9.

In the radial direction, the water at the top layers is pushed to the outer wall due to the effect of the surface shear stress applied, resulting in a water level rising near that wall. However in the lower layers, water flows inwards, to the inner wall, due to pressure gradient formed as the water rises near the outer wall.

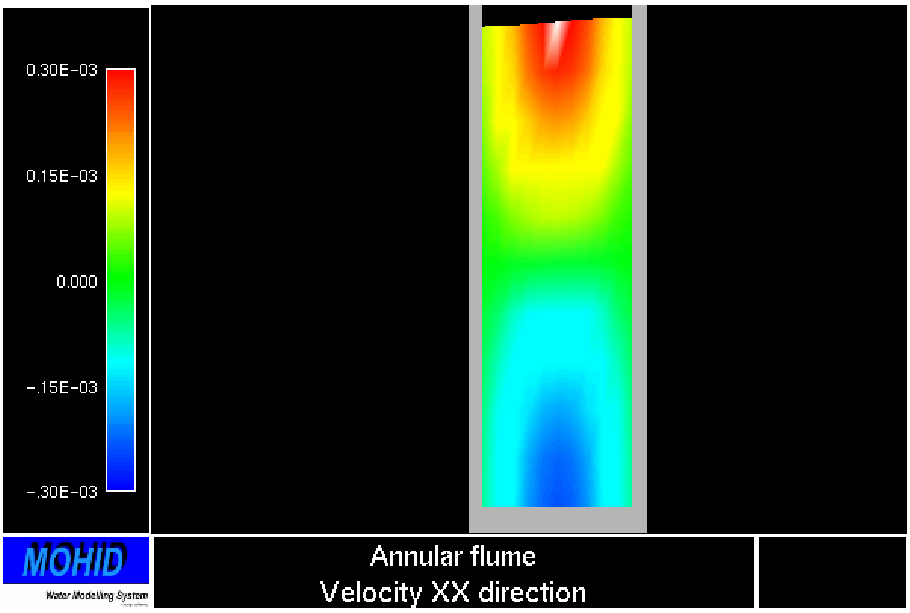

Figure 8 - Velocity XX direction (XZ cut)

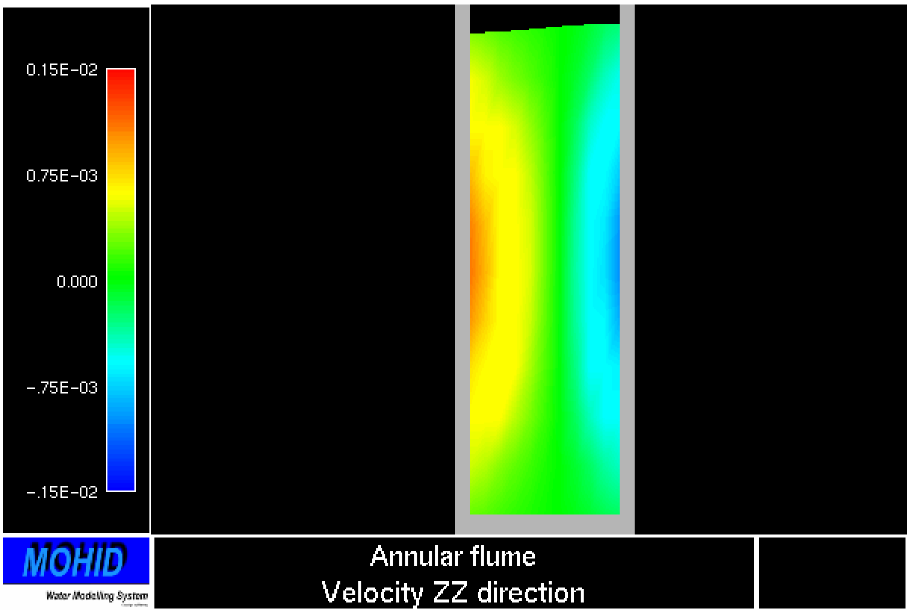

Figure 9 - Velocity ZZ direction (XZ cut)

In the vertical direction, near the outer wall the water flows downwards, due to pressure gradient, just referred above, which is compensated by an upwards flow near the inner wall.

Cohesive sediment transport simulations

The model was also applied to cohesive sediment transport in the flume. There were no need for any changes, being used all the formulation currently used in cohesive sediment transport in estuaries.

One standard simulation was performed, consisting of starting the hydrodynamics for a determined period, so that bed erosion by shear stress at the bottom boundary would be observed and afterwards stop the water flow, so that water velocity decreased to values where cohesive sediments were enabled to deposited.

Erosion

Initial conditions were considered to be null cohesive sediment concentration in the water column and a 1 kgsed/m^2 pool of sediment in the bottom boundary. Bottom shear stress values in steady state conditions reached 1.1 Pa, resulting in erosion of the deposited sediments to the water column, as it was considered a critical shear stress for erosion of 0.2 Pa. As shear stress maintains constant in steady state conditions, the sediment bed erosion rate is also constant, leading to a linear increase of the water column cohesive sediment concentration.

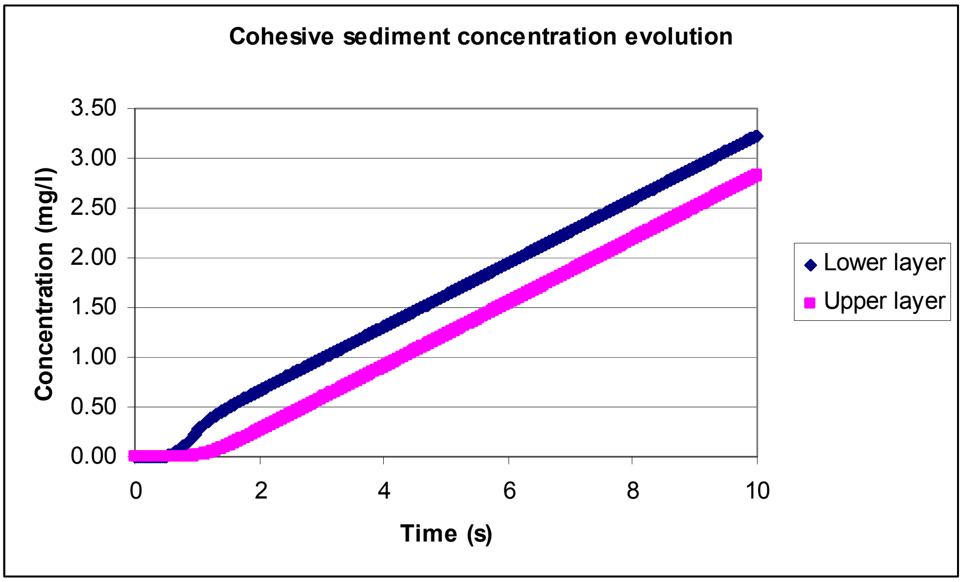

Figure 10 - Cohesive sediment concentration evolution (10 seconds simulation)

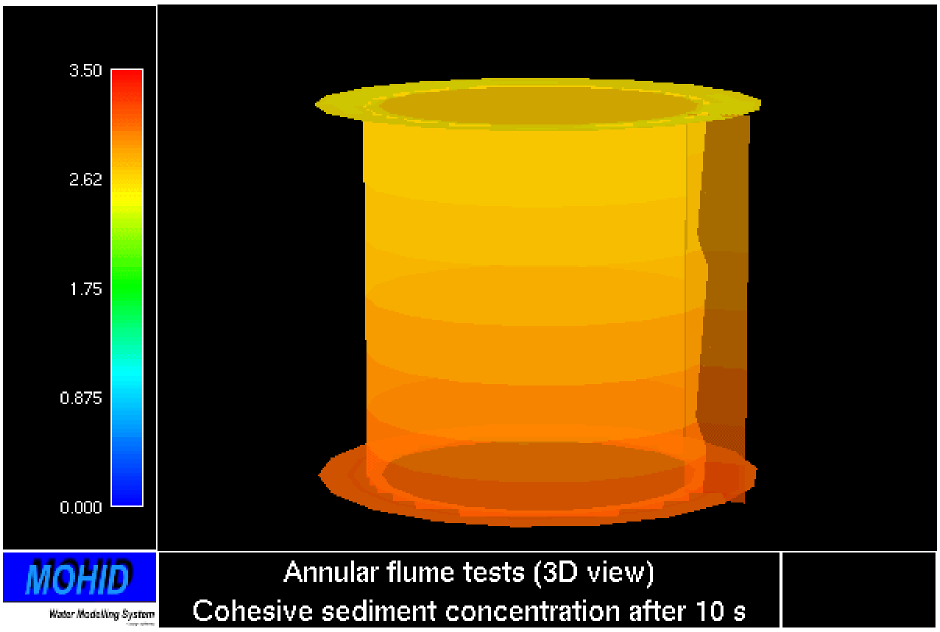

Figure 11 – Cohesive sediment concentration (mg/l) after 10 seconds of simulation with surface stress forcing

Deposition

After a 10 seconds period of bed erosion, surface stress was removed, leading water flow to eventually stop. Cohesive sediments deposition is observed.

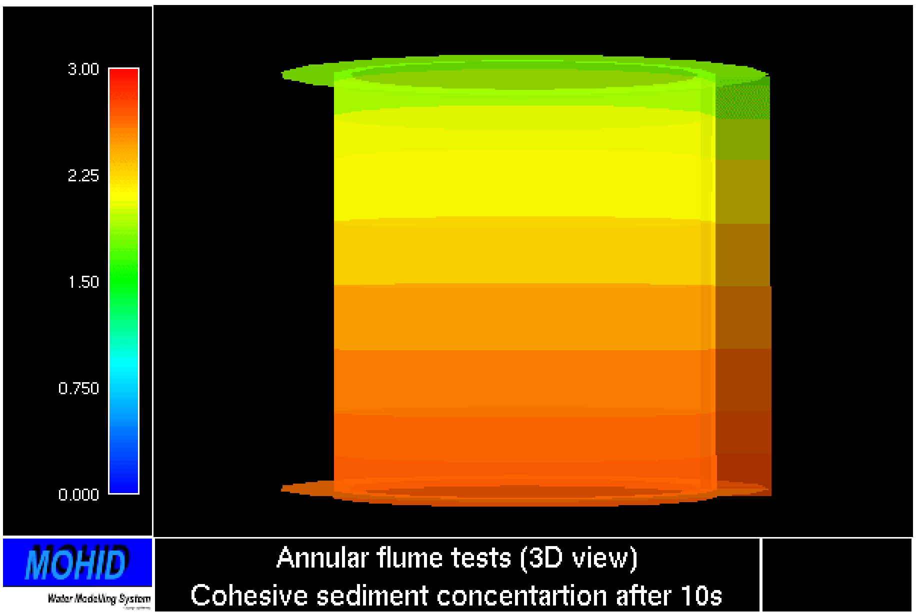

Figure 12 – Cohesive sediment concentration (mg/l) after 10s of simulation with no surface stress forcing

Main conclusions

The MOHID water modelling system is prepared to simulate water flow and cohesive sediment transport in an annular flume, therefore presenting to be an important numerical tool in this kind of studies.

Some basic results were presented and have shown to be satisfactory. Calibration of the model will be achieved with more experimental data, namely through water velocity measurements achieved with an ADV. Only then the cohesive sediment transport model can be calibrated, allowing then to simulate more accurately the sediment compartment, including the bioturbation effects.

Bibliographic references

Braunschweig, F (2001) – Generalização de um modelo de circulação costeira para albufeiras, MSc. Thesis, Instituto Superior Técnico, Technical University of Lisbon

Cancino, L. and R. Neves (1999) - Hydrodynamic and sediment suspension modelling in estuarine systems. Part II: Application to the Western Scheldt and Gironde estuaries, Journal of Marine Systems 22, 117-131

Leitão, P. C. (1996) – Modelo de Dispersão Lagrangeano Tridimensional. Ms. Sc. Thesis, Universidade Técnica de Lisboa, Instituto Superior Técnico

Neves, R., H. Coelho, P. Leitão, H. Martins, and A. Santos (1998) - A numerical investigation of the slope current along the western European margin. In: Burgano V.,

Martins, F. (1999) – Modelação Matemática Tridimensional de Escoamentos Costeiros e Estuarinos usando uma Abordagem de Coordenada Vertical Genérica. Ph. D, Thesis, Universidade Técnica de Lisboa, Instituto Superior Tecnico

Martins, F., P. Leitão, A. Silva and R. Neves (2000) - 3D modeling in the Sado estuary using a new generic vertical discretization approach, submitted to Oceanologica Acta

Montero, P., M. Gómez-Gesteira, J. J. Taboada, M. Ruiz-Villarreal., A. P. Santos, R. J. J. Neves, R. Prego and V. Pérez-Villar (1999) - On residual circulation of Vigo Ría using a 3D baroclinic model, Boletín Instituto Español de Oceanografía,„n o 15. SUPLEMENTO-1

Montero, P. (1999) - Estudio de la hidrodinámica de la Ría de Vigo mediante un modelo de volúmenes finitos (Study of the hydrodynamics of the Ría de Vigo by means of a finite volume model), Ph.D. Dissertation, Universidad de Santiago de Compostela, in Spanish

Pina, P. M. N (2001) – An Integrated Approach to Study the Tagus Estuary Water Quality. MSc Thesis, Universidade Técnica de Lisboa, Instituto Superior Técnico

Pérez-Villar, V. (1999) - ''Ordenación Integral del Espacio Maritimo-Terrestre de Gali-cia: Modelización informática'' (Integrated Management of the Galician Maritime-Terrestrial Space: Numerical Modelling). Final report by the Grupo de Física Non Lineal, Consellería de Pesca, Marisqueo e Acuicultura. Xunta de Galicia.

Santos, A. J. (1995) - Modelo Hidrodinâmico Tridimensional de Circulação Oceânica e Estuarina. Ph. D, Thesis, Universidade Técnica de Lisboa, Instituto Superior Técnico

Taboada J.J., R. Prego, M. Ruiz-Villarreal, P. Montero, M. Gómez-Gesteira, A. Santos and V. Pérez-Villar (1998) - Evaluation of the seasonal variations in the residual patterns in the Ría de Vigo (NWSpain) by means of a 3D baroclinic model, Estuarine Coastal and Shelf Science 47, pp. 661-670

Taboada, J.J., M. Ruíz-Villarreal, M. Gómez-Gesteira, P. Montero, A. P. Santos, V. Pérez-Villar and R. Prego (2000) - Estudio del transporte en la Ría de Pontevedra (NOEspaña) mediante un modelo 3D: Resultados preliminares, In: Estudos de Biogeoquímica na zona costeira ibérica,Eds. A.Da Costa, C. Vale and R. Prego, Servicio de Publicaciones da Universidade de Aveiro in press.

Taboada, J.J. (1999) - Aplicación de modelos numéricos al estudio de la hidrodinámica y del flujo de partículas en el Mar Mediterráneo (Application of numerical models for the study of hydro-dynamics and particle fluxes in the

Mediterranean Sea), Ph. D. Dissertation, Universidad de Santiago de Compostela. In Spanish

Villarreal, M.R., P. Montero, R. Prego, J.J. Taboada, P. Leitao, M. Gómez-Gesteira, M. de Castro and V. Pérez-Villar (2000) - Water Circulation in the Ria de Pontevedra under estuarine conditions using a 3d hydrodynamical model, submitted to Est. Coast. and Shelf Sc.