# II. The Tagus Estuary Pre-Operational Modelling System (MOHID Tagus Estuary)

## *II.1. Introduction*

Based on the modelling work of Leitão (2003), the Tagus Estuary Pre-Operational System (MOHID Tagus Estuary) was developed by Fernandes (2005) in the MARETEC research group[39], being in pre-operational stage since 2003.

Its main development motivation was to provide for the monitorization of the effect of pollution produced by the Guia wastewater discharge outfall operated by SANEST S.A. in the Tagus Estuary and adjacent ROFI area water and beaches quality.

It is composed by a forecast modelling tool, a measurement network and a set of tools for data transfer and processing. Additionally, there is a set of validation techniques used for the system assessment (Fernandes, 2005). The modelling tool is composed of a numerical model integrating hydrodynamics and water quality[40] and by an atmospheric model providing atmospheric forcing for the hydrodynamic and water quality model. The modelling, some measurements acquisition and data transfer and processing operations are processed in a nearly full automated way. The human intervention is concentrated in some measurement tasks, punctual in time, and the analysis and validation of measurement and modelling results.

In the next sections are presented the Tagus Estuary and the main components of the system which are relevant for this thesis work: forecast modelling tool, measurement network and validation techniques[41]. In the end of the chapter are presented deficiencies of the system, which motivated the work of this thesis.

[39] The MARETEC – Marine and Environmental Technology Research Center is a research center incorporated in the Instituto Superior Técnico, Technical University of Lisbon, created by Ramiro Neves.
[40] The model is operated, in an automated way in the MOHID Tagus Estuary case, using the graphic interface MOHID GUI. This application allows the manipulation of the files and directories required for MOHID Water simulations, the execution of these simulations and visualization of its results (Fernandes, 2005).
[41] The data management, storage and publication tools are presented by Fernandes (2005).

# *II.2. The Tagus Estuary*

## II.2.1. Characterization

The Tagus Estuary, presented in Figure II-1, is the transition area between the Tagus River and the Atlantic Ocean, being classified as inundated valley type (Martins, 1999).

With an area of 370 $Km^2$ in the high tide maximum and 265 $Km^2$ in the low tide minimum, it is one of the larger European estuaries and the larger wet area of the Portuguese territory, with about 1/3 of the surface (116 $Km^2$) being intertidal areas[42] (Fernandes, 2005).

Its width ranges from 2 to 14 Km (typically 10-14 Km) and the average depth is 10 m. Longitudinally, it spans for about 80 Km from its superior limit (near Muge) to the mouth (near S. Julião da Barra – Bugio)[43] (Martins, 1999; Fernandes, 2005).

Due to its morphological features, the Tagus Estuary can be understood as being composed of three distinct parts, each associated with distinct land use areas (Martins, 1999; Fernandes, 2005):

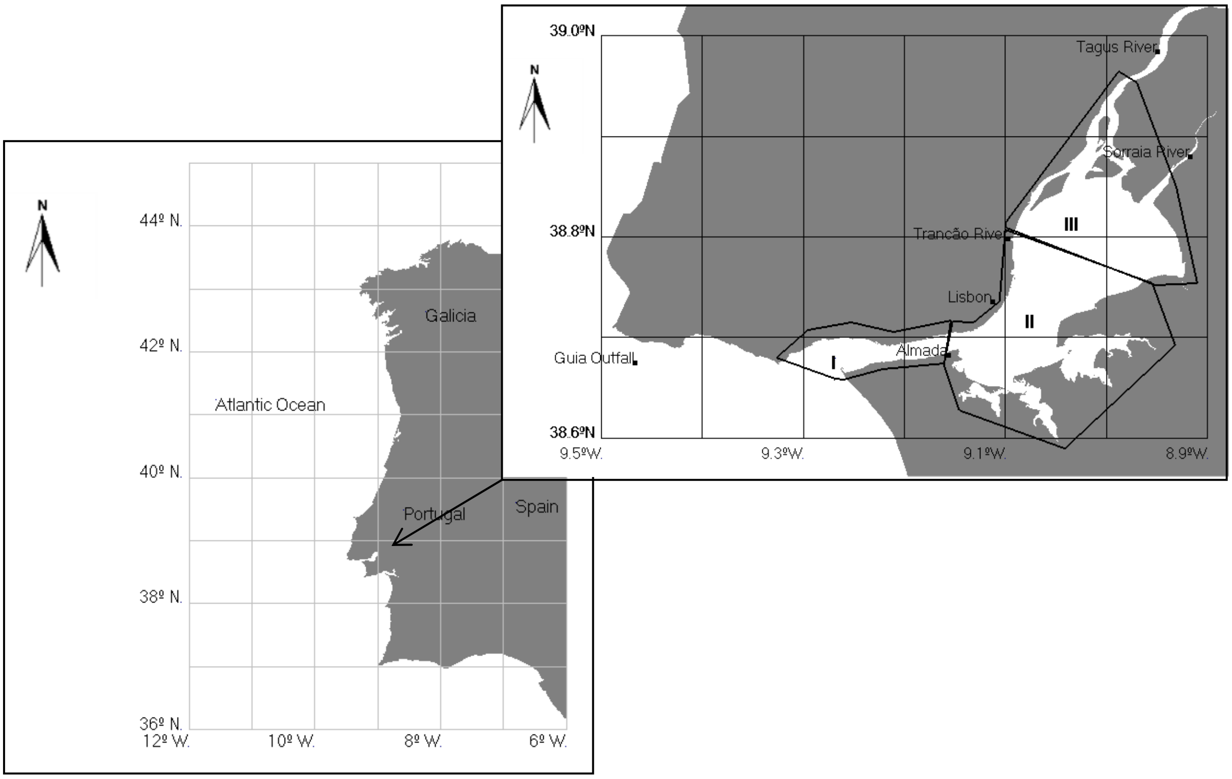
- the upper section (*troço superior*): a small depth area[44] comprising an inner delta and large marshland and tide spanning areas, directly influenced by the Tagus River flow; it comprises almost all of the Natural Reserve of the Tagus Estuary area, which has a large biological richness associated; it is the most important nursery area of the estuary for both fish and bird species[45];

- the central section (*troço central*): the one with the largest width, has average depth of 7 m, two main longitudinal channels and receives the input of rivers other than Tagus and streams and has in its margins most of the industrial facilities that surround the estuary; ship navigation in this area is intense with the existence of several navigation channels implying frequent dredging operations (Fortunato *et al.*, 1999);

- the last section (*troço terminal*): composed by small width[46] and large depth[47] channel, receives in its margins the cities of Lisbon and Almada; the end part is a mouth where the marine water is present.

[42] These are non-vegetated areas, old oyster farming facilities, sand banks and large marshlands (*sapais*) (Fernandes, 2005).
[43] Brackish waters are present till Vila Franca de Xira (50 Km from the mouth), the limit of the estuary according to Lemos (1972), and oceanic tides are still expressive in Muge, 80 Km from the mouth (Martins, 1999).
[44] Not more than 5 m in the deepest channels.
[45] Several fish species caught for human consumption, such as sole and seabass, can be found nursing there (Costa and Cabral, 1999). The estuary also shelters annually about 100 000 wintering birds (Martins, 1999).
[46] About 2 km wide.

**Figure II-1: The Tagus Estuary and its location in the Western Iberia Peninsula coast. The three areas of the estuary, according with Martins (1999) are shown: I – lower section, II – middle section and III – upper section. The main rivers, the cities of Lisbon and Almada and the Guia Outfall are also shown.**




In terms of hydrodynamics, the astronomic tide effect is very important inside the estuary and adjacent coast.

Both inside the estuary and the coast the dominant tidal period is half-diurnal ($M_2$ tidal component), with maximum tide amplitude of 2 m during spring tides, which induces currents of about 0.05 m/s in the Estremadura Promontory just north of the estuary[48].

Inside the estuary, the average volume involved in tide is significant relative to the water volume bellow the minimum tide water level. The maximum tide amplitude is about 2 m (spring tides) and the minimum value is near 1m (neap tides), being dominated by the flow heading for the ocean. At low tide time about 40% of the estuary area is emerged; the submerged area ranges from 30000 ha in neap tides and 34000 ha in spring tides (Fernandes, 2005). The high volume change induced by the tide and the small width of the last section of the estuary explain the large currents and bathymetry depth verified in this area (Martins, 1999).

[47] About 30 m deep.
[48] Diurnal tidal components are weak except in the Estremadura Promontory, where they induce currents with magnitude comparable to the $M_2$ ones.

The Tagus River flow influence on estuary hydrodynamics is not significant, except in flood times (Martins, 1999). Waves in the estuary are generated locally by the wind shear stress (Freire and Andrade, 1999).

The dominant fresh water source is the Tagus River[49]. The average flow is 600 $m^3/s$ (Fernandes, 2005) but with a large monthly variation and large peaks at flood times[50]. Other contributions, although much smaller, come from the Trancão and Sorraia rivers (Fernandes, 2005). The Tagus River induces a large variation of salinity in the estuary (Martins, 1999): in the upper section high horizontal density gradients[51] are observed, while in the other sections the salinity rapidly approaches oceanic values. The vertical density structure is homogeneous in the central and last sections[52] and, depending on the river flow and the spring-neap tidal cycle, between partially mixed and homogeneous in the upper section.

In what refers to biogeochemical conditions, the Tagus Estuary has high biological productivity, supporting profitable fishing activity (Baeta *et al.*, 2005). However, due to its extreme fluctuations of abiotic factors, namely salinity, temperature, currents and turbidity, the alternance of immersion and emersion periods associated with tidal motion and a large sediment mobility, it presents a harsh physical and chemical environment for animal and plant species, a heterogenic distribution of habitats, conditioning the diversity of estuarine life (Fernandes, 2005).

Just outside the estuary is a ROFI zone, where is located the outfall of the Waste Water Treatment Plant of Saneamento da Costa do Estoril S.A., at Guia (Fernandes, 2005). Leitão (2003) characterizes this area as having strong mixing and hydrodynamics: the main forcing factors are the wind and the tide[53]. The wind effect is processed at large scale, through the production of currents along the coast, and locally, by inducing vertical mixture. That vertical mixture is conditioned by the stratification conditions. Gama *et al.* (1994) analysis of a two year period of tide gauge measurements indicate important storm surge episodes frequency at the estuary mouth, observable in records for Cascais and Lisboa tide gauges. These episodes have a reported important influence on coastal degradation in Costa da Caparica (Ferreira, 2004), located at the immediate south coat of Tagus Estuary mouth.

[49] With spring in Serra de Albarracin, Spain, 1060 Km long, is one of the largest rivers in the Iberian Peninsula, inputting the Atlantic Ocean near Lisbon. Its watershed basin has an area of 80 500 $km^2$ approximately, with about a third in Portuguese territory (Fernandes, 2005).

[50] The flow depends of the year season, ranging from 30 $m^3/s$ in the dry season (summer) and 2000 $m^3/s$ at flood times (Martins, 1999), inter-annual changes and the regularization processes operated by the Spanish authorities. The fresh water residence time is variable: 65 days for a 100 $m^3/s$ discharge and 6 days for a 2200 $m^3/s$ discharge (Fernandes, 2005).

[51] Average salinity concentration ranges from null at Vila Franca de Xira to 27 p.s.u. in Sacavém-Alcochete (Martins, 1999).

[52] This happens because of high vertical mixing caused by the large velocities facing relatively small depth and small river flow (Martins, 1999).

[53] The density gradient caused by relatively fresh water discharges from the estuary is reportedly small in this area as stated by Martins (1999).

Fanjul *et al.* (1998) indicate the large scale atmospheric pressure as the main driver of storm surge events in the Iberian coast due to the relative small width of the Iberian continental shelf.

The currents patterns in this region along the year verify a constant residual current and overall current typically variable according to the year season (Haynes *et al.*, 1993; Coelho *et al.*, 2002; Leitão, 2003; Peliz *et al.*, 2005).

The residual current has a magnitude of 0.1 m/s and directed poleward (Coelho *et al.*, 2002; Peliz *et al.*, 2005)[54], of which about 0.02 m/s is due to the barotropic effect of tide, transporting to the ocean the fresh water plume coming from the estuary. This current is fed by the slope current (*corrente de vertente*)[55] and occasionally, by the wind[56]. The wind effect on this residual current is highly dependent on the land topography north of the Estoril Coast (mainly by the Sintra Mountain): when the wind blows from the quadrant between North and North-West the topography attenuates the wind effect (Fernandes, 2005).

The overall current in the ROFI is generally variable, as said, with the year season, strongly conditioned by the wind and precipitation conditions. In the winter, the Portuguese rain season, the high fresh water discharges cause in the ROFI a strong current in all water column directed poleward. This is usually fed by tide and by wind blowing from the South, which is generally associated to high precipitation. In the summer, the wind direction is more stable, blowing from the North/North West direction[57]. These wind conditions generate an equatorward flow on the continental shelf and slope, allowing for the occurrence of upwelling of cold water in the coast[58], which adds to the exchanges of water with the estuary in influencing the density gradients in the ROFI (Martins, 1999; Fernandes, 2005). Upwelling is classified by Coelho (2002) as the hydrodynamic process occurring in the continental Iberian margin which is more relevant for biochemical conditions.

North to this ROFI zone is located the Nazaré Canyon[59], a place where internal tide energy is generated and trapped, enhancing the local turbulence and mixing power of hydrodynamics and affecting the sediments transport along the continental shelf and slope regions.

[54] This is the dominant current in the depth range from 200-300 m to 1500 m.

[55] Documented by e.g. Ambar *et al.* (1986), Frouin *et al.* (1990) and Haynes and Barton (1990).

[56] According with wind direction.

[57] A succinct discussion of these wind conditions in the context of the general North Atlantic atmospheric circulation can be found in Coelho (2002).

[58] This is particularly noticeable in the area between 38º 30’ N and 39º 30’ N according to Coelho (2002).

[59] A 227 Km long *gouf* like structure (Vanney and Mougenot, 1990; Gomes, 2001-2002).

### II.2.2. Water quality problems

The Tagus Estuary is in direct contact with a population of about 2 million people, mainly concentrated in the city of Lisbon. Additionally, as pointed before, it is surrounded by several industrial facilities, belonging to diverse industrial sectors such as chemistry, concrete and oil refining (Martins, 1999). The estuary waters constitute the main destination of the domestic and industrial effluents thus produced[60], which are object of several degrees of water treatment. The industrial pollution has been connected to heavy metal presence in sediments and fauna in the estuary salt marshes (França *et al.*, 2005).

The current pollution loads seem not, however, by themselves to pose a main water quality problem, which has been explained by the strong hydrodynamics of the estuary associated with tide influence (Câmara *et al.*, 1987; Portela, 1996) and the small residence time near the north margin, where most effluents are discharged (Antunes, 1999). Similarly, and considering the work of INAG and MARETEC (2002), the main limiting factor for primary production in the Tagus Estuary is turbidity and not nutrient availability, making it a key element in the regulation of the biological production and water quality.

Being a ROFI zone, the water quality in Guia outfall area is very much conditioned not only by the outfall discharge but also by the water quality of the fresh water out flow from the estuary (Silva *et al.*, 2004; Fernandes, 2005).

Harmful algal blooms have been reported or derived toxins have been detected at levels sufficient to impact human and the environment health in the Portuguese continental coast (Van Dolah, 2000).

## *II.3. Forecast Modelling Tool*

### II.3.1. Hydrodynamic and water quality model (MOHID Water)

MOHID Water (Santos, 1995; Martins, 1999; Leitão, 2003) is a numerical tool[61] for modelling water hydrodynamics, dispersion phenomena (using a lagrangean and eulerian approach), wave propagation, sediment transport, water quality and biogeochemical processes within the water column and

[60] Most of the industrial effluents are discharged directly to the estuary (Caçador *et al.*, 1996).
[61] It is programmed in ANSI Fortran 95. According with Fernandes (2005) the use of this programming language ensures that the model can be executed and its code edited in any operating system (e.g. Windows, Linux, Unix) and environment.

exchanges with the water bottom, originally developed by Santos (1995) in MARETEC, Instituto Superior Técnico[62].

The different processes simulated are dealt within several modules, integrated in an efficient way. The modular organization of MOHID Water, supported by an object-oriented programming philosophy (Decyk *et al*., 1997)[63], allows the simulation of physical and biogeochemical processes using the same calculus grid and the integration of different time and space scales, through the use of one-way nesting (e.g. Leitão, 2003)[64], while assuring a robust use and model expansion (Miranda *et al.*, 2000). Additionally, it allows the simulation of different domains in parallel, communicating in MPI (Message Passing Interface) protocol, reducing significantly the calculation time.

Together, these features contribute to make MOHID Water a good tool for use in complex coastal and estuarine applications, with different process simulation requirements associated with different spatial areas. This is confirmed by the fact that, in its different versions, this model has been applied in very diverse applications for estuarine circulation, eutrofization and residence time studies (Cancino and Neves, 1998; Martins, 1999; Ruiz-Villarreal *et al.*, 2002; Braunschweig *et al.*, 2003; Vaz *et al.*, 2007)

Its architecture in terms of processes simulated can be understood as being composed of four main modules[65]:

- Hydrodynamic Module: managing the non turbulent flow properties, such as water level, velocity, water fluxes, in a eulerian referential;

- Turbulence Module: managing the turbulent flow properties, such as viscosities, diffusivities, turbulent kinetic energy, in a eulerian referential;

- WaterProperties Module: managing the processes governing water properties, such as salinity, density and temperature, evolution in a eulerian referential;

- Lagrangean Module: managing the processes governing water properties evolution in a lagrangean referential.

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[62] However the model foundations can be traced back in time with the seminal modelling work of Neves (1985).
[63] According with the work of Decyk *et al.* (1997) the object-oriented philosophy has proven very useful in the development of complex software, especially those having as objective the simulation of "real world" applications, as is the case of marine and estuarine processes. Although Fortran 95 language is not a object oriented language (OOL) *per se*, the Fortran modules can work as classes of a OOL and objects derived from classes, communicating between then in a client/server base, as explained by Fernandes (2005).
[64] As an example of model versatility it is referred that the number of nested domains is only limited by the available calculus capacity (Fernandes, 2005).
[65] In this classification are presented the modules names as in the Version 4 of MOHID Water. The MOHID Tagus Estuary version presented in this chapter and developed by Fernandes (2005) is based in Version 3 of MOHID Water and the modules names are not the same. As the type of processes involved in each module are maintained from Version 3 to Version 4 the last version module names are used in this text for simplicity.

Due to their relevance for the present thesis work the three first modules are described in more detail in the following sections[66].

### II.3.1.1. Hydrodynamic Module

It consists in a 3D baroclinic model which solves primitive equations for incompressible flows in orthogonal horizontal coordinates.

The space discretization of these equations is performed using the finite volume technique[67], allowing the application of the model in areas with diverse geometries and horizontal spatial resolutions[68], and the easy expansion to eventually more adequate coordinate systems (Fernandes, 2005). The geometries supported by MOHID Water include the sigma, cartesian and fixed depth. Several options are available for the discretization of the advection term, which include the centered differences, upwind and TVD schemes.

The time discretization, based in a Reynolds type decomposition[69], is half-implicit (*semi implícita*) of ADI (Alternate Direction Implicit) type (Neves, 1985; Martins, 1999)[70]. Two variants of this discretization are implemented:

- the S21 scheme (Abbott *et al.*, 1973): most adequate to large water depths due to the smaller computational cost and lower incidence of areas with non permanent water coverage (e.g. because of tide) which are not so well described (Martins, 1999)[71];

[66] The ecological and biogeochemical part of MOHID Water, dealing with ecological and water quality processes, is a relevant part of MOHID Tagus Estuary but falls beyond the scope of this thesis and will not be considered here. Information on this issue can be found in the work of Miranda (1999), Pina (2001) and Mateus (2006), with a good introduction being provided by Fernandes (2005).

[67] This technique consists in applying directly to a control volume the laws governing the simulated processes (physical, biochemical, etc.) in the form of a flux divergence. It is used to allow the use of a generic vertical coordinate system, as explained by Martins (1999) and Coelho (2002), and allows for the simulated properties mass conservation (Adcroft *et al.*, 1997).

[68] This versatility is due, as explained by Fernandes (2005), to the fact that the geometry is introduced in the model explicitly, through the areas and volumes of each cell.

[69] This decomposition acts as a time filter where the instantaneous values of hydrodynamic properties are substituted by average quantities and turbulent fluctuations.

[70] This discretization has effect for resolution of the momentum and continuity equations of hydrodynamics: in each iteration one of the horizontal components of momentum is calculated with barotropic term implicit and the other component of momentum with this term explicit, in next iteration the components considered implicitly and explicitly are inverted. The vertical transport terms are calculated implicitly (Martins, 1999).

[71] In this scheme in each time step are solved four algebraic equations, two for each half time step: in the first step is calculated the water level and one of the horizontal components of velocity implicitly and the other velocity component is considered as the one resulting from the previous half time step; in the second is calculated the water level and the velocity component which is calculated implicitly and the one considered from the previous step changes. The vertical velocity is calculated in each half time step based on the new water level.

- the Leendertse scheme (Leendertse, 1967): higher computational cost but better description of non permanent water coverage (Martins, 1999).

This ADI discretization has as effect that only barotropic pressure, bottom shear stress and vertical diffusion, the terms that introduce in the equations of motion more stability problems, are discretized implicitly. The others are discretized using the explicit approach[72].

The model considers vertical and horizontal boundary conditions. The vertical boundary conditions, expressing the effect of viscous tangential forces, can be defined at the water column bottom, using a formulation expressing the shear stress as the product of the Chezy coefficient and the water velocity square, and at surface, considering the shear stress as the shear stress derived from wind[73].

The model allows the use of open or closed horizontal boundary conditions. The open boundary conditions can be of imposed value, radiation[74] or a mix between these two types. Tide forcing is interpolated by the model for the boundary based on tidal components files containing the amplitude and phase of tidal harmonic components and time series of average water level at specific locations near the model domain boundary (tidal points). The closed boundaries are dealt with a slipping or no slipping condition and can have mobile location[75] (Fernandes, 2005).

The approximations considered in the model to simplify the calculus are:

- Coriolis force: account of the Earth rotation effect over flow through the inertial force due to Coriolis effect;

- Boussinesq approximation: density is considered constant for mass and inertial forces calculation, excepting for forces which are derived from the gravity acceleration[76];

- Hydrostatic approximation: vertical pressure gradient is assumed in equilibrium with gravity force, being the pressure determined only by depth and density vertical gradient[77];

72 The system of equations created by the discretization is solved easily by the Thomas algorithm (Fernandes, 2005).
73 The wind shear stress can be calculated by the model based on the wind velocity and direction or imposed directly as forcing.
74 Radiation condition is defined considering several options of local solution to account for nesting applications (Flather, 1976), tide (Blumberg and Khanta, 1985) and waves.
75 Mobile closed boundaries are considered to model intertidal areas.
76 This is concurrent with the fact that in ocean and coastal flows the water density variations are small (less than 3% according with Coelho, 2002).
77 In the ocean and coastal areas the vertical velocities are small, because of the vertical scales of velocity but also due to vertical stratification, which tends to inhibit vertical movements through impulsion, the small vertical accelerations and viscous forces (Coelho, 2002).

- Pressure term divided into barotropic and baroclinic components[78].

### II.3.1.2. Turbulence Module

The Turbulence Module controls the terms not derived from average hydrodynamic properties (Reynold tensors)[79], assuming the Reynolds decomposition used in Hydrodynamic Module to solve equations.

The general approach for the calculation of this turbulent term used in the module is to assume that it is proportional to the spatial gradient of the average property which is transported, using a constant turbulent viscosity, defined for the horizontal and vertical directions[80]. This turbulent viscosity is assumed defined mostly based on the horizontal and vertical resolutions considered in each specific model application[81] .

In 3D applications the vertical turbulence term can be parameterized using the turbulence module of model GOTM (General Turbulence Ocean Model)[82], incorporated in MOHID Water in the GOTM Module, which provides turbulent viscosities from the average flow properties.

### II.3.1.3. WaterProperties Module

This module calculates the water properties evolution, including salinity and temperature, through the general advection-diffusion equation. The calculation of advective and diffusion terms, horizontal and vertical, can be solved explicitly or implicitly. As in the Hydrodynamic Module, several discretization schemes are available for the advection term, which include the centered differences, upwind and TVD schemes.

Density is calculated based on the state equation for salinity and temperature from UNESCO (1981).

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78 The first component accounts for the effect of the water surface slope over pressure and the second component accounts the effect of the density gradient. The advantage of this approximation is that the water surface elevation can be used to calculate the control volume and also to estimate the barotropic pressure (Coelho, 2002).

79 These terms represent the contribution of the turbulent transport to the average field.

80 The unique value used for horizontal turbulent viscosity in all horizontal spatial directions is supported by the fact that in horizontal space the processes are normally homogeneous with direction, as explained by Fernandes (2005).

81 This dependence on resolution is explained by Fernandes (2005) as due to the resolution scales usually considered in MOHID Water applications, in the order of meters, which is several orders of magnitude larger than the molecular viscosity.

82 For applications and theory of the turbulence module of model GOTM please refer to the Internet site http://www.gotm.net.

The processes influencing the temperature and salinity comprise the effects of transport due flow from point discharges and surface fluxes, i.e., those related to solar radiation, infrared radiation, latent and sensible heat, in the case of temperature, and evaporation and precipitation, in the case of salinity.

Fine sediment processes are modeled based in the WaterProperties Module's approach and using specific formulations for falling velocity exchanges with the bottom and flocculation[83].

## II.3.2. Atmospheric model (MM5)

The MM5 (Meteorological Model 5) is a mesoscale non-hidrostatic meteorologic model, which solves the 3D Navier-Stokes equations, the thermodynamic equation and the water conservation equation in sigma coordinate system (Dudhia et *al.*, 2004), originally developed by the Pensylvania State University and the Nacional Center for Atmospheric Research in the late 1970 decade years but suffering several improvements since then.

The MM5 application used in MOHID Tagus Estuary is an operational model (since 2002) forecasting for the Portuguese coast[84], operated by the Environment and Energy Section coordinated by J.J. Delgado Domingos of the Mechanical Department of Instituto Superior Técnico (Sousa, 2002), providing daily forecasts for the continental Portuguese territory.

This model uses Internet based information and is composed of several domains, connected through the nested modeling approach, exchanging information in two-way mode. The smaller domain, higher resolution domain, has a horizontal grid composed of 70x43 cells, a time step of 27 seconds and a horizontal spatial step of 9 Km. Forecasts are obtained for the 72 hours following the beginning of simulation, which happens four times a day at 0, 6, 12 and 18h CET.

No data assimilation is used in this model.

[83] Flocculation and erosion/sedimentation processes are modelled using empirical formations (Fernandes, 2005).
[84] Forecasts are published in the Internet site http://meteo.ist.utl.pt.

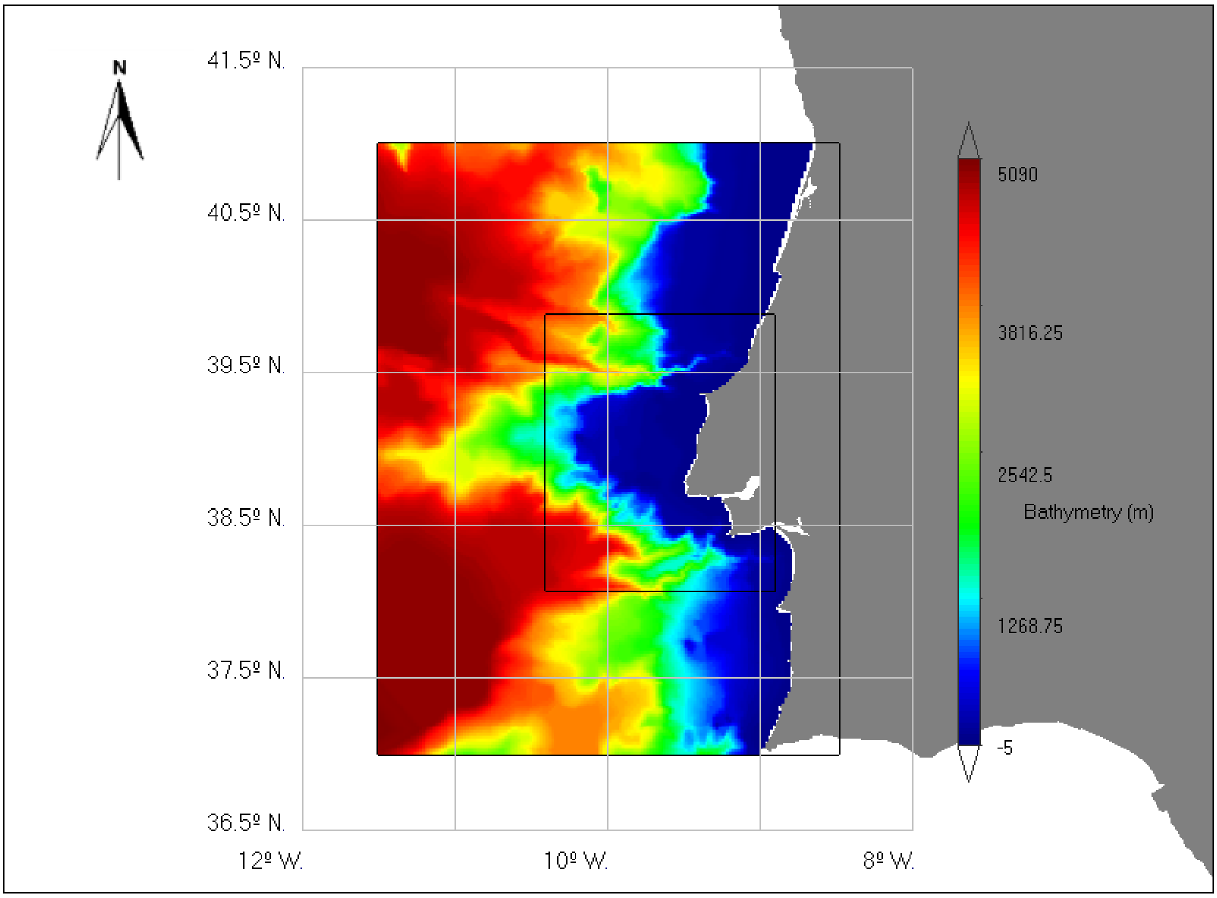
### II.3.3. Present configuration

Based on the modelling components presented in the previous sections, MOHID Water is used in MOHID Tagus Estuary to (Fernandes, 2005):

- simulate coastal circulation, hydrodynamics and biogeochemical conditions, in order to monitor the water quality in the Estoril coast and the nutrient and primary production dynamics in the Tagus Estuary;
- simulate, in an integrate way, the pollutant dispersion in the near and far field of the Guia wastewater outfall, assessing its impact in the water quality of the ROFI area, mainly due to bacteriologic contamination.

The forecast needs are diverse, which explains that the configuration architecture follows the approach of nested modeling, using three domains, as presented in Figure II-2 and Figure II-3 and in Table II-1.

**Figure II-2: Bathymetry of domain 1 of MOHID Tagus Estuary. Spatial area of domain 2 is shown inside smaller black rectangle.**



The domain 1 (Figure II-2) was developed to provide the open boundary conditions for the second nested domain. It is a regional domain simulating the barotropic tidal propagation and wind stress effects: is forced by the global tide solution FES 95.2 (Le Provost *et al.*, 1998) and wind, and has 2D resolution (Fernandes, 2005).

The domain 2 (Figure II-3 a) covering all the Tagus Estuary comprises two, 2D and 3D, domains. Both domains have surface boundary conditions and freshwater discharge characterization intended to support an adequate modeling of temperature and salinity evolution. The discharge values used have, however, different quality: while Tagus river discharges are obtained from Ómnias automated hydrometric station real time water level measurements (see section II.4. for details)[85], Sorraia river discharges are daily averages and the remaining discharges represent several years annual averages (Fernandes, 2005). The temperature and salinity evolution is required in both models for distinct purposes:

- 2D domain: intends to simulate the hydrodynamics and biogeochemical processes in the estuary; as the tide is the dominant forcing in the estuary, it has shallow depths and is well mixed in the vertical direction for most of its extension (as shown in Chapter I) a 3D vertical discretization is not a requirement;

- 3D domain: intends to supply adequate hydrodynamic boundary conditions to domain 3; 3D discretization is here required because of the large depth at which is implanted the Guia outfall.

Domain 3 comprises local scale domains which are intended for the monitorization of the Guia submarine outfall impact on water quality, which must be operational (domain 3 – Guia, presented in Figure II-3 b), and study water quality problems near Estoril coast beaches (Carcavelos – Paço de Arcos), which is not required to run every day (Fernandes, 2005).

The atmospheric forcing of all domains is provided by a time series extracted from the higher resolution domain of MM5 model for a location near Guia station. Spatially variable atmospheric properties are not considered because of the poor resolution of the MM5 model domain relative to the Tagus Estuary dimension (Fernandes, 2005).

[85] This information is converted to water flow on a daily basis (Fernandes, 2005).

**Figure II-3: Bathymetry of domain 2 (a) and domain 3 – Guia (b) of MOHID Tagus Estuary. Interest sites comprised in the domains' area are shown.**

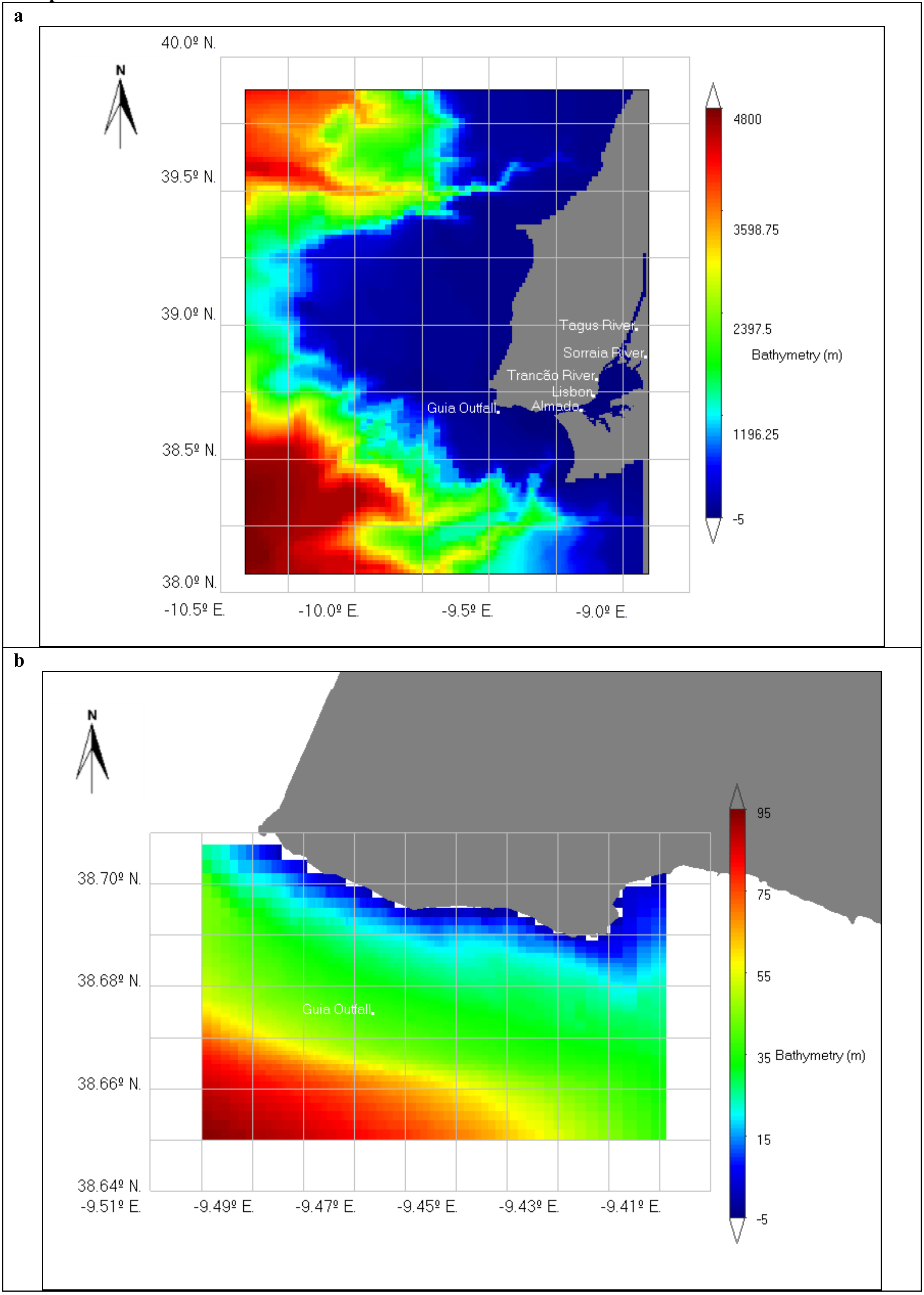


**Table II-1: Configuration of MOHID Tagus Estuary (adapted from Fernandes, 2005).**

| Domain | 1 | 2 | | 3 | |
|---|---|---|---|---|---|
| Location | Nazaré – Setúbal | Tagus | | Guia | Carcavelos – Paço de Arcos |
| Spatial span | -11.5ºE to -8.5ºE 37ºN to 41ºN | -10.5ºE to -8.8ºE 38ºN to 40ºN | | -9.5ºE to -9.4ºE 38.6ºN to 38.7ºN | - |
| Number of cells | 168 x 223 | 162 x 162 | | 100 x 60 | 301 x 105 |
| Minimum spatial step (m) | 2000 | 300 | | 35 | 10 |
| Time step (s) | 120 (double splitting) | 30 (double splitting) | 30 – hydrodynamic (double splitting) 60 – water quality | 15 (double splitting) | 7.5 (double splitting) |
| Vertical discretization | - | - | 11 layers (cartesian) | 11 layers (cartesian) | 11 layers (cartesian) |
| Processes modelled | Hydrodynamic | Hydrodynamic, Water Quality | Hydrodynamic | Hydrodynamic, initial dilution and dispersion of Guia outfall pollutant plume | Hydrodynamic |
| Flux | Barotropic | Barotropic | Baroclinic | Baroclinic | Baroclinic |
| Imposed tide | x | - | - | - | - |
| Advection spatial discretization scheme | Upwind order 1 | Upwind order 1 | Upwind order 1 | QUICK | QUICK |
| Discharges | - | Tagus, Sorraia, Trancão, WWTP | Tagus, Sorraia, Trancão, WWTP | Guia WWTP | - |
| Meteorological forcing | Wind | Wind, temperature, solar radiation, relative humidity, heat fluxes | Wind, temperature, solar radiation, relative humidity, heat fluxes | Wind, temperature, solar radiation, relative humidity, heat fluxes | Wind, temperature, solar radiation, relative humidity, heat fluxes |
| Bottom shear stress coefficient | 0.0025 | 0.0025 | 0.0025 | 0.0025 | - |
| Open boundary condition | Blumberg and Khantha (1985) radiation | Flather (1976) radiation (domain 1 providing reference water level and reference velocity), flow relaxation scheme for velocity to domain 1 solution (with decay times ranging from 900s in boundary to 7200000s inside) | Flather (1976) radiation (domain 1 providing reference water level and reference velocity), flow relaxation scheme for velocity to domain 1 solution (with decay times ranging from 900s in boundary to 7200000s inside) | Flather (1976) radiation (domain 2 providing reference water level and reference velocity), flow relaxation scheme for velocity to domain 2 solution (with decay times ranging from 30s in boundary to 7200000s inside) | - |
| Operation | Every day | Every day | Every day | Every day | When required |

The forecasts are made daily for the next 24 hours, with hourly graphic outputs, performing for the three-domain nested configuration simulated daily the calculus time of 6 hours without MOHID Water code parallelization and 4 hours with code parallelization use of the MPI protocol.

## *II.4. Measurement Network*

The main components of this network are the real time data acquisition systems and time discrete data acquisition through dedicated field campaigns[86].

The real time data acquisition systems aim at characterizing the most important forcing mechanisms of the study area which are not easily predicted[87], being composed by (Fernandes, 2005):

- a meteorological station, operated by the MARETEC team, located in the building of the Guia Wastewater Treatment Plan[88], measuring air temperature and humidity, atmospheric pressure, solar radiation, precipitation and wind direction and horizontal components of velocity;
- an automated hydrometric station[89], operated externally by INAG[90], measuring water level every 15 minutes at a Tagus River section in Ómnias.

The measurement network of MOHID Tagus Estuary included also for some time a buoy station for water quality monitorization, located in Paço de Arcos outside the last section of the Tagus Estuary[91], measuring water temperature, dissolved oxygen, conductivity/salinity, turbidity, depth, chlorophyll-a, horizontal component of velocity and direction of current (Fernandes, 2005). This system ceased to be operational due to anomalies in the data communication and storage device and logistic problems affecting the velocity measurements (for details see Fernandes, 2005).

The field measurement campaigns include:

- the water and sediment sampling for several water quality parameters, integrated in the Monitorization Program for the Estoril Coast developed for the main end-user of MOHID Tagus Estuary, SANEST S.A, and for the SimTejo Project;
- the sensor measurements for water quality, measured by a multiparametric sensor included in the MARETEC ship, acquiring at the same time of water and sediment campaigns;
- occasional mooring of ADCP devices in the sea floor, as happened in 2003.

[86] Remote sensing data acquisition is currently in operationalization stage (Fernandes, 2005).
[87] As presented in the Chapter I, tide is also an important forcing mechanism for local hydrodynamics but it is derived of well known and easily predicted astronomic forces.
[88] The location has geographic coordinates 38º 41' 41'' N and 9º 26' 48'' W, WGS84 (Fernandes, 2005).
[89] The location has geographic coordinates 39º 13' 05'' N and 8º 40' 05'' W, WGS84 (Fernandes, 2005).
[90] The measurements are posted in the Internet at http://snirh.inag.pt.
[91] The location had geographic coordinates 38º 40' 29'' N and 9º 17' 36'' W, WGS84 (Fernandes, 2005).

Although its use is not fully automated, the MOHID Tagus Estuary relies occasionally on remote sensed sea surface temperature (SST) and chlorophyll data for validation purposes and efforts are being made for making the access and processing to this type of data (mainly from the Seawifs, Meris and Modis sensors) more efficient[92].

[92] This is being pursued namely by the adaptation of existing MOHID Water support tools for the use of this kind of data.

## *II.5. Validation Techniques*

Operation validation of MOHID Tagus Estuary results consists in the graphic comparison of water level results of the 2D model domain 2 with tidal harmonic reconstruction water levels for 14 tidal gauge locations, mostly concentrated in the estuary and adjacent ROFI coast. The tidal components data for each location are based on water level measurements performed by Instituto Hidrográfico. These comparisons are generated and published in an automated way in the MOHID Tagus Estuary Internet site.

Non operational validation is performed, in a non automated way and with annual frequency, in the context of the estuary and ROFI water quality monitorization services provided by the MARETEC team to SANEST S.A., since the birth of MOHID Tagus Estuary, and for SIMTEJO, in the years from 2004 to 2006. In these studies, MOHID Tagus Estuary results are validated with campaign data (water sampling, ship sensor, ADCP) and remote sensed (SST, chlorophyll and suspended sediment) data. The types of comparison performed, focused on water quality parameters, are based on graphic comparison and eventually the calculation of general statistics such as averages and standard deviation. More advanced statistics, such as correlation coefficients and RMSE, are generally not calculated due to the low time frequency of measurement acquisition.

## *II.6. Knowledge Deficiencies*

Fernandes (2005) has performed the first assessment of the performance of the described MOHID Tagus Estuary configuration. Following are presented the main findings of this study.

The first phase of this assessment is a validation of the meteorological forecast provided by MM5 model for MOHID Tagus Estuary forcing relative to the Guia meteorological station measurements for the whole year of 2004. By relying mostly on the contrast between instantaneous model results and measurements this study concludes that:

- solar radiation evolution in MM5 model prediction is well characterized in the daily and annual cycles although in the summer the model overestimates its value;
- atmospheric pressure evolution is well represented in MM5 model;
- precipitation predictions by MM5 show the qualitative patterns present in measurements but also a large underestimation of quantitative values;
- wind predictions by the model although overall expressing the dynamics of measurements represent generally overestimations of the measured wind, which seem to be due to the fact that the MM5 resolution does not account for the specific effect of the Serra de Sintra topography in the local atmospheric dynamics;
- temperature daily evolution present in measurements is not reproduced by the model, which is explained by the fact that the model assumes a constant sea surface temperature as forcing and that the model result is in a sea location while the measurements are taken at a land location, where daily temperature amplitude is expected larger;
- relative humidity evolution predicted by the model show the same drawbacks of temperature prediction, which is explained with the correlations between relative humidity and temperature and between relative humidity and wind.

This author concludes that the meteorological forcing is validated but identifies as the two main meteorological model forcing deficiencies the fact that the spatial resolution of the grid does not allow for the small scale effects representation and the Sintra Mountain topographic feature and the use of a constant sea surface temperature in the meteorological forecast production.

The MOHID Tagus Estuary results are assessed in terms of hydrodynamics (water level, currents), temperature and salinity, microbiologic parameters (fecal coliforms) and biogeochemical parameter (cohesive sediments, chlorophyll, nitrates, dissolved oxygen) by comparing with measurement data (Fernandes, 2005).

In terms of water level model results, comparisons are made between model results and tide components reconstructed water level[93] in areas where the bathymetry is better described in base data and where the grid resolution is higher, as is the case of the Estoril coast, for a 45 days period. Inside the estuary the model bathymetry is less representative of real conditions[94] and the model results presents a lower concurrence with tidal reconstructed levels expressed by a generally negative bias, a relatively lower correlation coefficient[95] and larger RMSE. It is observed that a larger RMSE happens generally at locations where tide predictions have a greater variability. The author points that a higher resolution grid, possibly using a curvilinear type of grid, would benefit the water level results in these locations inside the estuary.

Model results for currents are contrasted with two measurement data sources: surface data acquired in the buoy in Paço de Arcos for two months in the summer of 2003 and the water column data acquired by the ADCP for one month in autumn of 2003. The buoy data is reportedly bad in situations of strong velocity but in situations of velocity bellow 1 m/s the concurrence in model and measurements in current direction and intensity seems high, with the inflow and outflow periods happening simultaneously in both model and measurements data. The comparison with the ADCP data[96] leads to the observation that the model reproduces adequately the instantaneous velocity measured for most of the water column and the average flow observed considering all water column. The residual velocities are also adequately reproduced, although the situation is variable through the water column with the correlation coefficient (averages of 0.49 and 0.42, respectively for the zonal and meridional current components) and RMSE (averages of 0.14 and 0.13, respectively for the zonal and meridional current components) degrading with depth, particularly for the meridional current component. The deficiencies of the model are linked with the poor vertical resolution of the domain grid, low resolution of the atmospheric model forcing, poor representability in the model for large scale processes and eventually an inadequate calibration of the bottom shear stress.

[93] 45 days of data for 16 locations are analysed and the model and tide reconstructed time series are object of harmonic analysis and reconstruction using T_Tide application (Pawlowicz *et al.,* 2002), to compare the water level resulting from similar effects (the forces expressed by the tidal components which can be characterized with 45 days of data).

[94] These are locations associated with lower depths and/or with underwater channels, but also where the horizontal grid resolution is smaller.

[95] All correlation coefficients are, however, above the 0.9 value.

[96] This data was previously interpolated for the layers used in MOHID Tagus Estuary domain 2 (Fernandes, 2005).

Relative to temperature and salinity, the comparison with surface, mid water column and bottom campaign measurements in the ROFI for the first semester of 2004 and with ROFI and adjacent coast MODIS SST data for spring 2004 and early 2005, concludes that the surface values in the ROFI are well characterized but not the water column stratification or the temperature surface values in offshore locations. This deficiency is connected with the lack of large scale forcing in the model.

As for microbiologic parameters, indicated by fecal coliforms concentration, the water column data comparison, performed for important locations in the ROFI zone near the Guia outfall for the year 2004, seems to indicate that the model represents well the time evolution trend detected by measurements, although the instantaneous values representation appears poor. The disparities are linked with the modeling options used in the version of MOHID Tagus Estuary operating through 2004, which were corrected in the 2005 version. In terms of biogeochemical parameters, the comparison with remote sensed suspended sediment data (MERIS), for a longitudinal section included in the estuary and in the ROFI zone in the spring, summer and autumn of 2004, show a good consistency between model and measurements. The comparison with campaign data for the year 2004[97] for the area near Guia outfall shows a good representabiliy of water column integrated values for chlorophyll-a and nitrates; ammonium nitrogen and dissolved oxygen figures show a poorer concurrence, which is linked to water quality processes not simulated in MOHID Tagus Estuary and the 2D discretization of the model.

Overall, Fernandes (2005) suggests a set of improvements to the MOHID Tagus Estuary configuration implemented which can be classified in the following points:

1. Improve the large scale phenomena description, both in terms of currents and of stratification.
2. Study the effect of meteorological forcing, especially wind conditions, and possibly improve the spatial resolution of meteorological model.
3. Increase grid resolution or use data assimilation inside the estuary to improve water level forecasts.
4. Improve the vertical grid resolution in the ROFI zone to improve stratification reproduction.
5. Use an advanced water quality modeling tool, such as the one implemented in MOHID Water by Mateus (2006).

[97] The exception is chrolophyll, for which data are available only for the first semester of 2004 (Fernandes, 2005).

6. Improve the measurement network, for validation and data assimilation purposes, namely by increasing the acquisition of coastal data and using spatially more continuous acquisition methods[98].

[98] This is already being partially dealt with the multiparametric sensor operating in campaigns using MARETEC ship.