AN INTEGRATION METHODOLOGY TO ESTIMATE WATER FLUXES AND CONSTITUENTS BUDGETS IN COASTAL AREAS: APPLICATION TO THE TAGUS COASTAL AREA

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CHAPTER SYNOPSIS

Background
Coastal models use fine vertical and horizontal grids for accuracy and, consequently, the output files contain large volumes of information. The interpretation analysis effort of these data is simplified if integration tools are employed. This is particularly important for long simulation periods. This chapter describes the strategy followed in the case of Tagus Estuary mouth, where a three dimensional (3D) operational model is used to simulate the flow generated by the tide, the density currents and the atmospheric forcing, and the biogeochemical processes controlled mostly by vertical transport and by the Tagus Estuary discharge.

Results
The hydrodynamic model was validated using tidal data collected at the mouth and inner estuary. Instantaneous results of the biogeochemical model in the vicinity of the outfall were validated using field data from the submarine outfall monitoring program. Fluxes were temporally and spatially integrated using three layers of five boxes. Results are presented for two contrasting situations, respectively during upwelling and downwelling conditions. Results show that in both scenarios the tidal flow associated to the estuary flood/ebb dynamics dominates the transport processes in the Tagus inlet vicinity and that the effect of the wind and global circulation role increase as one moves of the inlet.

Conclusions
With this methodology integration boxes may show the influence of systems with different hydrodynamic and biogeochemical properties (river, estuary, mouth, coastal area) to the circulation/property patterns of a particular area. The spatial and temporal versatility of boxes in MOHID implementation allows also differentiating periods in which each of the forcing actors are more significant. The use of integration boxes with vertical discretization of the water column also reproduced the effect of upwelling or downwelling, typical of this coastal area.

1 INTRODUCTION

Climatological data or monitoring campaigns allow instantaneous characterization and describe the main trends of coastal systems. However, this is insufficient to understand the processes that determine the spatial and temporal patterns. Thus, model results can provide continuous information about the system status and aid in the interpretation of observed data values.

The hydrodynamic of coastal areas influences the biogeochemical processes and determines the fate of both incoming constituents to that area and of materials produced locally. Since the velocity fields provided by these models presents a great spatial and temporal variability, which renders the hydrodynamic characterization and analyses difficult, most of the times their integration (residual circulation) provides significant information. In this context, mathematical models are essential tools for a spatial and temporal integrated characterization. The use of integration boxes with vertical discretization of the water column also reproduces the effect of upwelling or downwelling, typical of this coastal area. A way to obtain results for areas that have distinct hydrodynamic and ecological patterns is to consider each zone as individual volumes, but nevertheless allowing the interaction between them. MOHID model allows such approach, making possible to set a number of boxes with variable shapes and sizes in function of the objectives.

Recently modelling approaches and integration boxes have been used to describe the fluxes of the main constituents between areas of interest [1], as a complement to field data estimations. As an example, Hydes et al. [2] studied seasonal nutrient and sediment patterns in North Sea using measurements, and their work was followed by Skogen and Moll [3] using a three dimensional model for the same area to estimate the role of river inflow and modelled physics on primary production.

2 STUDY AREA

The study area is located in the West Iberian coast (Figure 1), and is under the influence of one of the largest estuaries in the Europe, the Tagus Estuary, with an approximately area of 320 km^2. Residual circulation in this coastal area depends mainly on four main forces: alongshore coastal currents, tides, the Tagus Estuary outflow and local wind. The interaction between these four factors determines the dominant regime at any given moment.

The Western Iberian currents systems present a seasonal variability, with distinct summer and winter regimes. In the surface layer, a current towards south associated to the wind regime (the Portugal current [4]) occurs predominantly during the upwelling the May-September period creating upwelling conditions. At the end of the summer and during winter, the predominant wind inverts (towards east and north) and surface currents to north occur. At intermediate depths, a poleward current (slope current) persists during all the year [5].

The Tagus Estuary outflow is forced mainly by tides and therefor is oscillatory. The maximum velocities occur in the estuary mouth, with spring tide ebb values around of 2 $m\,s^{-1}$ are reached. The Tagus River is the main freshwater source of the estuary with a mean flow rates of 300 $m^3\,s^{-1}$. During winter, river flow can eventually reach around 2000 $m^3\,s^{-1}$ while summertime river flows of around 50 $m^3\,s^{-1}$ are common. The instantaneous values are strongly controlled by several dams in the Tagus River. The estuary fresh water affluence is determinant for the estuary residence time. However, only in extreme river flows conditions the circulation pattern and consequently the water characteristics that reach the estuarine mouth.

3 METHODOLOGY

3.1 Tagus Estuary mouth operational model

MOHID model was first implemented for the Tagus Estuary and adjacent areas in the early 1990s to provide answers to coastal management issues, such as residual water discharges, eutrophication sensible areas, bathing waters protection, etc. Along the years, the model has been continuously validated and improved through calibration with *in situ* data collected in several monitoring campaigns. Both monitoring programs and modelling efforts provide a significant knowledge of the system, in terms of hydrodynamics and biogeochemical processes in this coastal area.

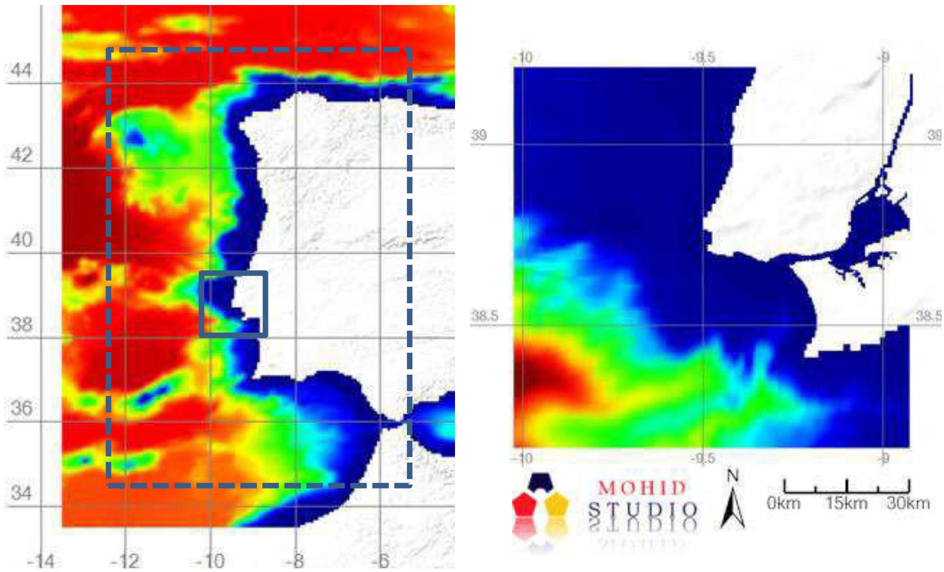

Figure 1. *Modelled domains in this study: regional model for the Portuguese coast (left) and nested model domain for the Tagus Estuary and adjacent coastal area (right).*

Recently, results were greatly improved with open boundary conditions obtained from the Portuguese Coast Operational Model System (PCOMS) (www.mohid.com/operational) [6, 7]. Velocity fields, water level, density, temperature, salinity, nutrients concentration and other parameters needed by the biogeochemical model are obtained with a 15 minutes time step (Figure 1). In the open boundary, PCOMS is forced by results from Mercator-Océan PSY2V4 [8] and its water levels are obtained from the global tide model FES2004 [9]. Both PCOMS and Tagus Mouth models are forced in the surface by operational meteorological models also running at IST (http://meteo.ist.utl.pt, [10]) which provide hourly fields of surface wind, temperature, relative humidity, pressure and solar radiation. PCOMS is forced with MM5 meteorological model with 9 km of spatial resolution, while the Tagus Mouth model is forced by the WRF meteorological model with 3 km of spatial resolution, allowing for a better differentiation of land use within the estuary and adjacent areas.

Rivers discharging into the estuary (Tagus, Sorraia and Trancão) and the submarine outfall from Guia WWTP are imposed as discharges in Tagus Mouth model with time series for flow and nutrients concentration values. The Tagus discharge has hourly values obtained in real time from hydrometric station, while the other affluent rivers values and WWTP correspond to monthly means from historical records.

The Tagus Mouth model has a 3D setup, thus allowing to study of the vertical stratification of density and coastal upwelling. The model runs operationally with 50 vertical layers (43 Cartesian and 7 sigma at the surface), in a similar configuration to the large-scale PCOMS model. The layers vary in thickness according to depth, increasing from 1 m at the surface to 450 m at a depth of 5000 m. The model horizontal resolution is irregular with a higher discretization around the estuarine mouth and the submarine outfall area with values around 300 m while in the open ocean the resolution is around 2 km. This horizontal grid was defined in this manner to optimize computation time while keeping the necessary spatial resolution for the areas of interest.

3.2 Model validation

PCOMS model validation [6] is made using real-time with data from satellite imagery (temperature and chlorophyll-a from http://oceancolor.gsfc.nasa.gov/), tidal gauge data, currents and temperatures measured in buoys along the Iberian coast and data from ARGOS buoys, an ocean monitoring international network (www.argos-system.org) [6].

Tagus Mouth model was validated using data from monitoring campaigns. Figure 2 shows the temperature and chlorophyll-a concentration model results compared with *in situ* data from laboratorial samples and multiparametric probe, at three different water depths in the water column (surface, middle and bottom water column) from a sampling station in the study area (the emission point of the outfall). In this example it is possible to observe that the model was able to reproduce the more important seasonal tendency patterns as well as small time scale variations deriving from wind and river flow variations, which determine the influence area of the estuary plume.

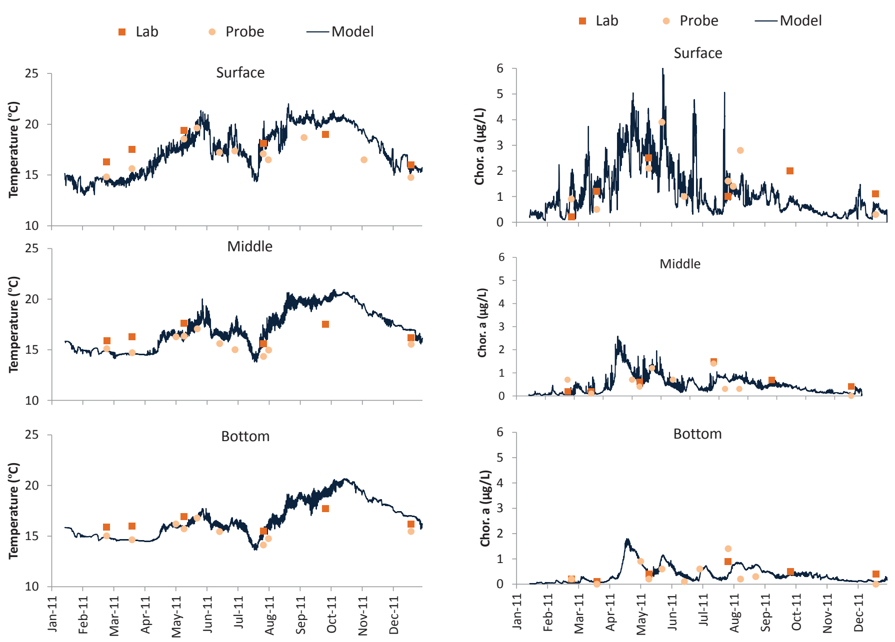

Figure 2. *Validation of model results with field data for temperature and chlorophyll-a during 2011 (outfall station).*

3.3 Fluxes

The model results comparison with field data, obtained at discrete locations, is a useful procedure for validation, but these results correspond to a specific cell in the model grid and to a given time instant. When the goal is to study areas or volumes as a whole, the representation of a specific area by a single cell make the model results simplistic and therefore unrealistic. Boxes definition is particularly useful to delimit zones or water masses with different characteristics and thereby to define and quantify processes within and between each other. In the MOHID model, the users can define boxes that could serve to determine the concentrations and the fluxes in the areas or volumes defined by them. Each box can be regarded as a finite volume where changes of proprieties exchanges between adjacent faces can take place. These exchanges are called fluxes, and can be defined as the product of the box interface flow rate and the concentration in each volume. Boxes concentrations mainly depend on the transport and transformation processes that occur in each box (mineralization of organic matter, consumption and excretion of phytoplankton, etc.).

The boxes are parallelepipeds that contain one or more cells, horizontally and vertically. Each box concentration results from the masses integration of all the cells that constitute the box. The flux between boxes is calculated by the sum of the fluxes between the adjacent cells that share a common face. An example of the MOHID box concept is shown in Figure 3. In the model each cell is defined by *i*, *j*, *k* coordinates.

To simplify the calculations, the regular or irregular polygon that defines each box is forced so that their faces coincide with the sides of the adjacent cells, that is, a cell cannot belong to two different boxes. Each box concentration results from the sum of the masses calculated at the center of each cell (green dots in Figure 3). The fluxes are calculated for all cells, partial fluxes, but for calculating the flux between the boxes, the model only considers the fluxes between cells that share one of the polygons faces (orange arrows oranges in Figure 3). The final flux results of the integration of the partial flows of each face. Water flux is calculated as:

$$\Phi_{a-b}^{water} = \int \int (\overrightarrow{v} \cdot \overrightarrow{n}) \cdot dA \tag{1}$$

Where *a* and *b* are the boxes, *v* is the velocity and *n* the normal.

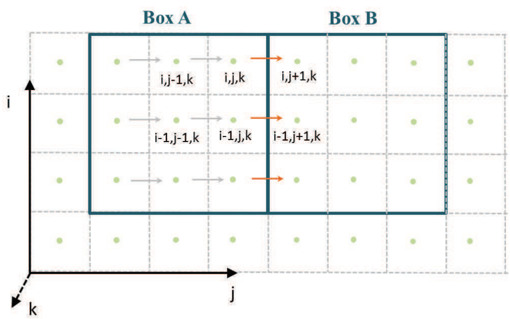

Figure 3. *Illustration of box fluxes calculated by the MOHID model.*

The flux of a given propriety is:

$$\Phi^{\beta}_{a-b} = \int_t \left(\int \int \beta \left(\vec{v} \cdot \vec{n} \right) \cdot dA + \int \int \gamma \left(\vec{\nabla} \beta \cdot \vec{n} \right) \cdot dA \right) \cdot dt \tag{2}$$

Where β is a given property and γ is the diffusion coefficient and ∇ the property gradient.

In dimensional form:

$$\left[\frac{M}{T}\right] = \left[\frac{M}{L^3}\right]\left[\frac{L}{T}\right]\left[L^2\right] + \left[\frac{L^2}{T}\right]\left[\frac{M}{L^4}\right]\left[L^2\right] \tag{3}$$

The number and size of the boxes result from the compromise between the computational process and the resolution of the process under study. A higher spatial resolution, horizontally and vertically, requires more computational time but the local scale phenomena are better represented, i.e., recirculation, punctual discharges.

Other studies [11, 12] used this box methodology to calculate residence times or nutrient and phytoplankton fluxes in several Portuguese estuaries. In both studies, a 2D model was used, since vertical stratification was not significant. When the upwelling process and the seasonal stratification or thermohaline are significant it is necessary to use a water column discretization approach. In the present study were considered five horizontal boxes, each discretized into three or four vertical layers, depending on the local depth. The study area was divided into three main areas namely: the estuarine, coastal and ocean areas. To understand the water column dynamics, the effort was centred in the coastal zone, which was represented by a total of nine boxes, three horizontal and three vertical (Figure 4). The analysed properties were water fluxes (flow), phytoplankton and nitrate, for being one of the key nutrients and for having a great variability depending on the Tagus River loads.

3.4 Upwelling Index

One way of quantifying the upwelling phenomenon is through the upwelling index [13, 14]. This index is a measure of the volume of water that upwells along the coast; it identifies the amount of offshore transport of surface waters due to geostrophic wind fields. Indices are in units of cubic meters per second along each 100 meters of coastline.[1]

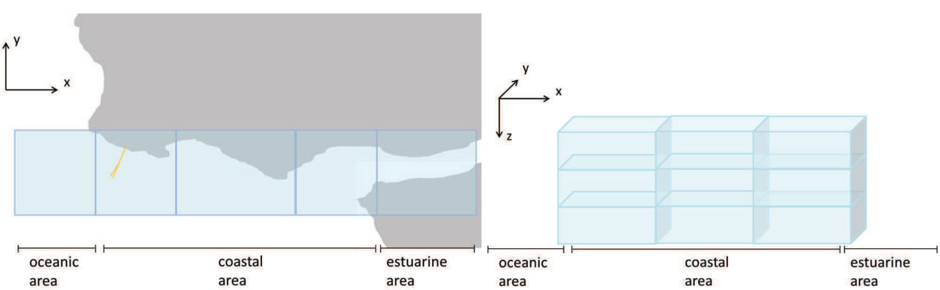

Figure 4. *Horizontal (left) and vertical (right) boxes used in the simulations.*

[1] Available at: www.indicedeafloramiento.ieo.es

4 RESULTS

The analysis focused on the first two weeks of September and November. These periods were selected based on the distinct coastal hydrodynamic patterns resulting mostly from rather different wind regimes [4]. Northerly winds dominated during September, while in November the wind regime was mostly dominated by south winds. In both periods, the Tagus River flow was relatively low ($\sim$40 m^3 s^{-1} and $\sim$180 m^3 s^{-1}, respectively). As previously mentioned, vertical movements in the water column are strongly induced by local wind direction and intensity. Upwelling is a common occurrence under northern winds regimes and the upwelling index calculated for 2011 is presented in Figure 5. Values were in the same order of magnitude in both months but opposite signals were recorded: 325 m^3 s^{-1} km^{-1} in September and -324 m^3 s^{-1} km^{-1} in November. This can be attributed to the upwelling and downwelling dominance, respectively. The study area shows significant variation in the upwelling index, with maximum values peaking $\sim$3000 m^3 s^{-1} km^{-1} [15].

Figure 6 presents wind directions and velocities and residual surface field velocity for September and November 2011. During September the dominant north wind induced a southward surface current, setting a pattern that characterized the general surface circulation during that period. Fresh water intrusion in the coastal area induced an E-W along shore transport. Together these two processes model the estuarine plume. River discharges determined the amount of water reaching the coastal area, and the upwelling current transported the plume outwards and induced its dispersion. Local topography is also known to play an important role in the general circulation patterns [16]. An opposite scenario was seen during November, when in general the dominant southern winds induced a surface general pattern of water transport towards north.

Figure 7 and 8 show the integrated fluxes obtained from the model results for the analysed months. It must be stressed that the values shown in this figures were the result of an in-depth integration, which might explain the similar fluxes patterns for both months. This pattern is characterized by a net transport of water from south into the coastal area, followed by an outflow towards west. However, when looking at individual surface boxes (results not showed), it is possible to observe that the general circulation in the upper layers is mostly determined by the wind pattern.

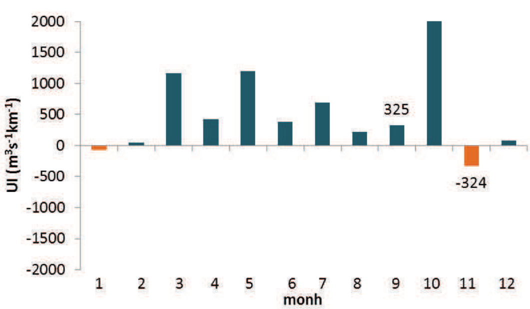

Figure 5. *Upwelling index for 2011.*

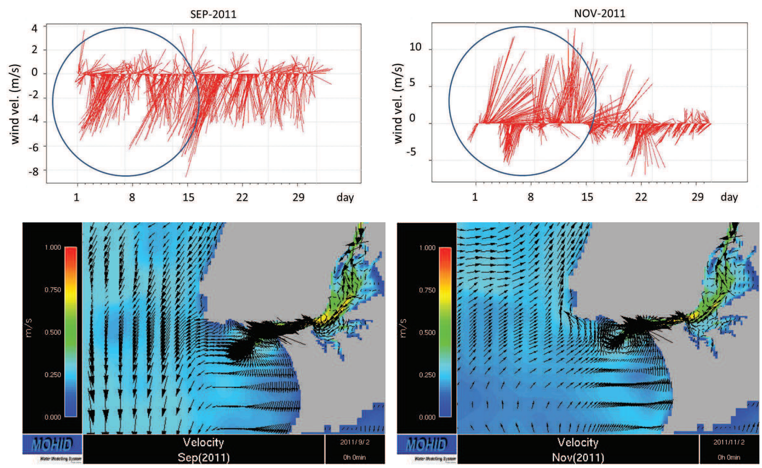

Figure 6. *Wind directions and velocities (top) and residual surface field velocity (bottom) for September (left) and November (right) 2011.*

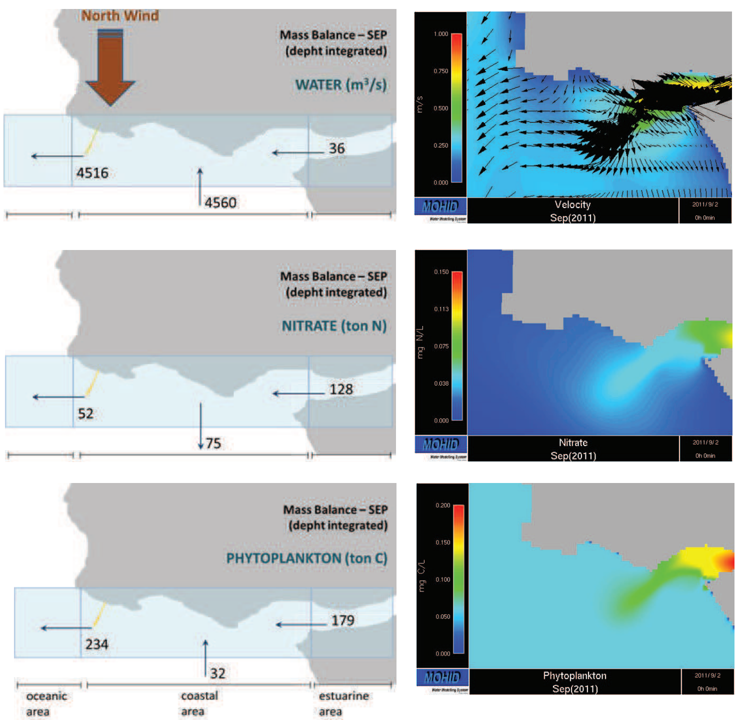

Figure 7. *Water, nitrate and phytoplankton fluxes (left) and respective residual field (right) from 2 to 15 September 2011.*

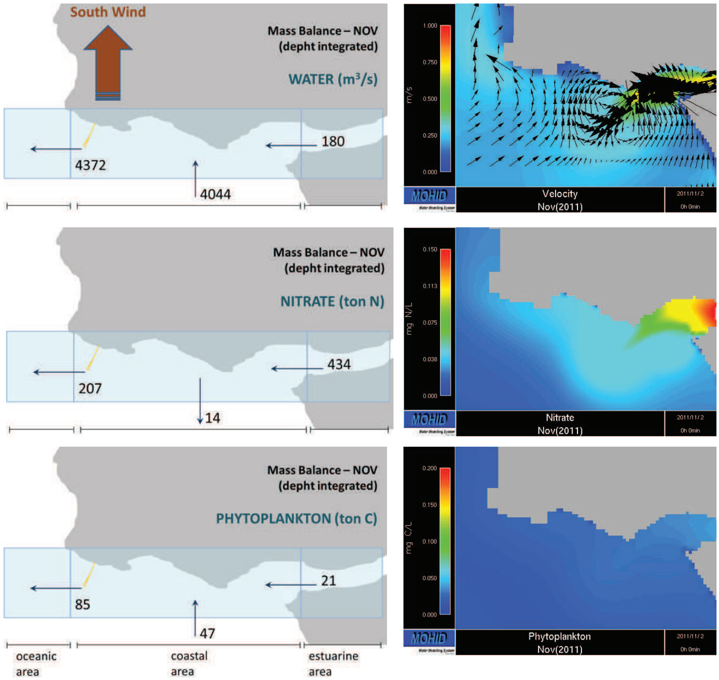

Figure 8. *Water, nitrate and phytoplankton fluxes (left) and respective residual field (right) from 2 to 15 November 2011.*

The nutrient flux is rather similar in both months, with a positive flux from the estuary to the coastal area and exportation of nutrients from this area into the open ocean. Nevertheless, the flux was higher in November, probably due to increased loads associated with the river discharge intensification and also because phytoplankton consumption decreased in response to lower light levels. The estimated values calculated in this work agree with previous data [12].

In general, phytoplankton (expressed in ton C) presented the same pattern found in the water fluxes. During the two analysed periods there was an export of phytoplankton from the estuary to the coastal zone. The low river flow caused a longer residence time within the estuary which could favour the growth of microorganism [17]. The difference lied in the balance for each of the periods, contrary to what was found for nutrients. During September, inside the estuary, the microorganisms still had favourable conditions for growing, therefore, the export from the estuarine area to the coastal area was around 10-fold higher than in November.

For a better understanding of the vertical fluxes in the water column, results for the near-coast boxes are shown in Figure 9. Flux direction suggests that upwelling condition predominated during September, with the exception of the estuarine mouth area, where the flux was downwards, most probably as a consequence of the effect of local topography. In the opposite situation, when the predominant wind was from south (Figure 10), downwelling occurred and the predominant flux was downwards for water and all the analysed properties.

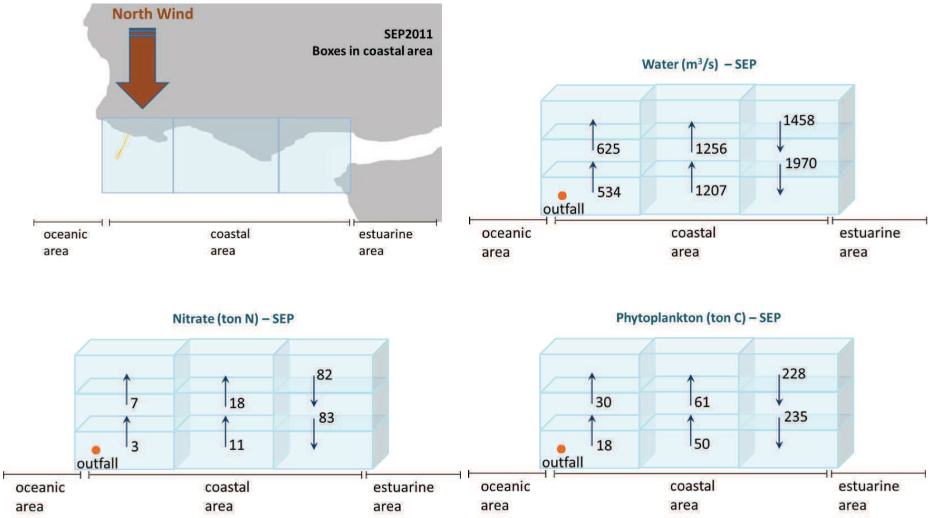

Figure 9. *Water, nitrate and phytoplankton fluxes in coastal area from 2 to 15 September 2011.*

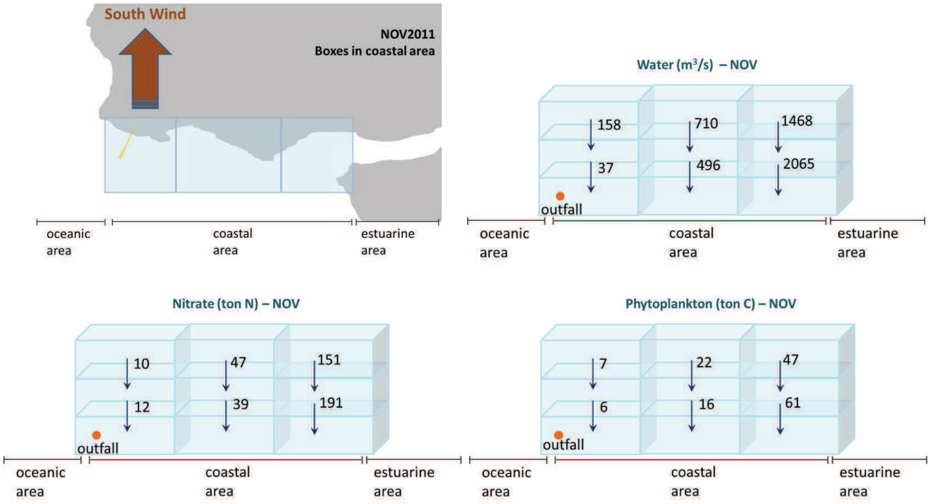

Figure 10. *Water, nitrate and phytoplankton fluxes in coastal area from 2 to 15 November 2011.*

5 CONCLUDING REMARKS

MOHID model runs operationally in forecast mode at the Tagus mouth and is validated using remote sensing data and field *in situ* data collection is continuously being performed. Field data sampled both on the Tagus Estuary influence area and on the coastal zone show that MOHID was able to reproduce both hydrodynamic circulation and water quality main processes.

The 3D biogeochemical model MOHID model reproduced the three-dimensional structure of the studied water masses. A 3D integration box approach was carried out and the model reproduced very satisfactorily the expected behaviour of circulation patterns. When the entire water column was integrated the expected north-south general circulation along the Portuguese coast was observed. When analysed only the surface boxes that cover the first few meters of the water column, flows were a function of the prevailing winds during the studied period, with circulation towards south with north wind and vice-versa. The use of integration boxes with vertical discretization of the water column also reproduced the upwelling or downwelling effect, typical of this coastal area.

Integration boxes may show the influence of systems with different hydrodynamic and biogeochemical properties (river, estuary, mouth, coastal area) to the circulation/property patterns of a particular area. The spatial and temporal versatility of boxes in MOHID implementation allowed also differentiating periods in which each of the forcing actors prevailed. For instance, in episodes with high river flow, the Tagus Estuary plume would be the most dominant factor in the physicochemical properties of the coastal zone, especially in the surface layers; episodes with intense winds would define the plume dispersion and possible redistribution of properties either at surface or in depth in upwelling / downwelling areas.

The possibility of different spatial boxes arrangements allows isolating smaller scale phenomena such as coastal recirculation or the submarine outfall effluent discharges local effects, making this a robust and versatile methodology for backing coastal management decisions.

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