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Integration of physical and water quality models

Intégration de modèles physiques et de qualité des eaux

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Cet article présente l'approche générale suivie au LNEC pour étudier des problèmes d'estuaires et de zones côtières, du point de vue de leur hydrodynamique, de leur morphodynamique et de la qualité des eaux. Le cadre conceptuel est présenté et permet de définir la problématique et les objectifs à long terme de ce type d'études. Les différents systèmes de modélisation, déjà disponibles ou en cours de développement et d'adaptation, sont ensuite présentés en mettant l'accent sur les aspects computationnels. L'importance de la prise en compte adéquate des processus physiques dans les études de qualité des eaux est enfin illustrée par l'analyse des temps de résidence et de la contamination fécale dans une lagune très dynamique (lagune d'Óbidos, Portugal).

I ■ INTEGRATED ANALYSIS OF PHYSICAL AND WATER QUALITY PROCESSES IN ESTUARINE AND COASTAL REGIONS

The ecological and recreational value of coastal systems has fueled many studies on hydrodynamics, residence times, morphodynamics and water/ecological quality. However, while water renewal in these systems is generally controlled by the combined action of waves, tides and river flows, most studies are system-dependent and discipline-specific, and resort to either field data analyses or numerical modeling of individual processes, disregarding their interactions. Hence, detailed characterization of these processes has improved, but holistic understanding of the systems remains limited.

The detailed understanding of the physical, chemical and ecological interactions and the ability to forecast the impacts of anthropogenic pressures poses multi-disciplinary challenges that cannot be solved through conventional, single-tool, analyses. A detailed characterization of coastal systems with field data alone has prohibitive costs. Numerical models are attractive low-cost alternatives, which have reached a maturity stage in some areas (hydrodynamics, wave propagation), but have limited accuracy in other areas (e.g., morphodynamics, water quality). These models can thus benefit significantly from the joint use of other methodologies such as field work and laboratory experimentation.

Integrated, multidisciplinary analysis emerges thus as the adequate approach to tackle the dynamics of coastal systems. It has been used successfully in estuaries without significant morphological dynamics [1] and in open coast systems [2]. This approach includes multidisciplinary field data analysis, to increase the knowledge on the system and to validate numerical simulations; integrated numerical modeling, to analyze the full variability of environmental conditions and the interaction between processes; and lab experimentation, to complement the current knowledge on relevant, specific processes under controlled conditions.

Simultaneously, the ability to forecast the long-term dynamics of estuarine and coastal zones is fundamental to assess the social, ecological and economical impacts of both human interventions and climate changes in these regions. This need has fostered the development of several computational nowcast-forecast systems in the U.S. and Europe (e.g. CORIE, for the Columbia River, USA; PORTS, for many ports and estuarine systems across the U.S.A.; POL for the Liverpool bay, U.K.; RIAMOM for the Sea of Japan), which provide predictions of several physical quantities at short time scales and are currently used for the management of harbors, marine resources and emergency operations.

The introduction of the European Water Framework Directive, as well as the new EU Bathing Water Directive, emphasizes the need to extend nowcast-forecast systems, typically developed for geophysical parameters, to water quality and ecological problems. Well-validated, reliable numerical models for simulating marine pollution and ecological issues, which account for the adequate interaction between physical, chemical and biological processes, are a key part of this process. However, the large temporal and spatial scales involved in the long-term integrated simulation of the water and sediment dynamics of coastal regions as well as the complexity and multitude of parameters involved in the water quality and ecological modeling require computational resources that were almost inexistent in the past.

High-performance computing platforms (e.g. PC clusters) and grid computing are now emerging as attractive and accessible tools for the modeling community to solve long term, large scale problems in estuarine and coastal areas, with pilot applications being developed in several places in the USA and Europe. The availability of vast shared computational resources within the grid computing community and a suite of parallel-processing models provide, for the first time, the means for an adequate scientific support for the sustainable long-term management of coastal systems. Using virtualization techniques, integrated modeling systems can take advantage, in a seamless manner, of a vast computational power that is physically distributed on several sites. The European projects Enabling Grids for E-sciencE (EGEE) and

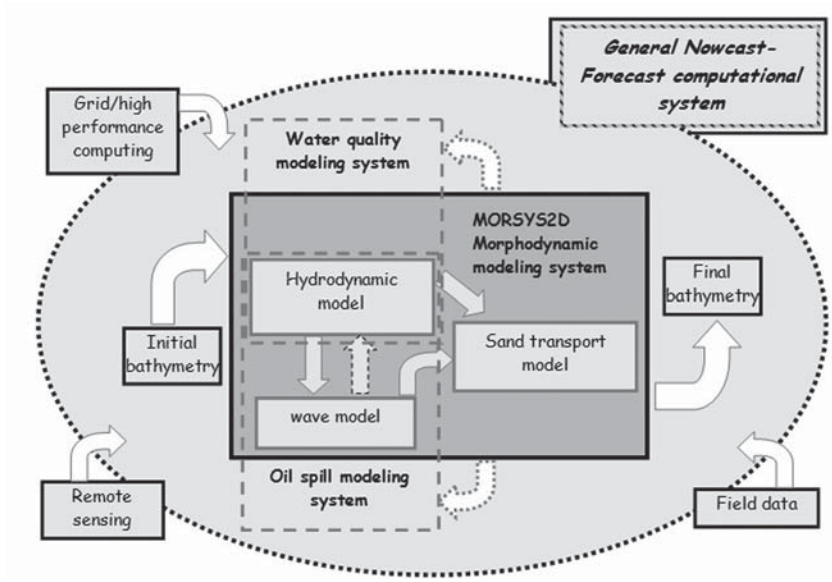

Figure 1 : Framework for the general nowcast-forecast computational system.

Interactive European Grid (int.eu.grid), are examples of the use of these computational resources.

In close cooperation with several institutes and universities, in particular with the staff of the new National Science Foundation (NSF) Science and Technology Center for Coastal Margin Observation and Prediction, led by the Oregon Health and Science University (OHSU, USA), the Estuaries and Coastal Zones division of LNEC is now developing a computational structure that integrates several numerical modeling systems for morphodynamics, oil spill analysis and other water quality problems, and targets forecasting capabilities. This computational structure is based on a new technology that enables the rapid deployment of forecast systems for any coastal system and the nowcast-forecast system for the Columbia River Estuary and the Pacific Northwest coast (www.ccalmr.ogi.edu/CORIE, [3]), both developed at the OHSU. Figure 1 illustrates the general framework of the computational structure, based in a core of hydrodynamic and short wave community models, including the ELCIRC/SELFE models from OHSU. These activities integrate several graduation projects, in collaboration with Portuguese universities, and other research projects, funded by national, European and American funding agencies.

II ■ CASE STUDY: THE IMPACT OF MORPHODYNAMICS ON THE RESIDENCE TIMES AND FECAL CONTAMINATION IN THE ÓBIDOS LAGOON

Physical settings

The Óbidos lagoon is a small and shallow coastal system located on the western Portuguese coast (Figure 2). The lower part of the lagoon consists of a web of channels and sand banks with strong velocities, while low velocities and muddy sediments characterize the upper lagoon. The inlet that connects the lagoon to the ocean meanders and migrates on monthly, seasonal and decadal time scales, with a general tendency for accretion [4]. The continuous evolution of the inlet bathymetry strongly affects tidal propagation and circulation patterns. For instance, tidal amplitudes can decrease by 50% in the lagoon during the maritime winter, as a result of the sedimentation of the tidal inlet [4]. The problems associated with the strong dynamics of the inlet have led to frequent dredging operations and to the search for more permanent solutions [5].

The hydrodynamics of the Óbidos lagoon were simulated with ELCIRC, a fully non-linear, three-dimensional, baroclinic shallow water model which is being developed as an open source community model at the OHSU [6]. This model uses a combination of finite volumes, Eulerian-Lagrangian methods and unstructured grids for mass conservation, domain discretization flexibility and stability at large time steps. Due to the shallow depths and negligible freshwater inputs in the Óbidos lagoon, circulation can adequately be simulated with a depth-averaged model. Hence, a single vertical layer is used, so ELCIRC reverts to two dimensions. The hydrodynamic model was forced by the eleven frequencies taken from a regional model [7], without any river flow. The model was calibrated and validated with field data, and results were condensed through harmonic analysis for the same constituents [8].

Hydrodynamic simulations were set up for two distinct bathymetries. In November 2000, a strong meander had developed near the inlet mouth, which strongly damped tidal propagation (Figure 3a). In contrast, the July 2001 bathymetry was measured right after an extensive dredging operation that had improved tidal propagation (Figure 3b). Hence, the two simulations are representative of two very distinct, but frequent, situations: velocities and tidal amplitudes are signi-

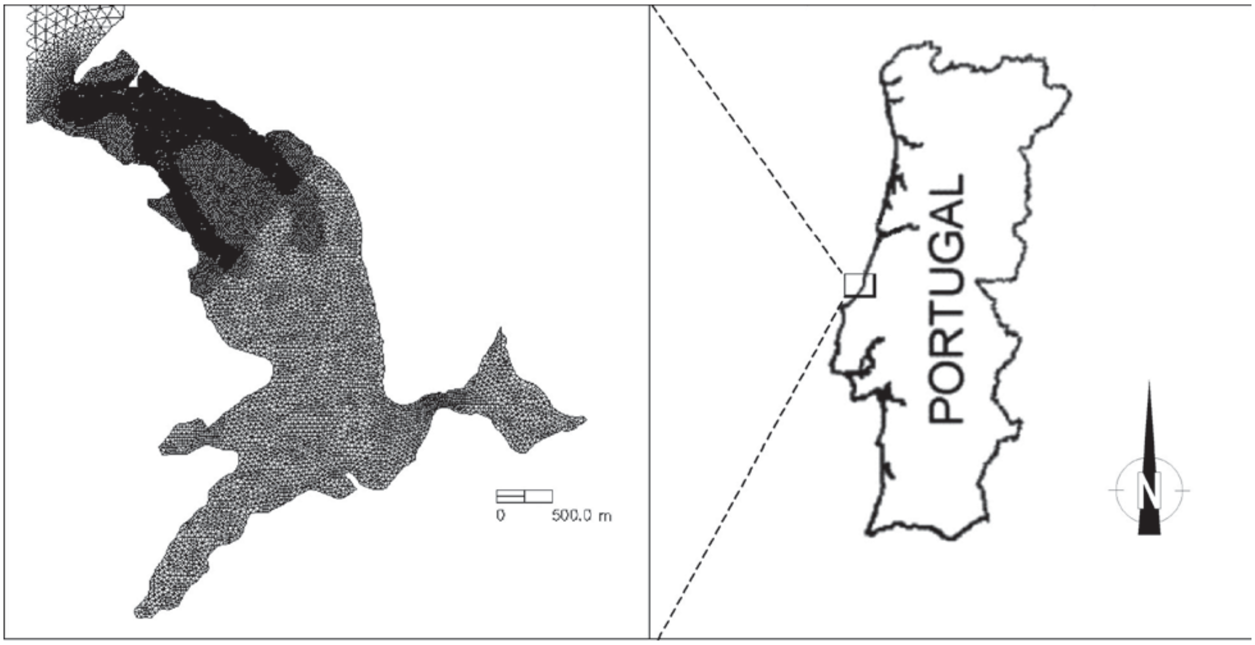

Figure 2 : Location and lagoon finite element grid.

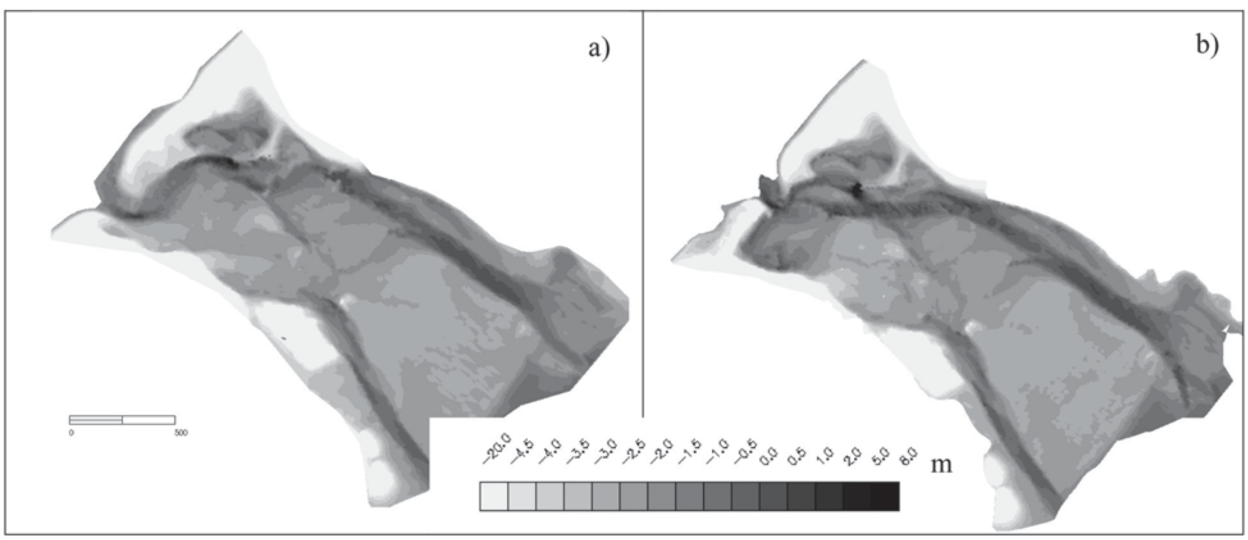

Figure 3 : Bathymetry for the lower lagoon: a) November 2000; b) July 2001.

ficantly larger in July 2001 (Figure 4b) than in November 2000 (Figure 4a).

Impact of bathymetry dynamics on residence times

Residence times (RT) are frequently used as indicators of the impact of the physical processes on the water quality and ecology of estuarine systems. RT were evaluated in the Óbidos lagoon to provide a base assessment on the impact of morphodynamics on both scalar and pollutant transport [8]. The analysis was based on the application of a particle-tracking model (VELApart, [9]), using a large number of particles scattered in the whole lagoon. These particles were released at 8 different instants, 4 on neap tides and 4 on spring tides, and their pathways were computed for 5 years.

Differences of average RT of each particle for the two situations (Figure 5) can be very important: of the order of 6 months to 1 year near the Arnóia delta and in the deeper areas, but generally smaller close to the margins. These patterns show the strong impact of bathymetric changes on scalar transport as the plumes will be mostly transported in the channels, where velocities are larger.

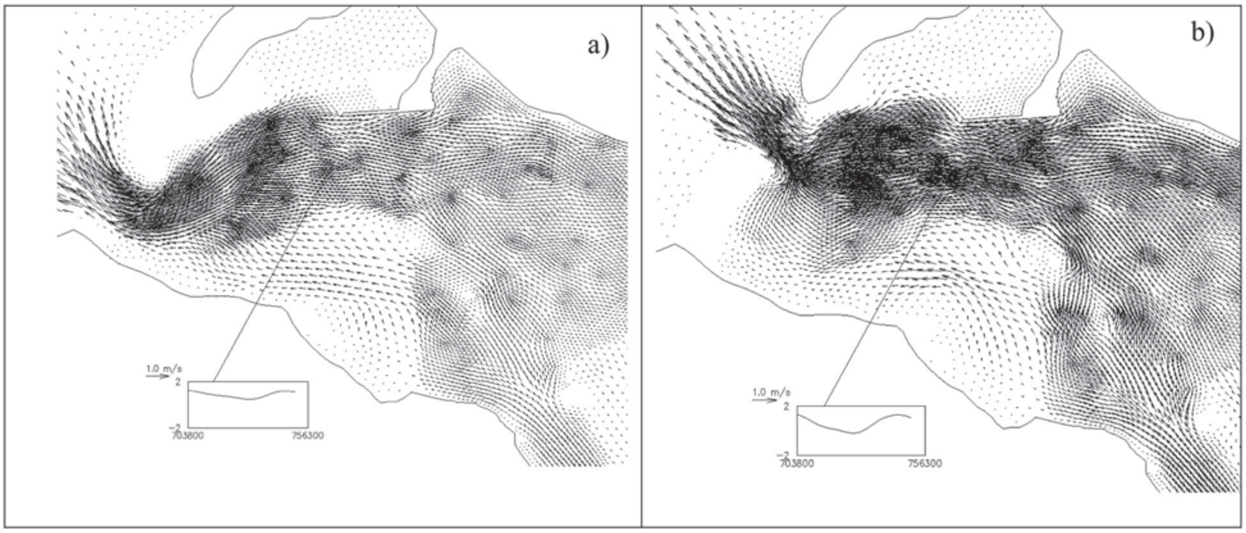

Figure 4 : Detail of the velocity field in the lower lagoon for the bathymetry of b) November 2000; b) July 2001.

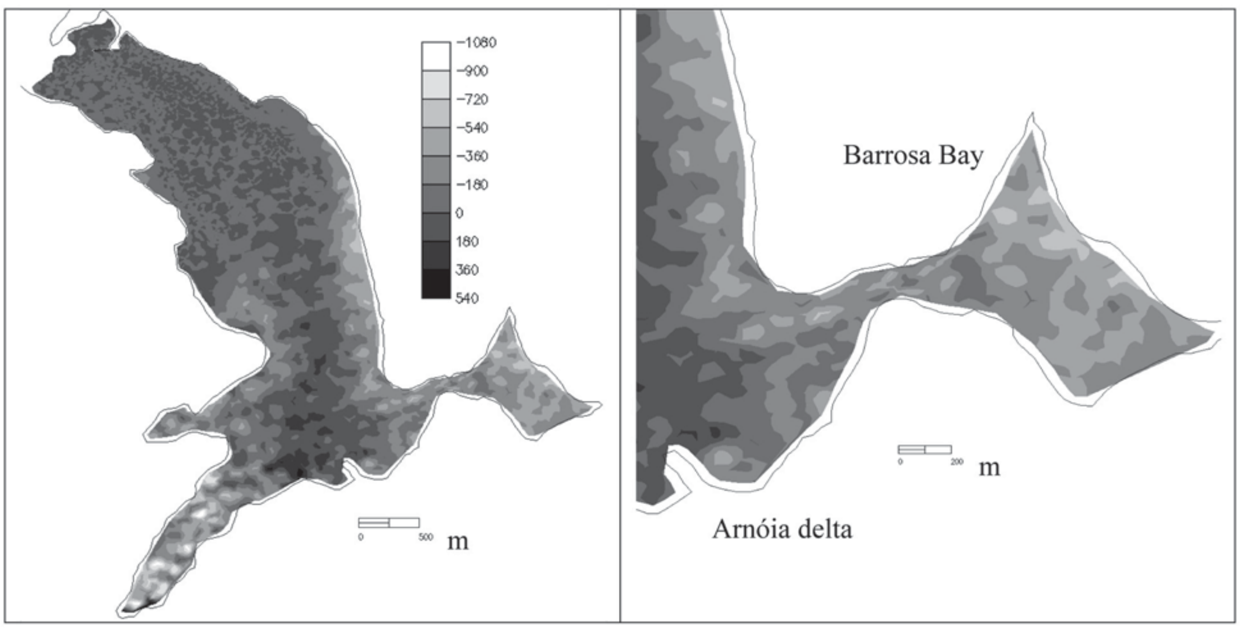

Figure 5 : Map of residence time differences (days) between July 2001 and November 2000: a) whole lagoon; b) detail of the Barrosa Bay area.

Analysis of the variability of the pathways of contamination plumes due to morphodynamics

To illustrate the impact of the bathymetric changes on water quality, the pathways of a synthetic sewage disposal discharge were simulated for the two bathymetries. The simulations were conducted with VELA [10], a depth-averaged transport model. This model combines Eulerian-Lagrangian and finite volume methods in an unstructured grid setting, providing very good accuracy, mass conservation and flexibility in discretizing complex domains. Several strategies to avoid spurious oscillations and unrealistic negative concentrations are also available in the model, which are defined using mass conservation principles [11]. The concentrations near the discharge are handled with a coupled near-field model based on the RSB model [12]. The evolution of the E. coli contamination plume is simulated using the formulation of [13], explicitly accounting for the dependence of the decay coefficient on solar radiation and water temperature and salinity.

Simulations were conducted for one day using a time step of 300 s, to evaluate the pathways and decay of a continuous discharge of sewage effluent characterized by the time series defined in Figure 6a. The salinity and the temperature were held constant at 25 and 18 ºC, respectively, based on recent field data. The simulations were forced by the two ELCIRC circulation fields, corresponding to the bathymetries of July 2001 and November 2000. To compare the effect of changes in bathymetry relative to a 50% reduction in contaminant mass, an additional simulation was performed using the grey time series from Figure 6a.

Concentration fields show very different plumes for the two bathymetries with the full discharge, as illustrated by the snapshots at hour 4 (Figure 6b,c). The smaller velocities in the Barrosa Bay in the November 2000 flow simulation relative to those observed in the July 2001 run are responsible for a smaller exchange of pollutant with the main body of the lagoon (which leads to higher concentrations inside the Barrosa Bay) and a smaller area of contamination (Figure 7).

The simulation for a 50% reduction in contaminant load leads to a similar pathway but smaller concentrations as expected. However, the differences in the maximum concentration observed in the whole simulations between the 100% load for the two bathymetries (Figure 8a) are much larger than those obtained by the difference between the 100% and 50% load runs in July 2001 (Figure 8b).

To analyze the impact of morphodynamics on the monitoring of a coastal system based on fixed sampling stations, two nearby synthetic sampling stations (A and B, Figure 8) were defined. Concentrations were interpolated for the three simulations for the two stations and are shown in Figure 9. Results show that different conclusions on the contamination level will be drawn, depending on the selected sampling station. Station A indicates a correct reduction of the contamination due to the 50% reduction of the load, while station

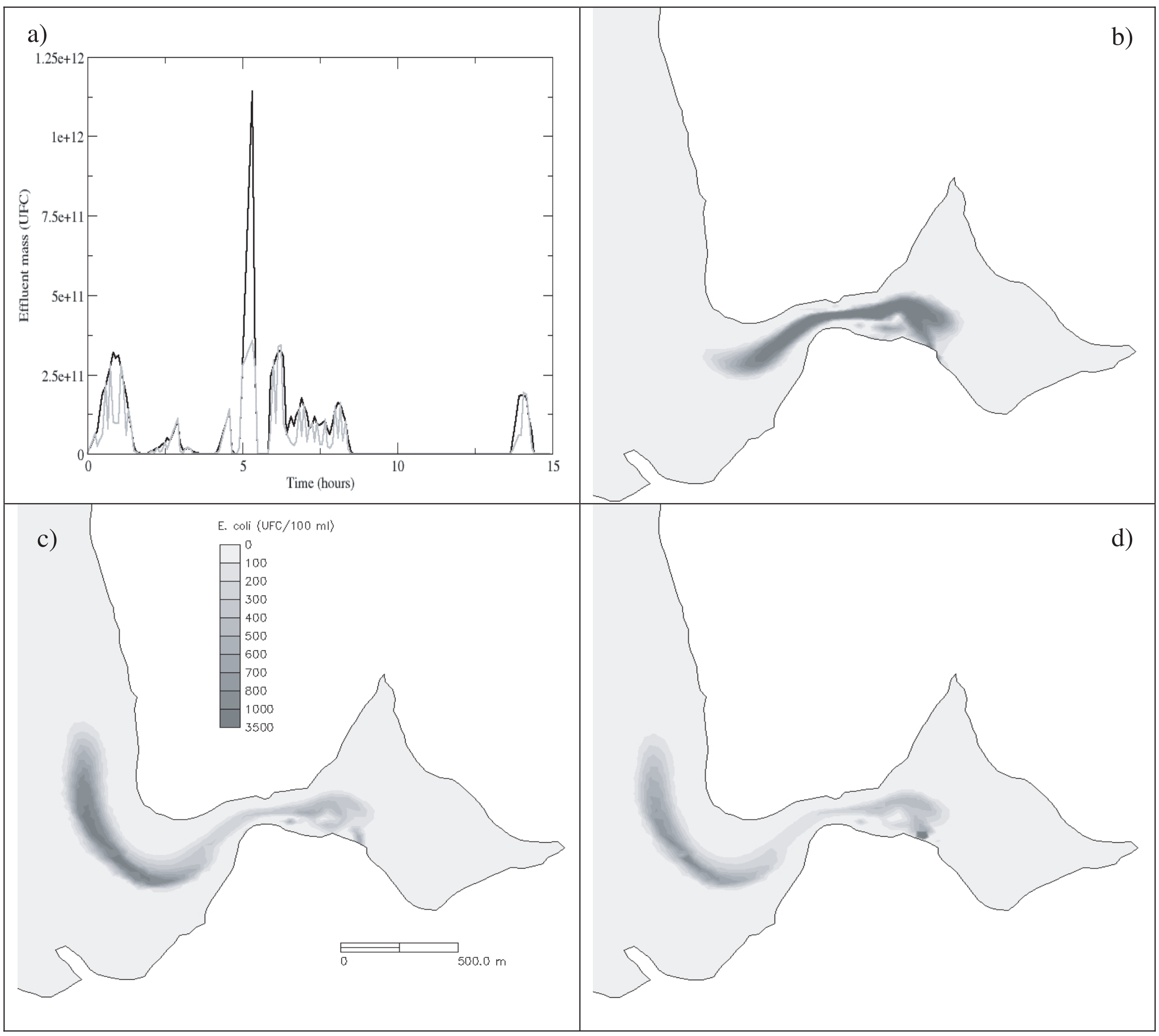

Figure 6 : a) Time series of the effluent mass for the full discharge (black) and the randomly 50% reduced discharge (grey). Concentration fields after 4 hours of discharge: b) November 2000, c) July 2001; d) July 2001 with reduced discharge.

B suggests that no gain was achieved by this reduction. Regarding the impact of the two bathymetries, both stations lead to incorrect interpretations of the conditions in the system: station A suggests that an increase in the pollution conditions from the November 2000 to the July 2001 simulations, while station B results suggest the opposite behavior. However, the pollutant load was indeed the same for both simulations.

This preliminary analysis shows that the bathymetric evolution in highly dynamic systems can have a stronger impact on the water quality of a coastal lagoon than significant changes in the pollutant loads. As such, traditional water quality analyses based on single bathymetries or few sampling stations may lead to incorrect conclusions, as changes in the renewal rates can mask important changes in the pollution conditions. Properly accounting for the relevant physical (morphological) processes is thus necessary to achieve an adequate coastal management of these dynamic systems. Integrated numerical modeling, which simultaneously accounts for morphodynamic and water quality, supported by detailed field monitoring, can be the best approach to quantify pollution pathways and the impact of changes in the input load conditions.

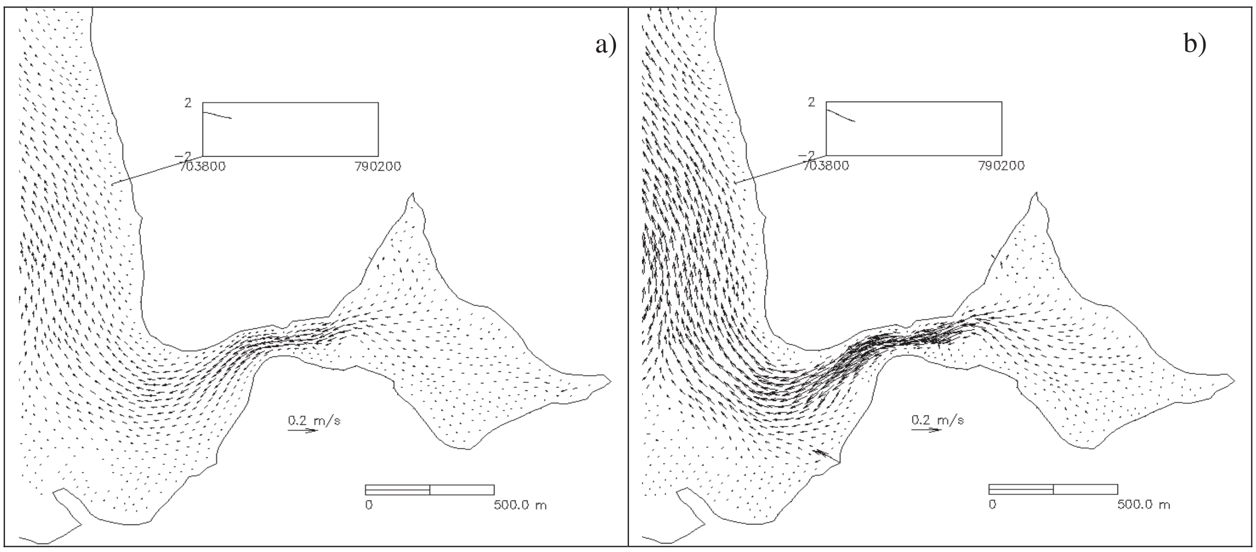

Figure 7 : Detail of the velocity field at hour 4: a) November 2000; b) July 2001.

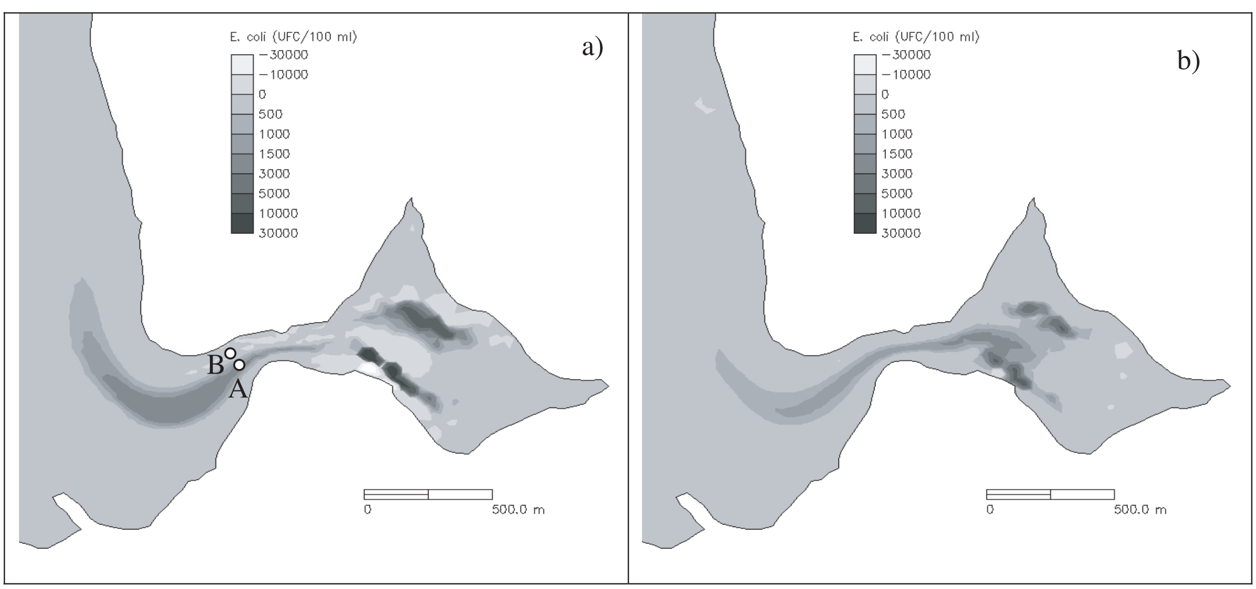

Figure 8 : Map of the maximum concentration difference in the whole simulation: a) July 2001 minus November 2000; b) 100% discharge minus 50% discharge for July 2001. Dark circles indicate the synthetic sampling stations.

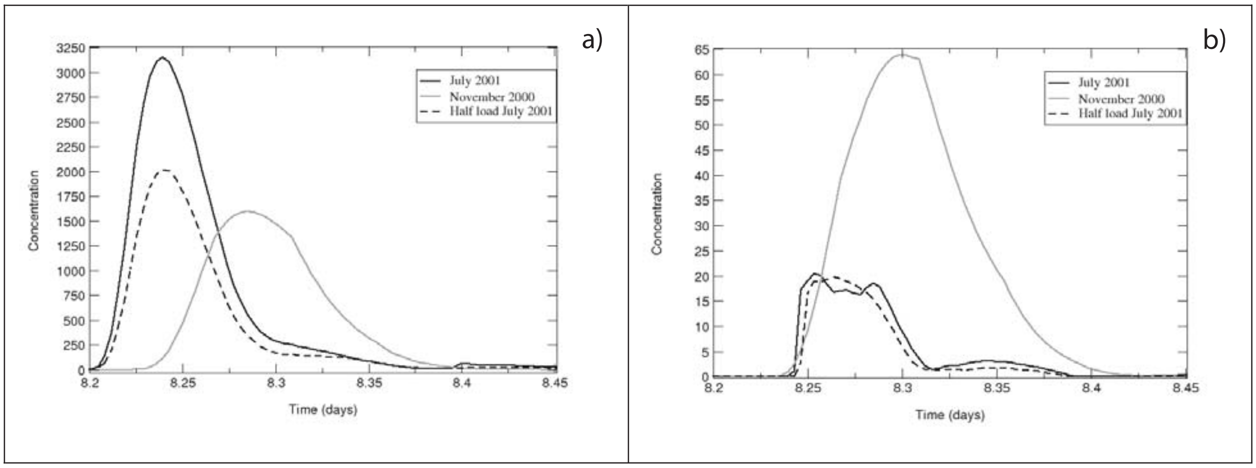

Figure 9 : Time series of concentrations for the three simulations at the "sampling stations": a) A; b) B.

III ■ FINAL REMARKS

This paper presented an overview of the conceptual framework under development at LNEC for studying estuarine and coastal problems in the fields of hydrodynamics, morphodynamics and water quality, which combines state-of-the-art models, nowcast-forecast computational systems and high performance computational resources. This framework is based on the explicit recognition of the importance of an adequate integration of physical, chemical and biological processes at the adequate spatial and temporal scales. The impact of morphological changes in a highly-dynamic lagoon on the residence times and fecal contamination was then used to illustrate this subject, based on an application to the Óbidos Lagoon in Portugal in two frequent bathymetric configurations. The analysis showed that residence times in the upper lagoon vary considerably with different bathymetries in the lower lagoon. The pathways of the synthetic fecal contamination plumes depend strongly on the bathymetric conditions in the lower lagoon, which may conceal the impact of reductions in the contaminant's load.

IV ■ ACKNOWLEDGEMENTS

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