Discussion and Conclusions

The research conducted evidences that the field of operational oceanography, through the development of operational forecasting systems, is regarded as a determinant knowledge area for providing the efficient and urgent management of water quality and hydrodynamic conditions in the important but sensitive estuarine areas. In order to fulfil this aim, operational forecasting systems are required to comprise a numerical model, for proving forecasts based on the system theoretical description, a measurement network, for providing model validation and the system bond to the real system, and a data assimilation scheme, to integrate the model and measurements in order to provide realistic forecasts having into account both model and measurement errors.

Although operational oceanography is expanding its object to water quality and ecosystems description, its main modelling focus still remains hydrodynamics. Perhaps the most relevant issue on coastal areas hydrodynamic modelling is the integration of different spatial and time scales providing an adequate grid resolution. In the context of operational forecasting this grid resolution is limited by computational and time acceptable costs. This determines the horizontal/vertical model grid resolution and increases the importance of boundary conditions such as bathymetry, atmospheric forcing and open boundary conditions. Advanced modelling techniques designed to tackle the operational constraints on modelling include the nesting of coastal models in regional or global models or the coupling of ocean and atmospheric models, in order to improve the boundary conditions.

One of the most relevant sources of measurements of the state of the ocean for operational oceanography is remote sensed satellite data which still remains inaccessible for coastal operational oceanography. However, coastal systems measurement networks can profit from in-situ measurement devices from the traditional tide gauges to the more recent moored sensors or the radar devices.

The most recently developed member of the operational forecast systems equation is the data assimilation scheme, which should be able to correct a model forecast considering information from measurements in an optimal way. Sequential methods based on Kalman filter are, capitalizing on their algorithm simplicity and capability to incorporate gradual developments, extensively used to improve global and regional operational forecast systems using predominantly remote sensed satellite data. However, issues such as measurement availability, non linearity of coastal dynamics, data assimilation schemes assumptions and computational costs make that data assimilation in coastal operational forecast systems is still a new and experimental field. Developments in theoretical and applied data assimilation research done approximately in the latest decade allowed the development of several sub optimal Kalman filter schemes with low computational cost and low filter initialization knowledge

demands which use in coastal operational systems seems promising. From these the most extensively used in the SEEK filter, from which several variants have been designed.

This work assesses the adequateness of the existing water quality forecasting system for the Tagus Estuary (MOHID Tagus Estuary), the most important Portuguese estuary and one of the largest in Europe, to reach the operational system status for assessing inside estuary conditions and performs the monitorization the Guia wastewater submarine outfall pollution. While possessing a modelling tool, MOHID Water, including most state-of-the-art modelling techniques, such as nesting modelling and atmospheric forcing from a meteorological model, it is found that it can benefit from an alternative model configuration and from a, currently absent, data assimilation scheme in order to reach that goal.

Being the astronomical tide the main driver of hydrodynamics in the Portuguese coast and while the tidal boundary conditions of the existent system are demonstrated to be adequate, an alternative domain comprising the whole Portuguese continental coast is presented and validated. This provides an equal quality boundary condition for the modelling in the Tagus Estuary interest area and supports the future nesting of other forecast systems for Portuguese coast.

A first-time contrast of the forecast system solution with tide gauge measurements from the existing tide gauge network, made available for the Tagus Estuary and adjacent coast, explicitly shows that one major problem affecting the water level forecast is the mean sea level misrepresentation. The existing forecast system modelling tool does not describes dynamic processes other than bottom and wind forcing shear stress which are capable to significantly affect mean sea level, although meteorological derived surge is known to be an important and frequent phenomenon the Portuguese coast. An improved boundary condition for the forecast model larger domain accounting for the large scale atmospheric pressure effect on mean sea level is shown to provide significant improvement in the mean sea level description for anomalies with period larger than 30h. These results provide evidence for this large scale effect being the underlying driver for previously unexplained variability with similar periods detected in water column integrated ADCP measurements at the Tagus Estuary adjacent coast by Leitão (2003).

A long known deficiency of the existing modelling tool is the complete absence of vertical stratification boundary conditions for the 3D version used to model the pollution of the Guia submarine outfall just outside the Tagus Estuary, which hampers considerably the forecast capability to adequately describe the pollution plume dispersion. A stratification derived from climatology imposed as open boundary condition, a more detailed vertical discretization of the model grid, a larger spatial resolution wind forcing and an improved advection scheme are implemented, causing large improvements in the description of stratification in the wastewater outfall area relative to CTD measurements and the accounting of surface temperature variability relative to satellite SST images.

Although the actualization with more detailed data of the bathymetry provides an improved forecast of tidal driven water level inside the Tagus Estuary, important tidal derived water level errors are still observed in channel areas inside the estuary. This error is known to affect negatively the water quality forecasts in the area, where the model grid horizontal resolution is inadequately small.

In order to avoid the increase of horizontal resolution, which should hamper the supply of operational forecasts, and capitalizing on the developments in data assimilation for operational oceanography and since the Tagus Estuary and adjacent coast is served by a tide gauge network, the data assimilation solution is envisaged as possible solution to water level misrepresentation, both in and outside the Tagus Estuary, while assuring that the forecast solution stays bond to real system variability.

An application of the Kalman filter for the correction of water level in a schematic linear model shows the potential of filter to correct the model forecast even if a drastic dynamic change is verified in measurements. It also highlights that the filter performance is very dependent of specification of filter parameters such as the system initial estimate, the model error, the assimilation frequency and spatial density of the assimilated measurements.

A data assimilation module is implemented in MOHID Water code comprising the SEEK filter and it fixed correction basis SFEK filter scheme, more adequate for non linear models for estuarine and coastal applications but not as computational resources demanding as other sub optimal Kalman filter schemes. Also a pre-processing tool is developed for performing EOF analysis and producing the dominant modes of system error variability, usable to provide the initial system correction directions for the filter.

A twin experiment data assimilation application to the improved 2D version of the system forecast modelling tool (but not accounting for the atmospheric pressure effect on water level and using the existing system bathymetry) assimilating tide gauge measurements and designed to correct a misspecification of mean sea level at the tidal boundary condition, shows that the original formulation of the SFEK filter while providing the effective reduction of water level forecast error in the range of 10-45% throughout the tide gauge locations does not accomplishes good corrections of velocity field in most of the locations. The original SEEK filter is also not useful in providing forecast corrections as these are found to be inexpressive or even inadequate, again in the velocity field for some locations.

The research suggests that these poor performances are linked firstly to an inadequate representation of the initial forecast error covariance derived from the EOF analysis of historical model results and secondly to the highly non linear dynamics of the model in some locations inside the Tagus Estuary. The very different horizontal and especially vertical resolution (because of 2D the water column depth ranges from 4km to 1m) present in the modelled domain and dynamic effects seem to prevent that a

representative initial state error covariance can be derived from historical model states. The model non linearities degrade the filter correction directions further in the SEEK filter, allowing the model dynamics to erode the unrealistic error covariance and causing small corrections, even at measurement locations. Compensation seems to be possible by increasing the number of measurements with the SFEK filter, although this is not a valid option as the tide gauge network has a limited number of locations.

Expressing that a SFEK filter can have a better performance than a SEEK filter in the same application, this work contradicts the general opinion expressed by published studies that SFEK is always a smaller cost but lower performance version of SEEK. However, this unusual finding is a consequence of the distinct characteristics of the model domain of the Tagus Estuary forecasting system relative to published work: areas of the domain with very different bathymetry depth together with a 2D setting and a very dominant and relevance tide influence.

These findings together with the known distribution of the model water level error relative to real tide gauge measurements strongly suggest that these original formulations for SFEK and SEEK filters should be inefficient in correcting the forecast with the assimilation of these measurements for the Tagus Estuary forecasting system. However, the same findings provide strong support that efficient corrections could be achieved with the improvement of the forecast correction directions evolution within the model or with the performance of data assimilation only in a sub domain comprising the Tagus Estuary and immediate adjacent coast.

The results of this work suggest that future research should be pursued in some issues.

Firstly, the study of astronomical tide propagation in the Portuguese coast should be consolidated. New boundary conditions using the recent FES2004 tidal model prediction should be implemented, studying the adequateness of boundary conditions in long time series of model results. The hypothesis for the degradation of tide propagation in the inner estuary channels due to insufficient bathymetry resolution should be explicitly tested with a bathymetry sensibility modelling study, quantifying the distortion of the tidal wave achieved with different resolution bathymetries.

Also, it is important to proceed with the study of factors affecting mean sea level time evolution in the Portuguese coast in general and in the Tagus Estuary in particular. This study should comprehend the analysis of long time series of tide gauge measurements and atmospheric pressure conditions (measured or provided by meteorological reanalyses), in order to assess the observed validity of the inverted barometer effect and adjust the reference mean sea level and atmospheric pressure used for the inverted barometer effect calculation. It also should be investigated, using model simulations, the

local effect of atmospheric pressure and wind velocity in mean sea level oscillations with period smaller than 30h, quantifying its importance in the several areas of the domain.

The baroclinic processes description in MOHID Tagus Estuary should be improved. The development of a baroclinic model for the Portuguese coast, with adequate vertical resolution, or the off-line nesting (due to operational exploration constraints) of MOHID Tagus Estuary in a large scale baroclinic model for the Atlantic Ocean and the improvement of the model vertical resolution at the Guia submarine outfall area should be studied, quantifying the quality of stratification conditions forecasts and the representation of the Guia submarine outfall pollution dispersion facing measurements. The downscaling of a large scale model solution from HYCOM model in a Portuguese coastal region is exemplified in the work of Leitão *et al.* (2005) for the Algarve coast. The phenomena of internal tide at the Tagus Estuary vicinity should be investigated using model simulations and measurements, identifying places of occurrence and explicitly testing its importance in the Lisbon canyon, just outside the Tagus Estuary.

The data assimilation capabilities of MOHID Water modelling tool ought to be improved. First, it should be included the learning mechanism adequate for applications of apprentice SFEK and SEEK filters as described by Brasseur *et al.* (1999) and implemented the SEIK filter as presented by Pham *et al.* (1998b). Also, the state-of-the-art EnKF scheme should be implemented to allow high quality data assimilation applications in non linear models. Additionally, it should be contemplated the possibility to add state variables representing a part of the state error and state error evolution models should be formulated and implemented in the code, for a better correction of state in data assimilation applications with non null average state error. The interface of reception of measurement files should be improved to allow the input of files in HDF5 format, such as remote sensed satellite or radar images. The observation operator specification should be improved to account for time change in the measurement number and for the assimilation of measurements not directly included in the state variables.

Finally, the usefulness of the data assimilation techniques for improving the MOHID Tagus Estuary is to be further investigated. Concerning the water level forecasts, it should be implemented an application of sub optimal Kalman filters in a nested domain comprising only the Tagus Estuary and immediate adjacent continental shelf for assimilation of tide gauge measurements. For improving the same forecasts, the apprentice filters and SEIK should be tested for assimilating tide gauge measurements in MOHID Tagus Estuary model domain 2. New sources of measurements suitable for operational use in data assimilation in MOHID Tagus Estuary must be investigated, such as temperature/salinity/chlorophyll sensors and remote sensed radar surface velocity images, for assimilation in the Tagus Estuary and continental shelf, and remote sensed satellite altimetry, for

assimilation in the ocean areas of MOHID Tagus Estuary model. The impacts of data assimilation in the forecasts of water quality of MOHID Tagus Estuary should be quantified.