Nomenclature

CTD	Conductivity-temperature-depth profiling system
EKF	Extended Kalman Filter
EnKF	Ensemble Kalman Filter
EOF	Empirical Orthogonal Functions
RMSE	Root Mean Square Error
RRSQRT	Reduced Rank Square Root Kalman Filter
SEEK	Singular Evolutive Extended Kalman Filter
SFEK	Singular Fixed Extended Kalman Filter
SEIK	Singular Evolutive Interpolated Kalman Filter
SST	Sea Surface Temperature

List of Symbols

a	State analysis indicator (in superscript) / amplitude of wave (1D schematic case)
c	Velocity of advection (1D schematic case)
f	State forecast indicator (in superscript)
I	Identity matrix
i	Index of time (in subscript)
K	Kalman gain
H	Observation operator (non linear)
H	Linearized observation operator
L	Matrix containing the correction directions of filter (correction basis)
M	Model operator (non linear)
M	Linearized model operator
N	Number of ensemble members
n	Dimension of state vector
P^a	Error covariance matrix of state estimate analysis
P^f	Error covariance matrix of state estimate forecast
p	Number of observations
Q	Error covariance matrix of model
R	Error covariance matrix of observations
r	Number of correction directions (rank of subspace approximation of P)
r_c	E-folding scale of correlation function (1D schematic case)

s	Number of time instants used for state sampling for EOF analysis
T	Period of wave (1D schematic case)
t	True state indicator (in superscript)
U	Matrix containing the weights of the correction directions of the filter
$\mathbf{x}^{a}(t_i)$	Analysis of state vector estimate at time t_i
$\overline{\mathbf{x}}^{a}(t_i)$	Ensemble average of analysis of state vector estimate at time t_i
$\mathbf{x}^{f}(t_i)$	Forecast of state vector estimate at time t_i
$\overline{\mathbf{x}}^{f}(t_i)$	Ensemble average of forecast of state vector estimate at time t_i
$\mathbf{x}^{t}(t_i)$	True state vector at time t_i
y_i^o	Observations at time t_i
α	EOF expansion coefficient
ε	Model linearization factor
λ	Eigenvalue / wavelength (1D schematic case)
η	Water level elevation (1D schematic case)
ν	Error of state estimate
ρ	Forgetting factor
ω	Error of observations

Preamble

When considering water bodies, estuaries are areas of high economical, social and ecological importance. In fact, they represent routes of transportation of economical goods, provide water and, directly or indirectly, several biological resources for economical activities, are used as disposal route for waste and provide aesthetic and recreation services. They are also an important habitat for ecological communities.

The broad spectrum of services and resources provided by estuaries made them, through the ages, a preferred site for human settlements. However, the amount of human exploitation of estuaries, although negligible at start, is nowadays, due to technological advances and the human population growth, threatening the sustainability of the future supply of these same services and resources and the whole health of the human population.

The seriousness of the situation makes estuaries the object of environmental protection national and international legislation, such as the Water Framework Directive, applied in the European Union space. This legislation stresses the importance of modelling in the monitorization of water quality in estuaries and coastal areas.

The only way for the model results to be really useful is if they are used to forecast in order to adapt or minimize the consequences of future hazardous situations both in short and long time terms. This implies that the modelling must be done incorporated in an operational system for forecasting water quality. However, models are affected by several errors, due to the way they or their specific applications are constructed and to errors in the data they use (e.g. initial and boundary conditions). In this context, to ensure that the model results are adequately reliable in reproducing the true system conditions, such operational system has to include also a measurement network. Measurements should be used in a first instance for model calibration and validation.

With the improvements of measurement techniques, namely in remote sensing, observed in the latest decades one of the most useful ways of using measurements in an operational forecasting system consists in using them in the context of data assimilation. In this process, the information from models and measurements are combined taking into account the uncertainty in both model results and measurements. A data assimilation technique is today an important part of most operational forecast systems.

One of the most important estuaries in the Portuguese territory is the Tagus Estuary, in the border of which is the Portuguese capital city Lisbon. Due to its social, economical and ecological importance,

the stresses that it is being submitted to and to the environmental legislation driving force, an observation and forecast system for water quality has been developed for the site and adjacent coastal area, which is in pre-operational phase. The Tagus Estuary Forecasting System (MOHID Tagus Estuary) is based in a state of the art modelling tool, MOHID Water, but has known deficiencies mainly due to insufficient use of measurement data, which hamper the developments of the system to full operational status. The main limiting factor seems to be the absence of a data assimilation tool.

This thesis presents the research made on the possible contribution of both advanced modelling and data assimilation techniques for the improvement of the MOHID Tagus Estuary forecasts of hydrodynamics, which will affect the water quality forecasts as well.

The objectives of the thesis are to:

- assess and implement the modelling improvements still required to adequately forecast the hydrodynamics in the Tagus Estuary and adjacent coastal areas;
- implement a data assimilation scheme usable in an operational setting to improve hydrodynamics forecasts made by MOHID Water for estuaries and coastal areas;
- assess the efficiency of the use of this scheme in the MOHID Tagus Estuary.

The research is conducted through the test of four hypotheses. The first three concern alternative modelling configurations accounting for the large scale effects on circulation of tide, atmospheric pressure and stratification. The fourth hypothesis refers to the use of data assimilation with SFEK and SEEK filters.

The thesis is composed of three main parts: the first part (first two chapters) concerns the state of the art of the operational modelling of water conditions in estuaries and the presentation of the existent MOHID Tagus Estuary tool; the second part presents the research plan (third chapter); the third part (last four chapters) presents the research results.

The information presented in the state of the art focus on the relevant hydrodynamic and water quality problems of estuaries and adjacent coastal areas, the modelling approaches used to deal with them, existent operational modelling systems and data assimilation techniques. The chapter dedicated to MOHID Tagus Estuary details the hydrodynamic and water quality characterization of the Tagus Estuary and adjacent coast and the main components of the existing modelling tool, the measurement network developments and the validation techniques used to assess the system forecast quality.

The research plan details the objective and the research question of the thesis, the research hypotheses, methodology to test the hypotheses and the data required to support this methodology. This methodology contains the details of the improved configuration of MOHID Tagus Estuary, developed to deal with the large scale tidal driven circulation representability, the large scale atmospheric pressure effect, stratification representability and the data assimilation developments.

The research results comprise the assessment of the performance of the improved MOHID Tagus Estuary configuration for the 2D and 3D versions relative to measurements and the existent MOHID Tagus Estuary configuration, the test of a data assimilation method in a schematic case, the implementation of a data assimilation module in MOHID Water code, and the implementation and test of the first improved 2D MOHID Tagus Estuary configuration with data assimilation.