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PROJECT UBEST: UNDERSTANDING THE BIOGEOCHEMICAL BUFFERING CAPACITY OF ESTUARIES RELATIVE TO CLIMATE CHANGE AND ANTHROPOGENIC INPUTS

Final Report

Abstract

The final technical report of the project "UBEST – Understanding the biogeochemical buffering capacity of estuaries relative to climate change and anthropogenic inputs" (ref. PTDC/AAG-MAA/6899/2014), funded by the Portuguese Foundation for Science and Technology (FCT), is presented. The project contributed to improve the knowledge on the biogeochemical dynamics in estuaries and coastal lagoons, in particular the Tagus estuary and the Ria Formosa. A detailed characterization of the current water quality and biogeochemical dynamics in these systems and further insights about their response to climate change and anthropogenic pressures are provided. The use of an integrated approach, combining field observations and numerical modelling, was fundamental as it allowed to effectively cover the relevant temporal (past-present-future) and spatial scales. An innovative coastal observatory was developed, the UBEST coastal observatory (http://portal-ubest.lnec.pt), which integrates all the main results of the project as layers of information with different levels of aggregation.

Keywords: UBEST coastal observatory / Hydrodynamics / Water quality / Tagus estuary / Ria Formosa

PROJETO UBEST: COMPREENSÃO DA CAPACIDADE DE REGULAÇÃO BIOGEOQUÍMICA DE ESTUÁRIOS NUM CONTEXTO DE ALTERAÇÕES CLIMÁTICAS E DAS FONTES ANTROPOGÉNICAS

Relatório Final

Resumo

Apresenta-se o relatório final do projeto "UBEST - Compreensão da capacidade de regulação biogeoquímica de estuários num contexto de alterações climáticas e das fontes antropogénicas" (ref. PTDC/AAG-MAA/6899/2014), financiado pela Fundação para a Ciência e a Tecnologia (FCT). O projecto contribuiu para melhorar o conhecimento sobre a dinâmica biogeoquímica em estuários e lagoas costeiras, em particular no estuário do Tejo e na Ria Formosa. Foi realizada uma caracterização detalhada da qualidade da água e da dinâmica biogeoquímica actual e uma análise da resposta dos sistemas às alterações climáticas e pressões antropogénicas. O uso de uma abordagem integrada, combinando observações de campo e modelação numérica, foi fundamental, pois permitiu abranger de forma efetiva as escalas temporais (passado-presente-futuro) e espaciais relevantes. Foi desenvolvido um observatório costeiro inovador, o observatório costeiro UBEST (http://portal-ubest.lnec.pt), que integra os principais resultados do projeto em camadas de informações com diferentes níveis de agregação.

Palavras-chave: Observatório costeiro UBEST / Hidrodinâmica / Qualidade da água / Estuário do Tejo / Ria Formosa

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1 | Introduction

The present document constitutes the final report of the project UBEST – Understanding the biogeochemical buffering capacity of estuaries relative to climate change and anthropogenic inputs, funded by the Portuguese Foundation for Science and Technology (FCT – Fundação para a Ciência e a Tecnologia). The project was developed within the scope of the LNEC's Planned Research Program (P2I) for 2013- 2020 and contributed to two R&D&I strategic lines of the Hydraulics and Environment Department, namely Environment and Aquatic Systems and Information and Decision Support Technologies.

The major identifying elements of the project are listed below:

- Project reference: PTDC/AAG-MAA/689/2014
- Scientific Area: Environment and Global Changes
- Scientific Sub-area: Environmental Modelling and Assessment
- Principal Investigator: Marta Filipa Gomes Rodrigues
- Principal Contractor: National Laboratory for Civil Engineering (LNEC)
- Participating Institutions: University of Algarve (UAlg)
- Project advisor: Prof. António Melo Baptista, Oregon Health & Science University, USA
- Starting date: 01-07-2016
- Final date: 31-03-2020
- Funding: € 152.460,00

This report is structured in 12 sections, including the present introduction. Section 2 presents a general overview of the project, including the context and objectives, the workplan, the presentation of the team and a brief description of the case studies. The following sections, from 3 to 8, present the main objectives and results of each task of the project. Section 9 summarizes the advanced training of research fellows that was integrated in the project. Section 10 presents the list of publications. In section 11 a list of the institutions and people that collaborated with the project is presented. Finally, the main results and a critical appraisal are presented in section 12.

2 | The UBEST project

2.1 Context, objectives and workplan

In a context of shrinking habitats and loss of biodiversity, the good ecological quality of coastal areas is a key issue. Estuaries and coastal lagoons are among the most productive ecosystems on Earth and provide multiple ecosystem services (e.g., Barbier et al., 2011; de Groot et al., 2012). They harbor ecologically important habitats for fish, shellfish and birds, and, due to their buffering capacity, protect the coastal ocean from increased nutrient loads and other terrestrial contaminants (Cloern, 2001; Paerl, 2006). These coastal systems also support diverse human activities (e.g. marine transportation, fishing, tourism, and repository waters for domestic wastewater), providing economic resilience to coastal communities and protecting them from natural and anthropological hazards. However, over 400 coastal systems worldwide have been identified as eutrophic or hypoxic areas due to a significant growth of nutrients loadings from terrestrial anthropogenic activities (Selman et al., 2008). The growing human activities in coastal areas (Rabalais et al., 2009) and climate change (CC) may increase the hazards in these systems (Statham, 2012), and alter the ecosystems dynamics. CC effects, such as sea level rise, represent a major threat to the world's estuaries, via potential changes in the hydrologic regimes, increases in salinity, acceleration in the nutrients cycling and disruption of aquatic ecosystems (Pethick, 2001; Statham, 2012). Recent and predicted increases of nutrients loads to coastal systems (Rabalais et al., 2012) may exacerbate these impacts, reducing the regulating services provided by them, which value was estimated at about 25000 '2007 International\$'/ha/year (de Groot et al.; 2012). Thus, assessing how human-induced or climate drivers threaten the estuaries and coastal lagoons is fundamental for the daily and the long-term management of these water bodies (Paerl, 2006), as it can support the establishment of protection measures and foster better-informed decision-making.

Several data-based or model-based studies aimed to evaluate the physical and biogeochemical dynamics in coastal systems (e.g., Cravo *et al.*, 2014; Romero *et al.*, 2018; Dan *et al.*, 2019; Rodrigues *et al.*, 2019; Suari *et al.*, 2019; Aveytua-Alcazar, 2020). However, integrated anthropogenicclimate studies and management approaches combining the potentialities of numerical modelling and data analyses remain scarce (e.g., Rodrigues *et al.*, 2015b), mainly due to the challenges to integrate different sources of information that cover the relevant temporal and spatial scales. In this context, coastal observatories can be effective tools to overcome some of these challenges.

Coastal margin observatories are fundamental components of management in coastal regions (e.g., Baptista, 2006; Baptista *et al.*, 2015; Fortunato *et al.*, 2017a; Fennel *et al.*, 2019), as they offer the flexibility to handle both early-warning and long-term planning and to easily access large amounts of disparate data. These systems can comprise several layers of information, including the provision of historical and real-time monitoring data, short-term forecasts and hindcast scenarios. Crossing different temporal scales, coastal observatories allow to: i) identify and understand shifts in the

systems by providing long time-series of environmental data, ii) anticipate hazardous events by providing forecasts of water conditions (e.g., water levels, temperature), and iii) assess future trends (e.g., in response to CC) through the analysis of available simulations of scenarios.

Although there are many detailed and broad-scope monitoring systems of the ecological status of coastal systems worldwide (e.g. the LTER network, https://lternet.edu/), linking data with physicalbiogeochemical models is necessary to achieve a thorough understanding of the coastal dynamics in a context of CC and growing anthropogenic pressures. Coastal observatories, combining monitoring data and numerical models for physical processes (e.g., water levels, waves), are relatively wellestablished tools (e.g., Fortunato *et al.*, 2017a), but operational systems for assessing the biogeochemical status of coastal waters are still in their infancy (e.g., Fennel *et al.*, 2019). Numerical models, which simulate the physical and biogeochemical processes at the relevant spatial and temporal scales, are useful tools to complement the data and to exploit the ecosystems response to different scenarios (e.g., Megrey *et al.*, 2007; Charria *et al.*, 2016; Rodrigues *et al.*, 2019). In turn, consistent data allow the models' validation and provide complementary means to investigate the ecosystem evolution. Implemented in operational frameworks, integrated data-model approaches offer a continuous surveillance of the systems, allow the adjustment of existing monitoring strategies and provide a valuable repository of data and model predictions to support coastal management and science.

The scientific goal of UBEST was to improve the global understanding of the biogeochemical buffering capacity of estuaries and its susceptibility to future scenarios of anthropogenic inputs and climate change by deploying an innovative "coastal observatory". This observatory integrates several layers of information, from real-time data and forecasts to indicators, in a user-friendly web portal (Figure 2.1). To support the development of the observatory, demonstrate its applicability and promote the generalization of the conclusions, two Portuguese case studies were considered, the Tagus estuary and the Ria Formosa, a coastal lagoon.

The specific objectives of UBEST were:

i) the deployment of a monitoring network for biological and chemical parameters (e.g. chlorophyll-a, dissolved oxygen and nutrients) that will include an online biogeochemical station and a set of conventional stations;

ii) the implementation/improvement and validation of state-of-the-art, process-based, coupled hydrodynamic-biogeochemical models in each system;

iii) the quantification of the biogeochemical buffering capacity of each estuary under present conditions and for projected scenarios of sea level rise, changes in the hydrological regimes, air temperature and nutrients loads;

iv) the assessment of the estuarine physical and trophic conditions of the two estuaries under global classification metrics, and their comprehensive comparison with other estuaries worldwide.

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Figure 2.1 – Overall concept of the UBEST observatory and location of the application sites (Tagus Estuary and Ria Formosa)

To accomplish the proposed objectives, the research plan was built on six interlinked tasks (Figure 2.2):

- Task 1 Historical data compilation and analysis;
- Task 2 Monitoring network: conventional field campaigns and online station deployment and validation;
- Task 3 Implementation, validation and operational deployment of the coupled hydrodynamicbiogeochemical numerical models;
- Task 4 Quantification of the estuarine biogeochemical buffering capacity for present and future scenarios;
- Task 5 Global estuarine classification;
- Task 6 Management and knowledge transfer.

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Figure 2.2 – UBEST project workplan

2.2 Team

The project team is presented in Table 2.1. The project benefited from the advisory of the scientific consultant Professor António Melo Baptista from the Oregon Health & Science University (USA) and the Center for Coastal Margin Observation & Prediction (USA).

Institution	Researcher/Technician				
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2.3 Case studies

2.3.1 Tagus estuary

The Tagus estuary, located on the Portuguese west coast, is one of the largest estuaries in Europe with an area of about 320 km² (APA, 2016). The estuarine margins are intensively occupied, with a population of about one million inhabitants, and support diverse uses and activities (urban, industrial/harbors, agriculture, shellfish harvesting) and a major natural reserve, which is one of the most important sanctuaries for wintering or staging birds in Europe. There are sharp contrasts in the occupation of the margins: urban and industrial facilities dominate in the right margin, while agriculture predominates in eastern and southern marginal areas (Tavares *et al.*, 2015). The Tagus estuary has a complex morphology, with a deep and narrow inlet channel and a broad and shallow inner basin and an intertidal area of about 40% of the total estuarine surface (Castanheiro, 1986).

The circulation in the Tagus estuary is primarily driven by tides and, to a small extent, by river flow, wind, atmospheric pressure and surface waves (Fortunato *et al.*, 2017b). Tides are semi-diurnal, ranging from 0.55 m to 3.86 m at the coast (Guerreiro *et al.*, 2015), and the tidal propagation within the estuary is complex (Fortunato *et al.*, 1997, 1999). The main source of freshwater discharging into the estuary is the Tagus River, with an average flow of 370 m³/s (APA, 2012a). The Sorraia and the Trancão rivers also contribute to the freshwater inflow into the estuary. The estuary is often considered well-mixed, but stratification has been observed at high flow rates and low tidal ranges (Neves, 2010; Rodrigues and Fortunato, 2017).



Figure 2.3 – General overview of the Tagus estuary. Source: Portuguese coastline, Instituto Hidrográfico

In the context of the Water Framework Directive (WFD), the Tagus estuary is classified as a transitional water¹ of the typology A2 – mesotidal well-mixed estuary with irregular river discharge (Bettencourt *et al.*, 2004). Four water bodies² are delimited within the estuary (Ferreira *et al.*, 2005, 2006; Figure 2.4): Tejo-WB1, Tejo-WB2, Tejo-WB3 and Tejo-WB4. Tejo-WB1 (182 km²) corresponds to the downstream, narrow area of the estuary, and includes two lateral bays. Tejo-WB2 (159 km²) corresponds to the inner bay, with the exception of Cala do Norte that corresponds to Tejo-WB3 (96 km²). Tejo-WB4 (16.5 km²) is located in the upstream area of the estuary, in the area more influenced by the freshwater input from the Tagus river. The estuary is bound downstream by coastal waters (CWB-I-4, coastal waters adjacent to the Tagus estuary) and surrounded by several river water bodies (Figure 2.4).

Many studies showed the importance of the Tagus estuary in terms of sediments, nutrients, contaminants, plankton and fisheries dynamics and its interaction with the adjacent coastal area (e.g. Caçador *et al.*, 1996; Cabeçadas and Brogueira, 1997; Costa and Cabral, 1999; Cabral *et al.*, 2000; Moita, 2001; Cabeçadas *et al.*, 2004; Brogueira *et al.*, 2007; Gameiro and Brotas, 2010; Valente and Silva, 2009; Caetano *et al.*, 2012).



Figure 2.4 – Water bodies in the Tagus estuary (green) and adjacent coastal waters (blue), and surrounding river water bodies (grey). Data source: SNIAMB, http://sniamb.apambiente.pt/, December 2016

¹ Transitional waters are bodies of surface water in the vicinity of river mouths which are partly saline in character as a result of their proximity to coastal waters but which are substantially influenced by freshwater flows.

² Water body: a sub-unit in the river basin (district) to which the environmental objectives of the Water Framework Directive must apply.

2.3.2 Ria Formosa

The Ria Formosa, a coastal lagoon located in the south coast of Portugal, is the most important ecosystem in the region and is classified as a Natural Park, a Ramsar wetland and a Natura 2000 site. This ecosystem provides valuable resources for several economic activities in the region, namely tourism, aquaculture (e.g. major national producer of clams), shipping, fishing and salt production (50% of the national salt production) and it is used by several species as spawning and nursery areas.

This coastal lagoon is a shallow barrier island system with about 100 km² that extends along 55 km in the west-east direction with a maximum width of 6 km in north-south direction. This coastal lagoon has a large intertidal area, which represents about 50% of the total area, mostly covered by sand, muddy sandflats and salt marshes. The Ria Formosa exhibits very dynamic and complex physiographic and morphologic features. The lagoon is delimited by five sandy barrier islands (Deserta, Culatra, Armona, Tavira and Cabanas) and two peninsulas (Ancão and Cacela) and connects to the Atlantic Ocean through six inlets. The inlets are linked by a complex network of interconnected channels, allowing the recirculation of water within the system and a permanent exchange with the adjacent ocean (Matias et al., 2008; Alcântara et al., 2012). The western sub-embayment (Ancão, Faro-Olhão and Armona inlets) is responsible for about 90% of the tidal prism of the lagoon (Jacob et al., 2013). The mean depth is 3.5 m, ranging from 6 to 13 m in the main channels and inlets (Falcão and Vale, 1990; Barbosa, 2010; Cravo et al., 2014). This lagoon is under the influence of semidiurnal tides, subject to a mesotidal regime, with a tidal range varying between 1.5 and 3.5 m (Jacob et al., 2013). Water renewal is high (between 50-75% daily; Tett et al., 2003) and the contribution of freshwater is negligible. The water characteristics of this lagoon are strongly regulated by the tidal exchanges and mixing with the coastal waters (Rosa et al., 2019).



Figure 2.5 – Location and general overview of the Ria Formosa lagoon. Source: ESRI. Retrieved in January 2016

In the context of the WFD, the Ria Formosa is considered a coastal water³, particularly a mesotidal shallow lagoon (A4 typology; Bettencourt *et al.*, 2004), rather than a transitional water, and was divided into five water bodies (Figure 2.6). These are affected by distinct circulation patterns and human pressures, which influence the water properties (Ferreira *et al.*, 2005, 2006). Ria Formosa-WB1 (4.7 km² – APA, 2015) corresponds to the Ancão basin and to the western end of the lagoon. Ria Formosa-WB2 (33 km²) corresponds not only to the innermost part of the Ria Formosa and to the weaker hydrodynamic regime, but also to the area most influenced by anthropogenic pressures from the Faro and Olhão populations. Ria Formosa-WB3 (30.8 km²) is characterized by larger exchanges of water through the Faro-Olhão inlet (the major inlet, artificially fixed in 1929). Ria Formosa-WB4 (10.7 km²) comprises the Armona and the Fuzeta inlets and is one of the area bordered by Tavira and is characterized by lower salinities, due to the presence of a permanent freshwater source, the Gilão River (Newton and Mudge, 2003). The adjacent coastal water bodies surrounding the Ria Formosa lagoon represent the water bodies CWB·If-6 and CWB·II⁻7 (APA, 2015).



Figure 2.6 – Water bodies in the Ria Formosa and adjacent coastal waters (blue), and surrounding river water bodies (grey). Data source: SNIAMB, http://sniamb.apambiente.pt/, December 2016

Understanding the functioning of the Ria Formosa is crucial to preserve the intrinsic values of this ecosystem. Along time, in addition to biological studies, several others have been developed, tackling diverse aspects such as physical, chemical, geological processes and the lagoon dynamics coupling numerical modelling with field data (*e.g.*, Pilkey *et al.*, 1989; Falcão and Vale, 1990; Williams *et al.*,

³ Coastal waters are bodies of surface water on the landward side of a line, every point of which is at a distance of one nautical mile on the seaward side from the nearest point of the baseline from which the breadth of territorial waters is measured, extending, where appropriate up to the outer limit of transitional waters.

1998; Vila-Concejo *et al.*, 2003; Newton *et al.*, 2003, 2010; Loureiro *et al.*, 2005, 2006; Goela *et al.*, 2009; Dias *et al.*, 2009; Pacheco *et al.*, 2010; Alcântara *et al.*, 2012; Fabião *et al.*, 2016; Malta *et al.*, 2016).

3 | Task 1: Historical data compilation and analysis

3.1 Overview

The main objectives of this task were to identify the main spatial and temporal patterns of the physical, chemical and biological variables along the Tagus estuary and the Ria Formosa coastal lagoon over the past decades, and to understand their variations in the context of the climatic and hydrological variability and of the anthropogenic interventions in these estuaries. Moreover, this task also aimed to develop the UBEST web portal, which is at the core at the coastal observatory providing the access to all the layers information (e.g., historical data, model forecasts and indicators).

The main results of this task, described below, were:

- an improved understanding of the past physical, chemical and biological evolution of the Tagus estuary and of the Ria Formosa and its relation to climatic and anthropogenic drivers;
- a new data repository that stores the historical data compiled and the data acquired during the project;
- an innovative web portal and associated services that provides access to the information to the users (http://portal-ubest.lnec.pt).

3.2 Historical data review, compilation and analysis

A literature review and compilation of historical data, from the 1980s until present, of hydrological (e.g. river flows), atmospheric (e.g. air temperature, precipitation, solar radiation), chemical (e.g. salinity, ammonium, silicates, dissolved oxygen) and biological (chlorophyll *a*) data was performed to provide a background characterization of the Tagus estuary and the Ria Formosa. This review also included an identification of the main anthropogenic interventions in these systems, that may potentially have affected the circulation and biogeochemical dynamics within each estuary (e.g. implementation of dredging plans, discharges of domestic and industrial effluents, agricultural practices, regulations of the river flows). The main spatial and temporal patterns of the physical, chemical and biological variables over the past decades were then characterized and their main variations were also analyzed in the context of the climatic and hydrological variability and of the anthropogenic interventions in the systems. The compiled data were then integrated in a data repository described in section 3.3 and the data or the metadata (depending on the owner of the data) are available to the users through the web portal (section 3.4).

Several environmental studies based on observations have been carried out in the Tagus estuary (e.g. Martins *et al.*, 1982, 1983; Silva *et al.*, 1986; Brogueira and Cabeçadas, 2006; Gameiro *et al.*, 2007; Valença *et al.*, 2011; Caetano *et al.*, 2016), providing important historical data to understand the Tagus estuary biogeochemical and water quality dynamics. Table 3.1 provides a summary of the main

environmental data compiled and analyzed for the Tagus estuary. Examples of dissolved oxygen and chlorophyll *a* variation in the Tagus estuary over the past years are presented in Figure 3.1 and Figure 3.2, respectively.

Dataset Title	Geographic Bounding Coordinates	Temporal Coverage	Variables	Sampling Description	Source
IBM	Three stations located along the estuary	1967- 1968	Physical and biological variables, including temperature and chlorophyll <i>a</i> .	Fortnightly sampling between June 1967 and May 1968	Silva <i>et al.</i> , 1969
CEPOL	-	1970- 1975	Several physical, chemical and biological variables, including nutrients	-	In Silva, 2003
EAET	Several stations covering the entire estuary and its main affluents (Tagus and Sorraia rivers)	1980- 1983	Several physical, chemical and biological variables, including salinity, temperature, pH, dissolved oxygen, ammonium, nitrate, nitrite, phosphate, silicate, TSS, chlorophyll <i>a</i> .	Monthly synoptic surveys, during high tide and low tide (1980-81) Samples were collected at several depths	Martins <i>et</i> al., 1982, 1983 Silva et al., 1986
INTAGUS	Longitudinal profiles in the downstream area of the Tagus estuary (Barra- Corredor, Cala do Norte, Cala de Samora)	1988	Salinity and water temperature	Vertical sampling during high tide and low tide	Neves, 2010
VQM	Several stations covering the entire estuary, from the adjacent coastal area until Muge	1985- 2009	Several physical, chemical and biological variables, including salinity, temperature, pH, dissolved oxygen, ammonium, nitrate, nitrite, phosphate, silicate, TSS, chlorophyll <i>a</i>	Sampling periodicity changed through time (six samples per year to two samples per year) Samples were collected during ebb conditions, at both bottom and surface	Valença <i>et</i> <i>al.</i> , 2011
FCUL_ CABRITA	Three stations covering the entire estuary, from the inlet until Vila Franca de Xira	1994- 1995	Several physical, chemical and biological variables, including salinity, temperature, ammonium, nitrate, nitrite, chlorophyll a	Samples were collected during high tide of neap tides, at several depths	Cabrita <i>et</i> <i>al.</i> , 1999a
IPMA0104	Several stations covering the estuary from the inlet until Salvaterra de Magos / Valada	2001- 2004	Several physical, chemical and biological variables, including salinity, temperature, dissolved oxygen, ammonium, nitrate+ nitrite, phosphate, silicate, TSS, chlorophyll a	Sampling in Mar/2001, Jul/2001, Feb/2004 Samples were collected during ebb conditions at several depths	Brogueira and Cabeçadas, 2006 Brogueira <i>et al.</i> , 2007

Table 3.1 – Summary of the Tagus estuary environmental data

Dataset Title	Geographic Bounding Coordinates	Temporal Coverage	Variables	Sampling Description	Source
EEMA	Several stations covering the estuary from the inlet until Vila Franca de Xira	2009- 2010	Several physical, chemical and biological variables, including salinity, temperature, pH, dissolved oxygen, ammonium, nitrate+ nitrite, phosphate, silicate, TSS, chlorophyll a	Three surveys (Oct/2009, Feb/2010 and Apr/2010) Samples were collected during ebb conditions, at both bottom and surface	Ferreira and Vale, 2010 Brito et al., 2012a Caetano et al., 2016
FCUL_ VALORSUL	Four stations covering the middle-upstream area of the estuary	1999- 2016	Several physical, chemical and biological variables, including salinity, temperature, pH, ammonium, nitrate+ nitrite, phosphate, silicate, TSS, chlorophyll <i>a</i>	Monthly surveys with some gaps during the sampling period Samples were collected during ebb conditions	Gameiro <i>et</i> <i>al.</i> , 2007 Gameiro and Brotas, 2010 Brotas, unpublished data
EPAL	Several stations covering the estuary	2004- 2016	Several physical, chemical and biological variables, including salinity, temperature, dissolved oxygen, pH, chlorophyll a	Sampling periodicity varied through time	EPAL, unpublished data
EPAL_ SIMTEJO	Online station located near Algés	2012- 2014	Several physical, chemical and biological variables, including salinity, temperature, dissolved oxygen, pH, turbidity, chlorophyll <i>a</i> , currents	Data is acquired in continuous (with gaps during the period)	EPAL, unpublished data
EPAL_ SIMARSUL	Online station located near Montijo/Alcochete	2012- 2013, 2015- 2017	Several physical, chemical and biological variables, including salinity, temperature, dissolved oxygen, pH, turbidity, chlorophyll <i>a</i> , currents	Data is acquired in continuous (with gaps during the period)	EPAL, unpublished data
PREPARED_SIGEA	Estuarine marginal area between Alcântara and Terreiro do Paço	2011- 2014	Several physical and chemical variables, including salinity, temperature, pH, dissolved oxygen, ammonium, nitrate+ nitrite and phosphate	Five surveys, covering one entire tidal cycle. Samples were collected at both bottom and surface	David <i>et al.</i> , 2014, 2015 Rodrigues <i>et al.</i> , 2015a
LNEC_ ALCANTARA	Online station located near Alcântara	2013- 2014, 2016- 2017	Several physical and chemical variables, including salinity, temperature, pH, dissolved oxygen	Data is acquired in continuous (with gaps during the period)	LNEC, unpublished data



Figure 3.1 – Dissolved oxygen in the water bodies of the Tagus estuary during the 1980's (Martins *et al.*, 1982, 1983; Silva *et al.*, 1986) and 2009-2010 (Caetano *et al.*, 2016) field campaigns



Figure 3.2 – Chlorophyll *a* concentrations in the middle Tagus estuary (Tejo-WB3) between 1980-1981 (A, Martins *et al.*, 1982, 1983; Silva *et al.*, 1986, at station 3.9), 2000-2015 (B, Gameiro *et al.*, 2007; Brotas, unpublished data, at station 4) and 2009-2010 (C, Caetano *et al.*, 2016, at station 4)

Many studies have also been carried out in the Ria Formosa, mainly after the 1960's-1970's, to analyze the water characteristics or evaluate its quality (e.g., Silva and Assis, 1970; Lima and Vale, 1977; Cunha and Massapina, 1984; Falcão *et al.*, 1985; Brockel, 1990; Cortez, 1992; Thiele-Gliesche, 1992). However, these data are scattered, with large temporal and spatial discontinuities, preventing an accurate evaluation of the historical evolution of water quality. Table 3.2 provides a summary of the main environmental data compiled and analyzed for the Ria Formosa. Figure 3.3 and Figure 3.4 present, respectively, examples of the nutrients and chlorophyll *a* concentrations in the Ria Formosa over the past years.

Geographic Dataset Temporal Bounding Variables Sampling Description Source Title Coverage Coordinates Three stations Two monthly sampling. covering the 1967-Temperature, salinity, Samples were collected Silva and NEIBM 1968 during low tide at surface western zone of chlorophyll a Assis, 1970 the lagoon level Several physical, Sampling in Jul/1976 in Several stations chemical and biological neap tide. Samples were Lima and SEP 1976 variables, including pH, collected during 3 covering the Vale, 1977 entire lagoon dissolved oxygen, %DO, complete tidal cycles at nitrite, phosphate different depths Several physical, chemical and biological Monthly surveys from Two stations variables, including July/1978 to located in the 1978temperature, salinity, Benoliel, CPOL December/1979. lagoon and one at 1979 dissolved oxygen, 1982 Samples were collected sea ammonium, nitrate, at several depths nitrite, phosphate, silicate, TSS Several physical, chemical and biological variables, including Several stations temperature, salinity, pH, Monthly surveys. Benoliel, located in the 1980-VCQA dissolved oxygen, %DO, Samples were collected 1984, 1989, lagoon and one at 1984 ammonium, nitrate, at several depths 1985 sea nitrite, phosphate, silicate, chlorophyll a, TSS Several physical, chemical and biological variables, including Several stations Sampling in May/1982. Cunha and covering the inner temperature, salinity, pH, Samples were collected INIP 1982 Massapina, area of the lagoon dissolved oxygen, %DO, during neap tide, in low 1984 and 3 at sea nitrate, phosphate, and high tide silicate, chlorophyll a, phaeopigments Several physical. Two monthly sampling chemical and biological between the period Three stations variables, including 1984-August/1984-Jan/1985. Falcão et INIP_8485 covering the Samples were collected 1985 temperature, salinity, pH, al., 1985 Tavira area nitrate, nitrite, in low, intermediate and phosphate, silicate high tide at surface level Several physical, chemical and biological Fortnightly sampling variables, including between Several stations temperature, salinity, pH, September/1985 to covering the inner 1985-Falcão. FALCAO dissolved oxygen, September/1986. area of the lagoon 1986 1996 Samples were collected nitrate, nitrite, and some inlets during spring and neap phosphate, silicate, chlorophyll a, tide, in low and high tide phaeopigments Several physical, Sampling periodicity chemical and biological changed through time Several stations variables, including (six samples per year to 1985-Valença et temperature, pH, %DO, VQM two samples per year) covering the 2009 al., 2011 entire lagoon ammonium, nitrate, Samples were collected nitrite, phosphate, at both surface and chlorophyll a, TSS bottom

Table 3.2 – Summary of the Ria Formosa environmental data

Dataset Title	Geographic Bounding Coordinates	Temporal Coverage	Variables	Sampling Description	Source
NEWTON	Several stations covering the entire lagoon	1987- 1989	Several physical, chemical and biological variables, including temperature, salinity, %DO, ammonium, nitrate, nitrite, phosphate, silicate	Monthly surveys from June/1987 to December/1989. Samples were collected during several tidal conditions	Newton, 1995
BARBOSA	Three stations, including two located in the inner area of the lagoon and one in the inlet zone in the western sector	1988	Several physical, chemical and biological variables, including temperature, %DO, Chlorophyll <i>a</i> , phaeopigments	Sampling period during April-October/1988. Samples were collected in mid-ebb tide at surface level	Barbosa, 1989
BROCKEL	Two stations, including Ancão inlet and Esteiro do Ramalhete	1988- 1989	Several physical, chemical and biological variables, including dissolved oxygen, nitrate, nitrite, phosphate, silicate	Sampling period between May/1988- Jun/1989. Samples were collected weekly, at several depths	Brockel, 1990
THIELE	Four stations covering the western area of the lagoon	1988- 1989	Temperature, dissolved oxygen, Chlorophyll a	Sampling during the period of October/1988- November/1989. Samples were collected every two weeks at surface level	Thiele- Gliesche, 1992
CORTEZ	Several stations covering the entire western sector of the lagoon	1989- 1991	Several physical, chemical and biological variables, including temperature, salinity, pH, ammonium, nitrate, nitrite, phosphate, silicate, TSS	Four surveys (Jul/1989, Feb/1991, May/1991, Oct/1991). Samples were collected at different depths	Cortez, 1992
BARBOSA	Two stations located in the western zone of the lagoon	1991- 1993	Temperature, salinity, chlorophyll <i>a</i>	Sampling from March/1991 to January/1993. Samples were collected in mid- ebb and mid-flood at surface level	Barbosa, 2006
CRAVO	Two stations located in the inner area of the lagoon, close to Faro	1991- 1992	Several physical, chemical and biological variables, including temperature, salinity, pH, dissolved oxygen, %DO, ammonium, nitrate, nitrite, phosphate, silicate, TSS	Sampling between April/1991 and May/1992. Samples were collected weekly at surface and bottom during low and high tide	Cravo, unpublished data
CONDINHO	Two stations located in the western zone of the lagoon	1998- 1999	Several physical, chemical and biological variables, including ammonium, nitrate, nitrite, phosphate, silicate	Sampling during October/1998- October/1999. Samples were collected in high tide at surface level	Condinho, 2004
PEREIRA	Three stations covering the bridge of Faro beach, Ramalhete and Ancão inlet	2000- 2002	Several physical, chemical and biological variables, including temperature, salinity, ammonium, nitrate, nitrite, phosphate, silicate	Sampling in 2000 (September, December), 2001 (March, June, September, December,) and 2002 (April, July). Samples were collected in low, mid and high water, during spring and neap tides	Pereira et al., 2007

Dataset Title	Geographic Bounding Coordinates	Temporal Coverage	Variables	Sampling Description	Source
LOUREIRO	Three stations covering the bridge of Faro beach, Ramalhete and Ancão inlet	2001- 2002	Several physical, chemical and biological variables, including temperature, salinity, ammonium, nitrate, phosphate, chlorophyll a	Sampling in 2001 (June, September) and 2002 (April, July). Samples were collected in low and high water at surface level, during spring and neap tide	Loureiro <i>et</i> <i>al.</i> , 2005
BRITO	Three stations covering the Ramalhete, Faro beach and its bridge	2006- 2008	Several physical, chemical and biological variables, including temperature, salinity, %DO, ammonium, nitrate, nitrite, phosphate, silicate, chlorophyll a	Sampling every two weeks between April- October/2006 and March/2007- February/2008.	Brito, 2010
ALCANTARA09	Station located in Ancão inlet	2009	Several physical, chemical and biological variables, including temperature, salinity, pH, dissolved oxygen, nitrate, nitrite, phosphate, silicate, chlorophyll a	One complete tidal cycle in April/2009. Samples were collected in spring tide at several depths	Alcântara et al., 2012
EEMA	Several stations covering the entire lagoon	2010	Several physical, chemical and biological variables, including temperature, salinity, pH, dissolved oxygen, ammonium, nitrate, nitrite, phosphate, silicate	Sampling in March/2010. Samples were collected in low and high water at surface and bottom levels	INAG, APA, 2010
OVELHEIRO	One station located in the channel of Faro beach	2010	Several physical, chemical and biological variables, including temperature, salinity, pH, dissolved oxygen, %DO, ammonium, nitrate, nitrite, phosphate, silicate, chlorophyll <i>a</i> , phaeopigments	Sampling in November/2010 during a complete tidal cycle. Samples were collected both surface and bottom levels	Ovelheiro, 2011
PONTAPE	One station located in the channel of Faro beach	2011	Several physical, chemical and biological variables, including temperature, salinity, pH, dissolved oxygen, %DO, ammonium, nitrate, nitrite, phosphate, silicate, chlorophyll a	Two complete tidal cycle in June and July 2011. Samples were collected at surface level	Pontapé, unpublished data
COALA	Several stations located in the western zone of the lagoon, including the three inlets and channels	2011- 2013	Several physical, chemical and biological variables, including temperature, salinity, pH, dissolved oxygen, %DO, ammonium, nitrate, nitrite, phosphate, silicate, chlorophyll <i>a</i> , phaeopigments, TSS	Sampling between November/2011- July/2013 with some gaps	COALA project, unpublished data



Figure 3.3 – Ammonium (NH₄⁺), nitrate (NO₃⁻), phosphate (PO₄³⁻) and silicate (SiO₄⁴⁻) annual minimum and maximum concentrations between 1976 and 2013 (all data) in each water body of the Ria Formosa



Figure 3.4 – Chlorophyll *a* minimum and maximum concentrations from 1967 to 2013 (all data acquired) along the water bodies of the Ria Formosa

Globally, regarding the biogeochemical dynamics of both systems estuaries presents seasonal patterns typical of temperate systems. In the Ria Formosa, the water characteristics depend strongly, not only on the seasonal variability, but also on tidal mixing, what is reflected in both spatial and short-term temporal dimensions (dependent on residence time and tidal range). The tides promote the propagation of the water masses into the lagoon and influence the physical-chemical and biological quality of the water, as well as the dynamics of the dissolved and particulate material (Falcão and Vale, 1990; Cravo *et al.*, 2014). Tides are also an important driver of the biogeochemical dynamics in the Tagus estuary, but the freshwater input also plays an important role in this system in controlling this dynamics. Residence time has been pointed out as the main factor influencing phytoplankton annual variability (Brotas and Gameiro, 2009) and varies considerably throughout the estuary (Oliveira and Baptista, 1997).

Anthropogenic pressures affecting the nitrogen and phosphorus loads are typically of the same type in the Tagus estuary and the Ria Formosa, including the discharge from urban and industrial effluents and agriculture practices. However, remarkable differences are found between the Ria Formosa and the Tagus estuary on the estimated magnitudes of nutrient loads, which are about two orders of magnitude higher in the Tagus estuary, highlighting the larger anthropogenic pressures in this system.

Significant variations occurred in nitrogen and phosphorous concentrations in the Tagus estuary between 1985 and 2009 (Valença *et al.*, 2011). A "Low" nutrient quality status was proposed for this estuary (Caetano *et al.*, 2016), due to the phosphate concentrations in the upstream area. The downstream area of the estuary was classified as "High" quality and the middle estuary was identified to be at risk, due to relatively high concentrations of both phosphorus and nitrogen.

Decreasing trends of nutrients concentrations since the 1970's have been found in the Ria Formosa. The highest concentrations of nutrients were found in the inner areas of the lagoon, where the water renewal is lower and the urban and agriculture inputs are more intense. The inlets and main channels of the Ria Formosa, where the water exchanges with the Atlantic Ocean are stronger, limit the impact of nutrients from anthropogenic origin and eutrophication problems (Newton *et al.*, 2003; Roselli *et al.*, 2013).

Light is often considered as the main limiting factor for phytoplankton growth in the Tagus estuary (Gameiro and Brotas, 2010). Regarding chlorophyll *a*, both the Tagus estuary and the Ria Formosa were classified as in "High" or "Good" ecological status (Brito *et al.*, 2012a,b) and are not considered sensitive to eutrophication (Ferreira *et al.*, 2003).

Further details about the historical data analysis can be found in Rodrigues et al. (2017b).

3.3 Data repository

A data repository was developed to store the compiled historical data and the data acquired during the project. This repository is a web-based application supported by a relational database. The application is built on the Django web framework, modeling a simplified version of the Observation Data Model 1.1

design specification (Tarboton *et al.*, 2008), and backed by a PostgreSQL (PostgreSQL, 2020) relational database management system.

The Data Model (DM, Figure 3.5) allows a detailed characterization of the data, as most models (data entities) describe meta-information related to actual measurements or results. Such models contain curated information about important aspects, like location (Site), collection (Dataset), among others. ScalarValue and the optional ScalarValueTideDetails models hold all the actual measurements or results.



Figure 3.5 – Data Model schema of the repository: entity-relation model diagram

The repository application is a simplified one and has only the essential components (apps in Django world) to fulfill its purpose, namely *datamodel*, *gateway* and *importer*. The *datamodel* implements the DM, which stores all the data and facilitates basic management through the Django's built-in administration portal. The *gateway* provides the means to fetch most data conveniently via a REST API. Finally, the *importer* offers several ways to load data into the repository, from local CSV files to specific probes, including a mini framework to simplify the addition of new methods.

3.4 UBEST observatory portal

The approach used to build the UBEST observatory portal relied on the concept of a user-friendly web portal that provides several layers of information, with different levels of aggregation and different access conditions depending on data access rules. Users may require information about the processes for different purposes. Hence, the observatory should provide information at different levels of aggregation. For instance, some users may want to look at time series of the basic variables, others may only want to examine their statistics, while others still may want to examine a higher level of aggregation through indicators based on several variables. Also, users may want to explore the answers with different datasets. Therefore, the observatory should provide information of different sources, namely both field data and model results.

The UBEST observatory portal (http://portal-ubest.lnec.pt/) is composed by a web portal, which provides detailed information to the user about the water conditions in a given coastal system, and the associated services, which provide that information, namely the data repository and the WFS/WMS map server (Figure 3.6).



Figure 3.6 – Architecture of the UBEST observatory portal

The web portal is developed in Django, a Python web framework aimed for full-stack web development. Thus this web portal has a Frontend, where the web framework provides the HTML pages for the user interactions, and a Backend (with PostgreSQL Database), where the web framework processes the user requests (e.g., as page loading or data fetch) and the web portal data are stored on the database (Figure 3.6). Other technologies are applied on the Frontend pages, such as Openlayers (map viewer) and Javascript (web scripting language). The following dashboards compose the UBEST web portal:

- 'Today' (Figure 3.7) is an operational dashboard that presents a snapshot of the current state of the coastal system, including all the available data and forecasts for the current day; this dashboard is easily configurable by the users for their particular interests, providing mechanisms to show or hide the features that they wish to see;
- 'Data' (Figure 3.8) gives the user the ability to access, view and download field data at all available stations. Available data are organized in several physical (e.g., water levels, salinity), chemical (e.g., dissolved oxygen, ammonium, phosphate, pH) and biological (e.g., chlorophyll *a*) variables. This dashboard allows the user to search and filter stations with available data by variable, value condition, date and/or water body. Several other functionalities are available, including charts of the selected variables (that can be exported as image files) and a 'View/Export Data' menu that lists the data and allows the user to export it as a csv file. The 'Data' dashboard also provides statistics of the data available at each station;
- 'Forecasts' (Figure 3.9) displays a 48-hour forecast of physical and biogeochemical variables from operational models. This dashboard allows the access to 1) model forecasts on a map and to follow its evolution by vertical level or by time (48 hours), 2) model comparison with available field data and to view/export these data, and 3) the access to 'virtual sensors' that allow users to probe the model results for any selected point in the computational domain and view/export the model forecasts;
- 'Scenarios' (Figure 3.10) presents the system's susceptibility to CC or anthropogenic pressures scenarios through hindcast model simulations results. The model results are made available through the ncWMS services as maps with statistics (means, maxima and minima) of the physical, chemical and biological variables. Besides viewing the maps, the user can also see the value of each variable at a selected location;
- 'Indicators' (Figure 3.11) provides synthesized information using indicators for the circulation and water quality status that allows the user to assess possible changes in the coastal system dynamics and biogeochemistry. The classification proposed by Geyer and MacCready (2014) is used to assess the circulation and the mixing conditions. Regarding the water quality/biogeochemistry two indicators are available: the chemical status of nutrients based on Caetano *et al.* (2016) and the Trophic index (TRIX, Vollenweider *et al.*, 1998).



Figure 3.7 – 'Today' dashboard: access to maps of model forecasts (e.g., water temperature) and to real-time field data (e.g., chlorophyll *a* and water temperature)



Figure 3.8 – 'Data' dashboard: access to data, both historical and real-time, and data statistics

Home UBEST-Today mfrodrigues (LNEC_ADMIN) (User) * Data -Forecasts -Scenarios Indicators FR 2-6 25.0 20.0 15.0 + 10.0 **i** 5.0 Model Comparison Virtual Sensors

Figure 3.9 – 'Forecasts' dashboard: access to model forecasts, model-data comparisons and virtual sensors



Figure 3.10 – 'Scenarios' dashboard: access to statistics of hindcast model simulations for climate change and anthropogenic pressures scenarios

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Figure 3.11 – 'Indicators' dashboard: access to indicators for circulation and water quality status

The UBEST observatory portal relies on information available from the data repository and the WFS/WMS map server. The data repository (section 3.3) provides data from several stations, obtained by in-situ sensors that measure different variables and automatically upload them in real-time by internet to the repository. The WFS/WMS map server provides information to the Forecasts, Scenarios and Indicators pages and is automatically fed by daily operational simulations (section 4.3).

Regarding the dependent services (Figure 3.6) – WFS/WMS map server and data repository –, requests to fetch data directly from the WFS/WMS map server are made on the Frontend, while requests to fetch data directly from the repository are made on both the Frontend and the Backend. To fetch the models' data from the WFS/WMS map server, the page (Frontend) sends a Javascript AJAX request to the ncWMS (Blower *et al.*, 2013) service to return an image of the model results that can be loaded to the page as a layer on the map viewer. To fetch data from the repository, the page (Frontend) sends a Javascript AJAX request to the Backend, which sends another request to Repository to return the JSON data back to the Frontend.

Further details about the UBEST observatory portal can be found in Rodrigues *et al.* (submitted, 2020).

4 | Task 2: Monitoring network: conventional field campaigns and online station deployment and validation

4.1 Overview

The main objectives of this task were to complement the existing data with field campaigns and to deploy an online monitoring station for physical-chemical-biological variables, with the goal to provide an overall biogeochemical characterization of the Tagus estuary and Ria Formosa over the relevant spatial and temporal scales.

The main results achieved, described below, were:

- the acquisition of complementary physical, chemical and biological data in the Tagus estuary and Ria Formosa through conventional field campaigns;
- the deployment of a state-of-the-art biogeochemical online probe and maintenance of real-time monitoring stations;
- the online acquisition of real-time data and uploading to the data repository;
- the conception, assembling and testing of a low-cost sensor for water levels.

4.2 Field campaigns

4.2.1 Tagus estuary

To characterize the seasonal variation along the Tagus estuary three main field campaigns were carried out in 2018 (May 10, September 27 and November 6). Samplings of physical, chemical and biological parameters were collected at seven stations (Figure 4.1, Figure 4.2). The seven sampling stations were chosen to allow the best coverage of the entire estuary, together with the boundary (end-members) water bodies (Tagus river in Muge/Valada – station 1, and coastal area in Cascais – station 7). Stations 2-6, in particular, cover all the Tagus estuary water bodies: station 2 – Vila Franca de Xira in TE-WB4, station 3 – Póvoa de Santa Iria in TE-WB3, station 4 – channel in TE-WB2, station 5 – channel in TE-WB1 and station 6 – Algés in TE-WB1. Stations 1, 2, 3, 6 and 7 were located on the shore; stations 4 and 5 were located in the middle of the channel and the sampling was performed using a boat that navigated between the two stations.

In-situ measurements of temperature, salinity, pH and dissolved oxygen (DO) (concentration in mg/L and saturation %) were performed with YSI multiparameter probes, which were duly calibrated prior to each field campaign. Water samples were collected (using Niskin bottles, Van Dorn bottles or sampling cups) for the determination of dissolved oxygen, nutrients, total suspended solids and chlorophyll *a*. The water samples were preserved in thermal containers with ice until the beginning of the laboratorial filtration processing. Measurements and water samples were collected only at the surface at stations 1 and 2 due to their shallowness, and at the surface and near the bottom in the
remaining stations. In addition, during the first field campaign vertical profiles were sampled at stations 4 and 5 to assess the variability along the water column. Measurements were performed during approximately one semidiurnal tidal cycle (~12 hours). Sampling intervals were: two hours at stations 2, 3 and 6; three hours at stations 4 and 5 (low and high tide, mid-flood and mid-ebb); and at low and high tide at stations 1 and 7 (end-members).



Figure 4.1 – Location of the sampling stations in the Tagus estuary



Figure 4.2 – Sampling stations in the Tagus estuary: a) station 1 – Muge/Valada, b) station 2 – Vila Franca de Xira, c) station 3 – Póvoa de Santa Iria, d) stations 4 and 5 – channel, e) station 6 – Algés and f) station 7 – Cascais

The water samples used for the determination of nutrients and total suspended solids concentrations were filtered using Gellman-Pall filters (mixed esters of cellulose) with 0.45 µm porosity. The water samples used for the determination of chlorophyll *a* were filtered with filters Whatman GF/F (0.7 µm porosity). The nutrients concentration (nitrate, nitrite, ammonium, phosphate and silicate) was determined through specific spectrophotometric methods described by Grasshoff *et al.* (1983). Chlorophyll *a* was determined using the spectrophotometric method described by Lorenzen (1967). Total suspended solids concentration was determined using the gravimetric method described by APHA (2002). The Winkler method (Winkler, 1888) was used to confirm the concentrations of the dissolved oxygen measured *in-situ*.

A summary of the water characteristics found at each sampling station is presented in Table 4.1. The variability of temperature, salinity, percentage of dissolved oxygen (measured *in-situ*), chlorophyll *a*, total suspended solids and inorganic nutrients are shown in Figure 4.3, Figure 4.4 and Figure 4.5. Data from the field campaigns are accessible in the web portal (section 3.4).

Variable	Station 1	Station 2	Station 3	Station 4	Station 5	Station 6 ¹	Station 7
Temperature	17.5	20.3	18.0	18.0	17.5	17.1	15.7
(°C)	(14.5-21.5)	(14.5-23.0)	(15.0-23.0)	(14.8-22.7)	(154-22.0)	(14.9-21.0)	(13.9-18.8)
Salinity	0.18	1.1	26.7	27.3	29.6	33.7	35.5
	(0.15-0.21)	(0.2-6.7)	(17.8-30.9)	(22.5-32.5)	(24.4-34.8)	(32.5-35.8)	(34.6-36.0)
рН	7.9	8.0	7.9	8.2	8.2	8.0	8.1
	(7.4-8.5)	(7.6-8.6)	(7.5-8.1)	(8.0-8.3)	(8.0-8.3)	(7.7-8.1)	(8.0.8.2)
Dissolved	9.2	9.4	7.3	7.8	8.2	7.3	7.7
Oxygen (mg/L)	(8.0-11.1)	(7.7-11.0)	(6.0-9.4)	(6.2-8.7)	(6.8-9.4)	(7.0-7.5))	(6.6-8.6)
Oxygen	96	105	90	97	102	93	96
saturation (%)	(82-118)	(77-126)	(73-111)	(83-107)	(87-116)	(89-98)	(81-113)
Chlorophyll <i>a</i>	4.9	11.6	2.4	1.5	1.5	1.0	0.6
(µg/L)	(1.6-9.2)	(4.8-23.9)	(0.3-9.1)	(0.7-3.8)	(0.4-4.2)	(0.3-3.7)	(0.4-0.8)
Ammonium	1.2	1.1	15.5	3.8	3.1	4.3	1.0
(µM)	(0.4-1.8)	(0.2-6.3)	(5.2-29.3)	(1.6-7.8)	(0.5-7.3)	(2.5-6.5)	(0.2-1.9)
Nitrate	50.5	59.2	23.2	18.0	13.8	9.5	6.0
(µM)	(16.9-64.3)	(39.9-74.5)	(9.6-40.4)	(9.7-29.5)	(4.6-22.8)	(4.7-13.8)	(2.4-8.9)
Nitrite	0.3	0.6	1.6	0.9	0.8	0.7	0.4
(µM)	(0.2-0.5)	(0.4-1.1)	(0.6-3.0)	(0.6-1.3)	(0.3-1.3)	(0.5-0.9)	(0.3-0.5)
DIN	52.0	63.2	40.4	22.7	17.6	14.5	7.3
(µM)	(18.1-66.3)	(40.9-75.8)	(17.5-65.4)	(13.0-38.6)	(6.4-31.4)	(7.7-20.8)	(3.7-10.4)
Phosphate	2.6	2.9	2.2	1.4	1.1	0.9	0.5
(µM)	(0.8-3.7)	(1.5-6.0)	(1.1-3.6)	(0.8-2.6)	(0.4-2.4)	(0.5-1.2)	(0.2-0.8)
Silicate	89.2	85.5	31.2	27.6	18.4	10.6	4.5
(µM)	(36.2-114.7)	(73.3-92.5)	(10.8-62.5)	(14.2-47.0)	(3.6-33.8)	(6.4-16.8)	(3.0-5.8)
Suspended	8.7	51.5	116.4	28.9	10.8	68.8	7.7
Solids (mg/L)	(5.8-13.7)	(7.2-161.6)	(10.4-547.0)	(3.1-160.3)	(1.0-57.5)	(18.3-213.4)	(2.8-16.6)

 Table 4.1 – Mean and range (minimum-maximum) of the water quality variables at each sampling station for the three seasonal campaigns. See Figure 4.1 for the location of the stations

¹ For station 6 the statistics are only presented for the September and November field campaigns.

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Figure 4.3 – Water temperature and salinity in the Tagus estuary. The water level variation at the Cascais tidal gauge (http://www.dgterritorio.pt/) is shown (gray line). See Figure 4.1 for the location of the stations; the location of station 6 was 6A during the May field campaign



Figure 4.4 – Oxygen saturation, chlorophyll *a* and suspended solids (SS) concentration in the Tagus estuary. The water level variation at the Cascais tidal gauge (http://www.dgterritorio.pt/) is shown (gray line). See Figure 4.1 for the location of the stations; the location of station 6 was 6A during the May field campaign

40 40 40 2 2 30 30 30 Ē -Ē Ē Water level ((M^{rl}) ₊[₽]HN o level o level (M 1) 20 ₩<u>1</u>20 Water Water Ť +"HN 10 10 -1 -1 10 + Ъ 7 ₽₽ X - \diamond 0 0 12:30 15:30 18:30 21:30 12:30 15:30 18:30 21:30 9:30 18:30 21:30 6:30 9:30 6:30 9:30 6:30 12:30 15:30 Hour (September 27, 2108) Hour (May 10, 2108) Hour (November 6, 2108) 100 100 100 2 2 80 80 80 Water level (m) - o -Water level (m) Ē ل Water level (ا 60 60 60 NO3- (µM) 00 -⁶⁰ 40 (MIL) No.-40 40 20 20 20 Ŧ 0 -2 0 -2 0 -2 6:30 12:30 15:30 12:30 18:30 21:30 15:30 18:30 21:30 12:30 15:30 18:30 21:30 9:30 6:30 9:30 6:30 9:30 Hour (September 27, 2108) Hour (November 6, 2108) Hour (May 10, 2108) 8 2 8 2 8 2 6 6 6 1 1 o 1 r level (m) 1 o level (m) 1 Ē o -level (PO4³⁻ (μM) PO₄³⁻ (μM) РО4³⁻ (µM) 4 4 4 ל Water ו∕ Water Water 2 2 2 0 12:30 15:30 18:30 21:30 12:30 15:30 18:30 6:30 9:30 9:30 21:30 12:30 15:30 18:30 21:30 6:30 6:30 9:30 Hour (May 10, 2108) Hour (September 27, 2108) Hour (November 6, 2108) 120 120 120 100 100 100 level (m) Ē Ē 80 80 80 ل Water level (ا o level () 편 60 (M1) (M1) 60 60 L Water ⊮ Water Sio4 Si04 °0 40 40 40 20 20 20 + 0 0 n -2 -2 -2 6:30 9:30 12:30 15:30 18:30 21:30 6:30 9:30 12:30 15:30 18:30 21:30 6:30 12:30 15:30 18:30 21:30 9:30 Hour (May 10, 2108) Hour (September 27, 2108) Hour (November 6, 2108)

Figure 4.5 – Ammonium (NH₄⁺), nitrate (NO₃⁻), phosphate (PO₄³⁻) and silicate (SiO₄⁴⁻) concentrations in the Tagus estuary. The water level variation at the Cascais tidal gauge (http://www.dgterritorio.pt/) is shown (gray line). See Figure 4.1 for the location of the stations; the location of station 6 was 6A during the May field campaign

Globally, results showed marked spatial gradients, typically with the highest concentrations of chlorophyll *a*, nitrate and silicate at the upstream stations. Silicate and nitrate presented a conservative behavior. Ammonium and phosphate were not conservative, which suggests anthropogenic inputs along the estuary. Seasonally, the highest nutrients and suspended solids concentrations were found in the Autumn, after a period of rainfall, pointing out to the relevance of land runoff for material supply into the estuary. These conditions were favorable for phytoplankton development upstream and chlorophyll *a* was maximum during this campaign (24 μ g/L in the upper estuary). Further discussion about these data can be found in Rodrigues *et al.* (2020).

In addition to the main field campaigns some specific exploratory field campaigns were also performed in the Tagus estuary in the beginning of the project. These field campaigns were performed in 2016

(October 28, November 5, December 20) and 2017 (January 11, April 27). Samplings were performed in several stations along the estuary. *In-situ* measurements of temperature, salinity, pH and dissolved oxygen (DO) (concentration in mg/L and saturation %) were performed with YSI multiparameter probes, which were duly calibrated prior to each field campaign. Water samples were also collected for the laboratorial determination of pH, turbidity, total suspended solids and *Escherichia coli*. Further details can be found in Mendes (2017) and Mendes *et al.* (2019).

4.2.2 Ria Formosa

To characterize the seasonal variation along the Ria Formosa three field campaigns were carried out in 2017 (May 30-31, September 14-15 and October 25-26). During this year, unfortunately, it was not possible to characterize the winter rainy season. In these campaigns seven stations were selected to cover all the water bodies established for the Ria Formosa (Figure 4.6, Figure 4.7). Five stations were located in the main channels, although at inner areas and comprise: station 1 – Bridge of Faro Beach representative of Ria Formosa WB1; station 2 – Cais do Combustível that represent the Ria Formosa WB2; station 3 – Fuzeta representative of Ria Formosa WB4; station 4 – Tavira under the influence of freshwater input that represents the Ria Formosa WB5-R; and station 5 – Cacela also located in the Ria Formosa WB3 and the Faro-Olhão inlet (main inlet) corresponds to station 7, the oceanic boundary station (BS). In addition, to evaluate the rainfall influence on the water quality, a field survey was carried out in 2019 (9 and 10 April) after 4 days of rain. In this field survey, only four sites were considered (BS, WB1, WB5, WB5-R). This field survey was conducted in April to characterize the rainy season, usually typical of Winter, so it is identified as Winter field survey from now onwards.



Figure 4.6 – Location of the sampling stations in the Ria Formosa

Four pressure transducers (PT - two Level TROLL, one Infinity and one DIVER) were installed at different locations, to measure the sea surface elevation and water temperature every 10 minutes (Figure 4.6). In-situ measurements of water temperature, salinity, pH and dissolved oxygen (concentration and saturation %) were made simultaneously at each station using YSI multiparametric probes. Previously to the field survey, all the sensors of the four YSI multiparameter probes were calibrated using the same calibration solutions. A 5 L Niskin bottle and/or a sampling cup of water were used for the water samples collection for further determination of chlorophyll a (2 L), nutrients and total suspended solids concentrations (1 L). At each station, measurements and sampling of water were carried out every two hours along a complete semidiurnal tidal cycle (~12.5 h), at the surface for those stations where the water column is shallower. At Tavira, due to the potential influence of freshwater input and at other stations with deeper water columns (>4 m), to identify if water stratification occurred, in situ measurements were performed along the water column, every 1 m and water samples were also collected both at the surface and at the bottom. In the last field survey (April 2019), at BS only slack waters were sampled, at low-tide and high-tide peaks. After water collection, the samples were placed in thermal containers to preserve their quality until further treatment in the laboratory. The laboratorial methods used for the treatment of the water samples were the same described previously for the water samples collected in the main field campaigns performed in the Tagus estuary (section 4.2.1).



Figure 4.7 – Sampling stations in the Ria Formosa: a) station 1 – Bridge of Faro Beach, b) station 2 – Cais do Combustível, c) station 3 – Fuzeta, d) station 4 – Tavira, e) station 5 – Cacela, f) stations 6 – Olhão channel and 7 – Faro-Olhão inlet

A summary of the water characteristics obtained at each water body is presented in Table 4.2. The variability of temperature, salinity, percentage of dissolved oxygen, chlorophyll *a*, total suspended solids and inorganic nutrients are shown in Figure 4.8, Figure 4.9 and Figure 4.10, respectively.

		-			•	-	
Variable	BS	WB1	WB2	WB3	WB4	WB5-R	WB5
Temperature	19.4	20.4	20.8	21.0	20.6	19.3	21.3
(°C)	(15.1-20.9)	(15.7-24.6)	(18.9-23.1)	(19.8-21.9)	(18.3-23.7)	(14.1-22.8)	(14.3-25.8)
Salinity	36.4	36.7	36.6	36.5	36.4	36.3	36.5
	(36.0-36.6)	(36.3-37.3)	(36.3-36.9)	(36.2-36.7)	(36.2-36.8)	(35.0-37.0)	(36.0-37.3)
pН	8.1	8.0	8.0	8.1	8.0	8.0	8.1
	(7.9-8.3)	(7.8-8.3)	(7.8-8.3)	(7.9-8.3)	(7.8-8.1)	(7.8-8.2)	(7.6-8.6)
Dissolved	7.4	7.4	6.9	7.6	7.2	7.2	8.9
Oxygen (mg/L)	(6.8-8.0)	(6.4-8.6)	(6.4-7.6)	(7.1-8.1)	(6.4-7.9)	(6.3-7.9)	(2.6-14.0)
Oxygen	100	102	96	106	99	98	126
saturation (%)	(92-109)	(89-128)	(87-105)	(97-114)	(89-115)	(84-109)	(37-192)
Chlorophyll <i>a</i>	0.4	0.8	1.1	0.7	0.4	0.3	0.7
(µg/L)	(0.0-1.1)	(0.3-2.7)	(0.1-2.9)	(0.3-1.2)	(0.0-0.9)	(0.0-0.7)	(0.3-1.7)
Ammonium	1.6	3.0	2.7	1.8	1.9	3.1	2.9
(µM)	(0.2-3.4)	(0.7-15.0)	(0.7-4.3)	(0.2-3.5)	(0.1-3.8)	(1.1-7.4)	(1.0-6.5)
Nitrate	0.8	0.5	0.5	0.4	0.6	2.4	0.6
(µM)	(0.0-3.6)	(0.1-1.0)	(0.0-1.2)	(0.1-0.6)	(0.1-2.0)	(0.0-9.6)	(0.0-1.8)
Nitrite	0.1	0.1	0.2	0.1	0.1	0.1	0.1
(µM)	(0.0-0.2)	(0.0-0.1)	(0.1-0.3)	(0.0-0.2)	(0.0-0.2)	(0.0-0.2)	(0.0-0.2)
DIN	2.5	3.5	3.4	2.2	2.6	5.6	3.6
(µM)	(0.4-7.0)	(1.2-16.0)	(1.0-5.4)	(0.7-4.0)	(0.3-5.4)	(1.2-15.8)	(1.5-7.3)
Phosphate	0.24	0.4	0.2	0.3	0.3	0.3	0.5
(μM)	(0.0-0.4)	(0.1-0.8)	(0.1-0.4)	(0.1-0.6)	(0.1-0.6)	(0.1-0.5)	(0.1-0.9)
Silicate	1.8	4.7	3.5	2.6	2.4	3.7	7.2
(µM)	(0.8-4.7)	(2.2-10.5)	(1.4-5.5)	(2.0-3.3)	(0.7-7.7)	(0.9-9.6)	(5.1-11.2)
Suspended	2.6	5.4	5.3	4.2	5.3	4.5	10.6
Solids (mg/L)	(0.4-5.1)	(1.6-8.8)	(2.4-8.9)	(2.2-19.6)	(1.5-16.4)	(1.7-12.3)	(3.5-37.5)

Table 4.2 – Mean and range (minimum-maximum) of the water quality variables at each water body (WB) of the four seasonal campaigns

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Figure 4.8 – Water temperature and salinity in the Ria Formosa along the tidal height variation recorded by the PT. See Figure 4.6 for the location of the stations



Figure 4.9 – Oxygen saturation, chlorophyll *a* and suspended solids (SS) concentration in the Ria Formosa along the tidal height variation recorded by the PT. See Figure 4.6 for the location of the stations

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Figure 4.10 – Ammonium (NH₄⁺), nitrate (NO₃⁻), phosphate (PO₄³) and silicate (SiO₄⁴) concentrations in the Ria Formosa along the tidal height variation recorded by the PT. See Figure 4.6 for the location of the stations

The results clearly depict a spatial variability pattern. The lowest variability occurred at the boundary station – the main inlet in permanent connection with the coastal ocean (station 7, BS), while the maximum variability was recorded at the lagoon edges (stations 1 and 5, WB1 and WB5, respectively). In these waterbodies, the highest nutrient concentrations were recorded, mainly due to the shallowness of the water column and benthic-pelagic coupling processes. Seasonally, the highest concentrations of nutrients were obtained during Winter (not shown). The maximum value of ammonium was at station WB1 and the maximum nitrate value at station WB5-R due to the influence of precipitation and runoff recorded previously to the field survey. The lowest concentrations of nutrients were generally recorded during the Summer survey, as a result of its consumption by phytoplankton, as confirmed by the highest concentrations of chlorophyll a (*ca.* 3 μ g/L). Phosphate

concentrations (and silicate to some extent) were higher during this time than in the remaining field surveys, associated with their release from the sediments to the water column, due to desorption processes promoted during higher temperatures. These data will be discussed in detail in a scientific paper that will be submitted soon to an international journal. Preliminary results of the assessment of the long-term evolution of the nutrients concentrations through the comparison of these data with historical datasets over the past 40 years, showed a decreasing trend, meaning that the water quality of Ria Formosa has been improving over the past decades.

Data from the field campaigns are accessible in the web portal (section 3.4).

4.3 Real-time monitoring

4.3.1 Tagus estuary

Two real-time monitoring stations were maintained in operation in the Tagus estuary. The equipment of these two stations and their installation were supported by other research projects (Rodrigues *et al.*, 2015a; Rodrigues *et al.*, 2017a). The maintenance of these stations was partly supported by the UBEST project and the acquired data integrate the UBEST data repository (section 3.3). During the project both stations became inoperative due malfunction of the equipment or to the end of the agreements with the companies that supplied some of the equipment (see below).



Figure 4.11 – Location of the real-time monitoring stations in the Tagus estuary: station 1 – Parque das Nações and station 2 – Alcântara

The Parque das Nações monitoring station (station 1) is located in the Tagus estuary in the Parque das Nações Marina (38°45'15.27" N, 9°05'34.17" W; Figure 4.11). This monitoring station was equipped with a SEBA MPS D3 multiparameter probe, which measures water pressure, conductivity and water temperature, and a SEBA Slimcom2 data logger, for data acquisition and transmission. The

probe and the data logger were supported and protected by a PVC tube, which was located near the gates of the marina (Figure 4.12). This station became operational on January 14, 2016. Data were measured continuously at the monitoring station with 10 minutes intervals, transmitted once a day to LNEC and stored in databases. Further details can be found in Rodrigues *et al.* (2017a).



Figure 4.12 – General overview of the Parque das Nações station and SEBA MPS D3 multiparameter probe with SEBA Slimcom2 data logger

During the period of the project, maintenance procedures were undertaken to guarantee the safety of the equipment, the acquisition of the data and their quality. Damage to the data logger, which required factory repairing, prevented the acquisition of data between July 2016 and December 2016. Moreover, abnormal water temperature values were observed from April 2016 onwards, which remained even after the calibration of the sensor. The probe was reinstalled in January 2017 and measured water pressure until June 2017. After this date, a malfunction and damage of the probe was confirmed.

In the scope of an agreement between the private company SenZ2 and LNEC, a sensor to measure water levels was also installed in the Parque das Nações (Figure 4.13). This sensor was installed in August 2017 and was operational until October 2019, measuring water levels with 5 minutes intervals. This sensor measures the distance between the sensor and the water surface. During low tide of high spring tides, the location below the sensor dries out, and the sensor measures the distance to the bottom, rather than to the water surface.



Figure 4.13 – General overview of the sensor SenZ2 installed in the Parque das Nações Marina

The Alcântara monitoring station (station 2) is located in the Tagus estuary at the Alcântara pier, in the vicinity of the Alcântara wastewater treatment plant discharge (38°41'52.7"N; 9°10'31.7"W; Figure 4.11). This monitoring station is equipped with S::CAN probes, including a conductivity meter (Condu::lyser S::CAN), a dissolved oxygen probe (Oxi::lyser S::CAN), a UV-Vis Spectrolyser (Spectro::lyser S::CAN) and a Con::cube S::CAN data logger. The probes are supported and protected by a structure suspended from the pier (Figure 4.11). The Condu::lyser S::CAN and Oxi::lyser are property of LNEC, while the Spectro::lyser was installed in August 2018 in the scope of an agreement with the private company S::CAN. The Spectro::lyser was factory calibrated to measure chlorophyll *a*. Regarding the measurement of chlorophyll *a*, this sensor is typically used in freshwater environments and the aim of the collaboration was to explore its usage in an estuarine environment.

This station started its operation in October 2013, although it was reinstalled several times due to damage of the equipment or of the supporting structures. Data are measured continuously at the monitoring station with 2 to 5 minutes intervals, transmitted to LNEC and stored in databases (Rodrigues *et al.*, 2015a).

During the period of the project, maintenance procedures were undertaken to guarantee the safety of the equipment, the acquisition of the data and their quality. The station was reinstalled in April 2016 and was in operation until November 2017, although with some flaws in the data acquisition. Due to large damage to the shelter that protects some of the equipment, the station was totally dismantled in December 2017. The Alcântara on-line monitoring station was then reinstalled in August 2018 and was in operation until December 2019 Flaws were found in the salinity and dissolved oxygen data and the station in currently inoperative to assess the sensors status. Moreover, the period established to evaluate the Spectro::lyse probe finished.



Figure 4.14 – General overview of the Alcântara station and supporting structure of the probes

Some examples of the data acquired at these stations are presented below. Water levels and salinity data acquired at the Parque das Nações station between January 2016 and February 2019 are presented in Figure 4.15 and Figure 4.16. In general, the water levels obtained with the two sensors are very similar, as they are located a few tens of meters apart. The major difference is the lack of

data during low spring tide at the distance sensor, due to the drying of the estuary below the sensor. This similitude allows us to use the distance sensor when the pressure sensor fails. Figure 4.17 presents salinity data acquired at the Alcântara station between June 2016 and February 2019.



Figure 4.15 – Water levels observed at the Parque das Nações pressure sensor between January 2016 and June 2017



Figure 4.16 – Salinity (psu) observed at the Parque das Nações station between January 2016 and March 2016

Regarding the exploratory use of Spectro::lyser to measure chlorophyll *a* in an estuarine environment, the probe was calibrated by comparison with data from water samples collected and analyzed in the laboratory using HPLC (in the scope of the PhD of Dr. Rui Cereja, see section 9.1). Results suggest that the relative main variations can be captured. However, due to the location of the probe, maintenance procedures are very demanding, and the data starts to degrade after 1 to 2 weeks after the maintenance.

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Figure 4.17 – Salinity (psu) observed at the Alcântara station between June 2016 and April 2017 and between October 2018 and February 2019 (after the reinstallation of the station)

4.3.2 Ria Formosa

A real-time water quality monitoring station was deployed in the Ria Formosa. The water quality monitoring station is located in the Cais do Combustível of the Port of Faro (37°00'9.92" N, 7°55'16.28" W; Figure 4.18), which is an old and disabled fuel dock under the administration of the APS - Ports of Sines and the Algarve Authority. The Cais do Combustível is located in one of the main channels of the western sector of the Ria Formosa, the Faro channel. Since about 90% of the water volume is exchanged in the western sector of the lagoon (Pacheco *et al.*, 2010), this location was selected aiming to be representative of the water quality in one of the main channels of the Ria Formosa. The selection of this site took also into consideration other criteria, namely the access to essential infrastructures (e.g., GSM/GPRS connectivity), the ability to obtain permission to install the equipment and the protection from vandalism (Caradot, 2012).

The water quality online monitoring station is equipped with an YSI EXO 2 multiparameter probe (Figure 4.19). This probe includes sensors to measure water temperature, conductivity, pH, dissolved oxygen, turbidity and chlorophyll *a*. The probe is also equipped with copper-alloy sensor guard and an anti-fouling wiper to reduce the biofouling in the sensors. Data acquisition and transmission are performed using an OBSERMET OMC-045-III data logger, which includes a GSM/GPRS modem. Data are transferred through the internet, from the remote site to LNEC's data center, using the FTP protocol. The transmission procedure happens every hour, producing a new csv formatted file encompassing the data sampled/acquired in that period.

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Figure 4.18 – Location of the water quality online monitoring station in the Ria Formosa: general (a) and detailed (b) views. Background image from ESRI basemap



Figure 4.19 – YSI EXO2 multiparameter probe

The probe is supported and protected by a PVC tube, while the data logger is protected by an environmental shelter (Figure 4.20, Figure 4.21). The power supply to the operation of the multiparameter probe and of the data logger is provided by solar panels (Figure 4.20, Figure 4.21).

The multiparameter probe was under operation since May 26, 2017 until March 2020. Data were measured continuously at the monitoring station with 15 minutes intervals. Measured data, transmitted hourly, were stored in the data repository developed in the project (section 3.3) and are accessible through the web portal (section 3.4).

<image>

Figure 4.20 – Installation of the online monitoring station: May 25 and 26, and June 23, 2017



Figure 4.21 – General overview of the Ria Formosa monitoring station

Maintenance procedures were established and implemented to guarantee the continuous acquisition of the data, the safety of the multiparameter probe and the quality of the data. These procedures were performed by the members of UAIg's team with the support of APS - Port of Faro, which provided the access to the place where the probe is installed. Two levels of maintenance procedures were considered:

 Periodic cleaning, verification and inspection – procedures of visual inspection and manual cleaning of the probe, verification and/or calibration of sensors. These procedures were performed with a periodicity of one to two weeks during the first two months of operation of the probes to ensure the quality of the acquired data. After this period, these procedures were performed with the periodicity of one month. For safety reasons at least two technicians were required;

 Out-of-schedule inspection – supplementary procedures for inspecting the probe were undertaken when needed (e.g., lack of communication from the probe, observation of out of the range measurements).

During the operation of the probe along 33 months maintenance visits were performed. Calibration was performed every month, after the first two months. One conductivity calibration solution of 50 mS/cm was used, three pH calibration solutions (pH 4, 7 and 10), two of deionized water (0 FNU) and 12.4 FNU for turbidity. All calibration solutions used were recommended and commercialized by YSI Inc. Chlorophyll a sensor was calibrated with two standards: deionized water (0 µg/L) and the concentration determined in water collected in the day before at the place where the probe is deployed, using a spectrophotometric method (Lorenzen, 1967). Dissolved oxygen was calibrated using the water-saturated air mode recommended by the manufacturer for 100% of saturation, placing the probe in a wet aerated calibration cup and checking if the 100% saturation percentage was maintained. The error was always < 5%. Winkler method (Winkler, 1888) was used several times to check concentration accuracy, recording a 2-4% error. During this period of deployment, the calibrations showed a good performance of the sensors, with deviation of 1-2%. The probe data records were inspected carefully for detection and removal of outliers and gaps. Spikes and unreliable values, based on criteria reported in the bibliography for other similar systems or outside the possible ranges of variation (e.g. negative values for chlorophyll a and turbidity, pH < 7, or values orders of magnitude higher than typical, like for turbidity values > 100 FNU and for chlorophyll a values > 10 µg/L) were discarded manually. The interdependence relationship between variables determined from measured data was also considered, for example, the percentage of dissolved oxygen data were not validated during the periods with no salinity records (Cravo et al., 2020).

Some examples of the data acquired at the station are presented below. Figure 4.22 presents water temperature, salinity, pH, chlorophyll *a* and dissolved oxygen (in concentration and saturation percentage) data acquired at the Ria Formosa monitoring station between May 2017 and May 2019. Further details can be found in Cravo *et al.* (2020).

The time series acquired by the RTO contains some gaps due to several reasons. A long gap period without pH data was identified, from 05/09/2018 to 05/08/2019 because the pH sensor had stopped working and could only be replaced in August 2019. Two shorter periods of data lost are present in the records: i) one month for all parameters, from 13/11/2018 to 15/12/2018, due to lacks of recording data on the probe memory and communication with the data logger; and ii) three months of salinity data, from 09/02/2019 to 15/05/2019, due to conductivity sensor malfunctioning, which also affected the calculation of DO saturation percentage.

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Figure 4.22 – Time series of water temperature (A), salinity (B), pH (C), chlorophyll *a* (filtered data; D), turbidity (filtered data; E), DO in concentration (F) and in percentage of saturation (G) data acquired by the RTO during two years (from May 2017 to May 2019) along with SSE data obtained from the OTIS tide model. In DO representations, the yellow and red lines correspond to 5 mg/L and 2 mg/L benchmarks, the minimum required for aquatic life in seawater and hypoxia concentrations, respectively (F) and the orange line represents 60% of saturation, the imposed benchmark value for shellfish waters (G)

4.4 Low-cost sensor for water levels monitoring

A new prototype for a low-cost sensor for water levels measurement was developed and tested in laboratory and in the field. The following components were acquired and assembled to build the prototype (Figure 4.23):

- Sonar XL-Max-Sonar-WR MB7066;
- Raspberry Pi 3 (with Rasbian as OS);
- Sleepy Pi 2;
- Breadboard;
- Inverter Max 232;
- Battery.

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Figure 4.23 – Prototype for a new low-cost sensor for water levels

Laboratory measurements at LNEC's wave channels demonstrated good performance and the capacity to measure at the intendent frequency for tidal elevation (Figure 4.24). Because the sensor only became ready for field deployment after the UBEST field campaigns, the field testing was done in the scope of other projects. Results evaluated against Hydrographic Institute official measurements at the mouth of the Mondego estuary confirm the good accuracy of the sensor (Figure 4.24). The sensor was able to measure the water distance with good accuracy and reliability, throughout the whole time.

However, further developments are required for long term deployment, as it doesn't fare very well in terms of power consumption, drawing about 2W continuously.

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a)



Figure 4.24 – Testing of the low-cost sensor for water levels:a) LNEC's wave flume; b) Mondego estuary site

5 | Task 3: Implementation, validation and operational deployment of the coupled hydrodynamic-biogeochemical numerical models

5.1 Overview

The main objectives of this task were to implement and validate the coupled hydrodynamic-biological models of the Tagus estuary and of the Ria Formosa and to deploy the validated models in forecast mode.

The main results were:

- validated three-dimensional baroclinic hydrodynamics and biogeochemical models of the Tagus estuary and of the Ria Formosa;
- extension of LNEC's Water Information and Forecast Framework (WIFF, Fortunato *et al.*, 2017a) to provide forecasts of physical, chemical and biological variables and the automatic comparison with online data for the Tagus estuary and Ria Formosa.

5.2 Implementation and validation of the hydrodynamics and biogeochemical models

5.2.1 SCHISM modelling system

The hydrodynamics and biogeochemical models of the Tagus estuary and the Ria Formosa were implemented using the community modeling system SCHISM – Semi-implicit Cross-scale Hydroscience Integrated System Model (Zhang *et al.*, 2016; http://ccrm.vims.edu/schism/, version 5.4.0). SCHISM evolved from SELFE (Zhang and Baptista, 2008) and is developed by several institutions, led by the Virginia Institute of Marine Sciences (USA). This modelling system is fully parallelized and includes modules for surface waves (Roland *et al.*, 2012), morphodynamics (Pinto *et al.*, 2012; Guerin *et al.*, 2016) and water quality (Rodrigues *et al.*, 2009, 2011; Azevedo *et al.*, 2014).

The hydrostatic version of the model solves the three-dimensional shallow-water equations, with the hydrostatic and Boussinesq approximations, and the transport equations for salt and heat. SCHISM has a user-defined transport module that allows the simulation of any given tracer through which the biogeochemical module is coupled. The biogeochemical model formulation was extended from EcoSim 2.0 (Bisset *et al.*, 2004) to simulate zooplankton and the oxygen cycle (Rodrigues *et al.*, 2009, 2012). This model includes the carbon, nitrogen, phosphorus, silica, oxygen, and iron cycles and simulates several ecological tracers (Figure 5.6). Several options are implemented within the model that allow the user to select the relevant variables for a specific application.

SCHISM is based on unstructured grids in the horizontal dimension and hybrid SZ coordinates or LSC² (Localized Sigma Coordinates with Shaved Cell) in the vertical dimension. It uses semi-implicit finite elements and finite volume methods, combined with Eulerian-Lagrangian methods, to solve the shallow water equations.

Further details about the model can be found in Bisset *et al.* (2004), Rodrigues *et al.* (2009, 2012) and Zhang *et al.* (2016).



Figure 5.1 – Sources and sinks of the biogeochemical module (Rodrigues et al., 2015b)

5.2.2 Tagus estuary implementation and validation

A new three-dimensional baroclinic model was developed for the simulation of the circulation and biogeochemical dynamics of the Tagus estuary (Portugal). An horizontal grid composed of triangular elements was generated with the softwares *xmgredit* (Turner and Baptista, 1993) and *nicegrid* (Fortunato *et al.*, 2011), based on grids from previous applications (e.g., Guerreiro *et al.*, 2015, Fortunato *et al.*, 2017a). The domain is over 110 km long and has a surface area of 1442 km². It extends from the ocean, 27 km away from the estuary mouth, to the river (Figure 5.2). The resulting grid has 83 000 nodes and a typical resolution of 15-25 m, which is lower in the channels to allow the proper propagation of the tide. Taking into account the results of preliminary simulations the vertical domain is discretized with a hybrid grid with 39 SZ levels: 30 S levels in the upper 100 m, and 9 Z levels between 100 m and the maximum depth.

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Figure 5.2 – Tagus estuary model domain and bathymetry relative to mean sea level (MSL). Location of the sampling stations: the circles represent the 1972 tidal gauges, the squares represent the 1983 survey stations and the red lines represent the 1988 campaigns longitudinal profiles (BC: Barra-Corredor, CN: Cala do Norte, CS: Cala de Samora)

The bottom stress was parameterized using a drag coefficient. The time step was set to 30 s and the Generic Length Scale KKL turbulence closure scheme, with the Kantha and Clayson's stability function, was used.

The numerical model is forced by tides at the ocean boundary, river flows at the riverine boundaries (Tagus and Sorraia) and atmospheric data at the surface. In all validation simulations the oceanic boundary was forced with 23 tidal constituents (Z0, SSA, MM, MF, MSF, O1, K1, P1, Q1, N2, M2, S2, K2, 2N2, Mu2, Nu2, L2, M3, MN4, M4, MS4, M6, 2MS6) from an application of SCHISM to the NE Atlantic Ocean (Fortunato et al., 2017). The Tagus river flow was established based on the data Sistema available at SNIRH Nacional de Informação de Recursos Hídrico _ (http://snirh.apambiente.pt), namely at the Ómnias or Almourol stations, depending on the period assessed. For lack of data, the river flow in the Sorraia River was taken as 5% of the river flow in the Tagus River, based on the ratios between annual averages in the two rivers. Salinity, water temperature and biogeochemical tracers (e.g., ammonium, dissolved oxygen and chlorophyll a) are also imposed at the open boundaries. Salinity was set as constant at the open boundaries (36 at the oceanic boundary and 0 at the riverine boundaries). The water temperature was estimated with the Atlantic-Iberian Biscay Irish-Ocean Physics model (http://marine.copernicus.eu/) and with climatology estimated based on SNIRH data at, respectively, the oceanic boundary and the riverine boundaries. For the biogeochemical tracers different approaches were followed depending on the data available. At the oceanic boundary, ammonium, nitrate, phosphate, silicate, dissolved oxygen, phytoplankton and chloropohyll a were imposed based on the Atlantic-Iberian Biscay Irish-Ocean Biogeochemical model (http://marine.copernicus.eu/). The other variables were estimated based on climatology or

derived from the previous based on estimations from literature review. At the riverine boundaries, the biogeochemical tracers were estimated based on climatology data when available or derived based on estimations from literature review. Depending on the simulated period, the atmospheric forcing was obtained from NCEP-NCAR Reanalysis (~50km/6h resolution, provided by the NOAA/OAR/ESRL PSD, http://www.esrl.noaa.gov/) or ERA-Interim (Dee *et al.*, 2011) produced by the European Centre for Medium-Range Weather Forecasts (ECMWF; https://www.ecmwf.int/).

The updated model was calibrated and extensively validated, namely by comparison with the following datasets: i) water levels from 1972 that were harmonically analyzed to extract the amplitudes and phases of the tidal constituents (Fortunato *et al.*, 1999; Figure 5.2), ii) salinity and water temperature data measured along the estuary in 1983 (Silva *et al.*, 1986; Figure 5.2), iii) salinity and water data along three longitudinal profiles in 1988 (Neves, 2010; Figure 5.2), iv) physical, chemical and biological data measured in April 2010 along the estuary (Caetano *et al.*, 2016), and v) data from the project field campaigns performed in 2018 (section 4.2.1).

Some examples of the model results and error measures are presented below in Table 5.1, Figure 5.3, Figure 5.4 and Figure 5.5). Overall, the results showed its ability to represent the circulation and water quality main spatial and temporal patterns of salinity, temperature, nutrients, chlorophyll *a* and dissolved oxygen observed in the Tagus estuary. The main differences observed between the observations and the model results arise from uncertainties in the boundaries conditions and the existence of other point sources, namely regarding the input of nutrients that was not considered in the model.

Further details about the Tagus estuary hydrodynamic model can be found in Rodrigues and Fortunato (2017).

Station	RMSE (cm) SCHISM 3D	U-RMSE (cm) SCHISM 3D*	RMSE (cm) SELFE 3D
Cascais	3.8	3.7	1.8
P. de Arcos	4.3	3.1	5.8
Trafaria	10.6	7.8	9.6
Lisboa	6.9	3.3	10.8
Pedrouços	5.0	3.4	5.9
Cacilhas	3.8	3.5	6.4
Seixal	5.5	5.0	9.4
Montijo	8.2	4.6	12.2
Cabo Ruivo	8.8	4.3	13.5
Alcochete	7.4	7.2	12.3
P. Sta. Iria	8.7	6.8	17.3
Ponta da Erva	7.3	6.9	20.2
V. F. de Xira	15.4	11.2	21.5

Table 5.1 – Water levels root mean square errors (RMSE) for the 1972 data: present application (SCHISM 3D) and previous application by Costa *et al.* (2012) (SELFE 3D). For the present application unbiased RMSE (U-RMSE) are also presented



Figure 5.3 – Observed and simulated vertical profiles of salinity during low-tide (February 11-13, 1988). Model results are presented for upwind and TVD numerical schemes



Figure 5.4 – Spatial variation: observed and simulated salinity, ammonium, silicate and chlorophyll *a* in the Tagus estuary during the May 2018 field campaign at stations 2, 4 and 5 (Suf – surface, Bot – bottom)

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Figure 5.5 – Seasonal variation: observed and simulated salinity, ammonium, phosphate, silicate and chlorophyll *a* in the Tagus estuary during the May, September and November field campaigns at station 5 (Suf – surface, Bot – bottom)

5.2.3 Ria Formosa implementation and validation

A new three-dimensional baroclinic model was developed for the simulation of the circulation and biogeochemical dynamics of the Ria Formosa.

The hydrodynamic model was first calibrated in three-dimensional barotropic mode. This application was based on the previous application of SELFE 3D (Zhang and Baptista, 2008) in the Ria Formosa by Fabião *et al.* (2016). The model calibration was performed by comparison of the model results with the sea surface elevation data measured by the Instituto Hidrográfico between October 1979 and October 1980 at 11 stations located along the Ria Formosa and in the adjacent coastal area (Figure 5.6). The model was then validated by comparing the model results with sea surface elevation and current velocity data sets from the field campaigns carried out in the western sector of the Ria Formosa between October and December 2011 within the scope of project COALA (Jacob *et al.*, 2012; Fabião *et al.*, 2016).

To implement SCHISM in baroclinic mode, the grid and the bathymetry were updated for the 2017 conditions. Regarding the grid resolution, some areas were refined, such as Cacela, Fuzeta, Armona and Ancão inlets, and some channels (Faro channel, from the Faro Commercial Port to the Bruce's Yard, and Faro beach channel) and the Gilão River were introduced in the domain. Additionally, the ocean part of the domain was extended due to instabilities in the current velocity simulations at the edges of the domain. The final grid used in the validation of the baroclinic model was characterized horizontally by 98308 nodes and 192824 elements (Figure 5.6). The bathymetric information from 1980 to 2010 was updated with the topographic and bathymetric surveys performed during 2011, along the Portuguese coast with LiDAR equipment (Light Detection And Ranging) (Silva *et al.*, 2012). This is an important dataset, with great detail and accuracy (resolution of 2 meters). This information was combined with the existing bathymetry, since the data obtained with LiDAR equipment are limited to a coastal band with an approximate width of 1 km. Additionally, the bathymetry in the upstream area of the Gilão River was developed based on local knowledge and unpublished works, given the scarcity of bibliographic information (Figure 5.6).



Figure 5.6 – Horizontal grid and bathymetry (MSL – mean sea level) of the Ria Formosa

The numerical model is forced by tides at the ocean boundary, river flows at the Gilão river and atmospheric data at the surface. Similarly to the Tagus estuary, in all validation simulations the oceanic boundary was forced with 23 tidal constituents (Z0, SSA, MM, MF, MSF, O1, K1, P1, Q1, N2, M2, S2, K2, 2N2, Mu2, Nu2, L2, M3, MN4, M4, MS4, M6, 2MS6) from an application of SCHISM to the NE Atlantic Ocean (Fortunato *et al.*, 2017). The river flow rate at the Gilão river was imposed based on climatology estimated from data from Bodega hydrometric station, ava Salinity, water temperature and biogeochemical tracers (e.g., ammonium, dissolved oxygen and chlorophyll *a*) are also imposed at the open boundaries. For salinity, the boundary conditions were constant and defined as 0 in the river and

36.5 in the ocean boundary. At the river boundary temperature was set based on climatology estimated from data of the Bodega station. At the oceanic boundary several options were tested, including constant values and time-space varying data from the Atlantic-Iberian Biscay Irish-Ocean Physics model (http://marine.copernicus.eu/). For the biogeochemical tracers different approaches were followed depending on the data available. At the oceanic boundary, ammonium, nitrate, phosphate, silicate, dissolved oxygen, phytoplankton and chlorophyll a were imposed based on the Atlantic-Iberian Biscay Irish-Ocean Biogeochemical model (http://marine.copernicus.eu/). The other variables were estimated based on climatology or derived from the previous based on estimations from literature review. At the riverine boundary, the biogeochemical tracers were estimated based on climatology data when available or derived based on estimations from literature review. The atmospheric dataset used in the simulations was the ERA-Interim (Dee et al., 2011) produced by the European Centre for Medium-Range Weather Forecasts (ECMWF; https://www.ecmwf.int/). Since the wastewater treatment plants are one of the main inputs of freshwater into the Ria Formosa, some exploratory simulations were also performed considering the input of these sources. Boundary conditions for the freshwater effluents discharge, ammonium, nitrate and phosphate were imposed based on climatology estimated from data provided by Águas do Algarve.

The updated model was validated in the Ria Formosa by comparison with data from the project field campaigns performed in 2017 (section 4.2.2).

Some examples of the model and error measures results are presented below in Figure 5.7, Figure 5.8, Figure 5.9, Figure 5.10, Figure 5.11 and Figure 5.12. Overall, the results show the model's ability to represent the main spatial and temporal patterns of salinity, temperature, nutrients, chlorophyll *a* and dissolved oxygen observed in the Ria Formosa. The main differences arise from uncertainties in the boundaries conditions, the existence of other point sources that were not considered in the model and processes related with the sediment-water exchanges that are not considered in the model.

Further details about the Ria Formosa hydrodynamic model can be found in Rosa et al. (2019).

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Figure 5.7 – Comparison of the Root Mean Square Error (m) for sea surface elevation between previous applications (ELCIRC – Bruneau *et al.* (2010), ELCIRC – Dias *et al.* (2009), SELFE – Fabião *et al.* (2016)) and the best result obtained from SCHISM model simulations for each station



Figure 5.8 – Observed and simulated water levels during the May 2017 field campaign: a) Faro-Olhão inlet and b) Cais Comercial de Faro

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Figure 5.9 – Observed and simulated salinity during the May 2017 field campaign: a) Cais Comercial de Faro and b) Tavira



Figure 5.10 – Seasonal variation: observed and simulated salinity and water temperature at the Cais Comercial de Faro considering the data from the online monitoring station



Figure 5.11 – Spatial variation: observed and simulated ammonium, phosphate, silicate and chlorophyll *a* in the Ria Formosa during the October 2017 field campaign at stations 1, 5 and 7

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Figure 5.12 – Seasonal variation: observed and simulated salinity, ammonium, phosphate, silicate and chlorophyll *a* in the Ria Formosa during the May, September and November field campaigns at station 2

5.3 Forecast engine

The Tagus estuary and Ria Formosa hydrodynamics and biogeochemical models were implemented operationally, providing daily forecasts of the physical, chemical and biological variables that are available in the UBEST web portal. The forecasts are performed daily, taking advantage of an established model and procedures to reliably and consistently produce the predictions. These procedures are assembled in the forecast engine, a software built on top of the Water Information Forecast Framework (WIFF, Fortunato *et al.*, 2017a; Rogeiro *et al.*, 2018), a Python-based framework, that is also used to enable the on-demand forecast systems in the OPENCoastS service (https://opencoasts.ncg.ingrid.pt, Oliveira *et al.*, 2020). WIFF provides most of the generic aspects required to operate a forecast system, such as coupling different simulation models, retrieving the necessary forcings, running simulations remotely or locally with MPI, chaining periodic simulations to make them a continuous series of events, post-processing the model results and providing

notifications to the users and administrators about progress or unexpected behavior. The modularity in this procedure also allows them to be customized and/or extended, by subclassing. Figure 5.13 depicts the forecasting software stack.



Figure 5.13 – Forecast engine: forecasting software stack

Forecasts are available for the following variables: water levels, velocity, salinity, temperature, ammonium, nitrate, phosphate, silicate, dissolved oxygen and chlorophyll a (Figure 5.14, Figure 5.15). Several forcings are available in the forecast engine to establish the boundary conditions for oceanic, riverine and surface (atmosphere) boundaries. Oceanic boundaries are forced by ocean forecasts, IBI ANALYSIS FORECAST PHYS 005 001 sourced from Copernicus' CMEMS and IBI ANALYSIS FORECAST BIO 005 004 (http://marine.copernicus.eu/), for physical and biogeochemical variables, respectively. The biogeochemical variables imposed at the oceanic boundary from the IBI model are ammonium, nitrate, phosphate, silicate, dissolved oxygen, phytoplankton and chlorophyll a. The other variables are estimated based on climatology or derived from the previous based on estimations from literature review, and a script was built to compute these variables automatically. Riverine boundaries can be forced by extrapolations of quasi real-time data or climatology. Regarding the surface boundary, atmospheric forecasts sourced from NOAA's GFS 0.25° are used as well (https://www.ncdc.noaa.gov/data-access/model-data/model-datasets/global-forcastsystem-gfs).

Further details about the forecast engine can be found in Rodrigues et al. (submitted, 2020).

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Figure 5.14 – Example of salinity forecasts in the Tagus estuary



Figure 5.15 – Example of chlorophyll a forecasts in the Ria Formosa

6 | Task 4: Quantification of the estuarine biogeochemical buffering capacity for present and future scenarios

6.1 Overview

The main objectives of this task were to quantify the individual and combined impacts of anthropogenic pressures (increased nutrients loads) and climate change (sea level rise, changes in the hydrological regimes and in the air temperature) on the estuarine biogeochemical dynamics.

The main results achieved, described below, were:

- estimation of the Net Ecosystem Metabolism (NEM) for the Ria Formosa for one year based on the dissolved oxygen data acquired at the Ria Formosa online monitoring station;
- database of physical, chemical and biological variables information for anthropogenic-induced and climate change scenarios development for each system and information uploading to the web portal;
- improved understanding of the Tagus estuary and Ria Formosa biogeochemical response to increased nutrients loads, sea level rise, and changes in the hydrological regimes and in the air temperature;
- assessment and quantification of anthropogenic-induced and climate change impacts.

6.2 Net Ecosystem Metabolism quantification in the Ria Formosa coastal lagoon

The Net Ecosystem Metabolism (NEM) metric (i.e. the balance between production and respiration) is a useful indicator of the trophic condition within estuaries (Needoba *et al.*, 2012). NEM was calculated for one year, from 30 May 2017 to 29 May 2018, based on the dissolved oxygen data acquired at the Ria Formosa online monitoring station (Figure 6.1). Daily NEM was estimated by the sum of the daily rates of organic matter production and aerobic respiration. The evaluation of NEM, net ecosystem production (NEP) and ecosystem respiration (ER) from high-resolution *in-situ* dissolved oxygen measurements taken in Ria Formosa follows the method described by Needoba *et al.* (2012), using the equations presented by Caffrey (2003, 2004) for the air-water and biological dissolved oxygen fluxes. Further details can be found in Cravo *et al.* (2020).

Data reveal a slightly heterotrophic behavior of Ria Formosa in the study area (Figure 6.1). This means that respiration process overpassed photosynthesis, suggesting the influence of pulses of organic matter inputs and benthic remineralization, which were more evident after storms and rainfall periods and land runoff. The NEM showed lower negative values for longer periods during autumn-winter than during spring-summer, when the study area can be considered slightly autotrophic for very short periods.
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Figure 6.1 – Top: air-water diffusion flux values, F₀₂, using a constant correction factor; middle: biological oxygen change (BDO flux); and bottom: daily calculated net ecosystem production (NEP, black line), ecosystem respiration (ER, red line) and net ecosystem metabolism (NEM, histogram)

6.3 Assessment and quantification of climate change and anthropogenic-induced and impacts for present and future scenarios

The relative impacts of increased nutrients loads, sea level rise, and changes in the hydrological regimes and in the air temperature were quantified. This evaluation supports the assessment of the susceptibility of the estuarine biogeochemical buffering capacity. Several scenarios of climate change and anthropogenic pressures were simulated in the Tagus estuary and Ria Formosa, using the validated hydrodynamics and biogeochemical models developed (section 5.2). The set of scenarios for conditions anticipated for the end of the 21st century was defined using a methodological approach similar to Rodrigues *et al.* (2015b). Since the numerical models developed are very demanding computationally, simulations were performed for the Spring season, when the primary productivity is highest.

For comparison purposes, a reference scenario was established based on climatology estimated from the historical data (section 3.2). The boundary conditions at the oceanic, riverine and surface boundaries were established following a similar approach to Rodrigues *et al.* (2019). To set up the

tide, the tidal amplitudes at Cascais (near the coastal boundary of the model) were determined between 1991 and 2010 using the tides from the regional model of Fortunato *et al.* (2016) and statistics were computed (mean and standard deviation). The comparison of these values with their global mean and standard deviations indicates that the year 2001 is the most representative of average conditions. A similar approach was used to define the atmospheric forcing for the scenarios simulations, using the data from ERA-Interim (Dee *et al.*, 2011, https://www.ecmwf.int/) and evaluating the main representative variables (wind, air temperature, surface pressure and solar radiation). This analysis indicates that the years of 2001 and 2012 are the most representative of average conditions in the Tagus estuary and in the Ria Formosa, respectively. The river flow was established based on climatology estimated based on data from the Almourol and Bodega stations for the Tagus river and the Gilão river, respectively. Salinity, temperature and biological tracers concentrations were established based on climatology.

The climate change and anthropogenic scenarios were established based on a literature review. In each scenario only one variable is changed relative to the reference scenario. The following scenarios were simulated for the Tagus estuary:

- Sea level rise (SLR) this scenario considers a mean sea level rise of 0.5 m. This value was defined taking into account that the median values of SLR between 1986-2005 and 2081-2100 depend on the Representative Concentration Pathway (RCP) and that typical values estimated for the end of the 21st vary between about 0.4 m for RCP2.6 and 0.7 m for RCP8.5 (Nauels *et al.*, 2017);
- River flow decrease this scenario considers a decrease of the river flow to 75% of the reference scenario. This scenario was based on the predictions for the average Spring precipitation in 2071-2100 in the Lisbon Metropolitan Area considering RCP8.5, available at http://portaldoclima.pt/;
- Nutrients increase this scenario considers an increase of 100% in the nutrients loads (ammonium, nitrate and phosphate) at the riverine boundaries;
- Nutrients decrease this scenario considers a decrease of 50% in the nutrients loads (ammonium, nitrate and phosphate) at the riverine boundaries.

For the Ria Formosa the future scenarios simulated were:

- Sea level rise this scenario considers a mean sea level rise of 0.5 m, similarly to the scenario simulated for the Tagus estuary;
- Air temperature increase this scenario considers an increase of 1.68 °C of the air temperature. This scenario was based on the predictions for the average Spring air temperature in 2071-2100 in the Algarve region considering RCP4.5, available at http://portaldoclima.pt/;
- Nutrients increase this scenario considers an increase of 50% of the nutrients loads (ammonium, nitrate and phosphate) at the wastewater treatment plants.

The results from these simulations were summarized in maps of statistics (mean, minima and maxima) that can be accessed through the web portal (section 3.4). To quantify the impacts, differences

between the reference scenario and the other were also computed. For the scenarios, the TRIX trophic index was also computed allowing an integrated comparison and the resulting maps are available in the web portal.

For the Tagus estuary, results suggest that for the evaluated scenarios changes in the sea level and river flow have a larger influence in the circulation and water quality dynamics compared to the changes in the nutrients loads at the riverine boundaries. Sea level rise and the decrease in river flow lead to an increase of the salinity (Figure 6.2) and a decrease of nutrients (Figure 6.3) and chlorophyll *a* (Figure 6.4) concentrations in the upper estuary.

For the Ria Formosa, results suggest that sea level rise promotes changes in the salinity mainly in the vicinity of the wastewater treatment plants (Figure 6.5), where the salinities are lower. Regarding the air temperature scenario, results suggest that an increase of the air temperatures of 1.68°C leads to changes of the water temperature in the lagoon of about 0-1°C (Figure 6.6). Results also suggest that sea level rise and the increase of the nutrients loads from the wastewater treatment plants have contrary effects on the inorganic nutrients concentrations: sea level rise leads to a decrease of the nutrients concentrations in the area of influence of the wastewater treatment plants, while an increase is observed in the nutrients loads scenario. Minimal differences were observed between the simulated scenarios regarding chlorophyll *a* concentrations.

These results provide further insight about the systems response to changes in the main drivers and constitute an important database to support their management.



Figure 6.2 – Salinity in the Tagus estuary: differences between the sea level rise and river flow scenarios and the reference scenario



Figure 6.3 – Ammonium and phosphate in the Tagus estuary: differences between the sea level rise, river flow and nutrients scenarios and the reference scenario



Figure 6.4 – Chlorophyll *a* in the Tagus estuary: comparison for different scenarios of climate change and anthropogenic pressures



Figure 6.5 – Salinity in the Ria Formosa: differences between the sea level rise scenario and the reference scenario



Figure 6.6 – Water temperature in the Ria Formosa: differences between the temperature increase scenario and the reference scenario

7 | Task 5: Global estuarine classification

7.1 Overview

The main objectives of this task were to the assess the Tagus estuary and Ria Formosa physical and trophic conditions under global classification metrics and to compare their behavior with other estuaries worldwide.

The main results, described below, were:

- the classification of the Tagus estuary and Ria Formosa for physical metrics;
- the classification of the Tagus estuary and Ria Formosa for different water quality metrics trophic status;
- setting the relative positioning of the Tagus estuary and the Ria Formosa physical and trophic conditions at a global scale.

7.2 Context

Several classifications schemes have been proposed for estuaries over the past decades (e.g., Hansen and Rattray, 1966; Engle *et al.*, 2007; Hume *et al.*, 2007; Geyer and MacCready, 2014). Since all estuaries are different, classification schemes are simplifications, whereby an estuary is represented by a limited set of characteristics. Estuarine classifications help generalizing behaviors identified in a given estuary to other, similar, estuaries. The underlying hypothesis is that different estuaries with similar characteristics exhibit comparable behaviors or responses to external forcings. This hypothesis implies that a particular classification should be consistent with the purpose for which it is used. For instance, a classification directed towards the morphological behavior of estuaries (Hayes and FitzGerald, 2013) may be inadequate for the analysis of circulation patterns. Hence, the choice of a classification scheme depends on the context of the study.

The goal of UBEST is to understand the buffering capacity of estuaries, and how this capacity will be affected by climate change. From a physical viewpoint, this capacity should be significantly affected by the time that river-borne nutrients remain inside the estuary before being flushed out to the sea. Hence, residence times and similar descriptors (flushing time, water age, etc.) are expected to play a significant role in the buffering capacity of estuaries. Other, secondary, physical quantities that should affect the buffering capacity of estuaries are light availability (determined by both incoming radiation and turbidity) and temperature. Residence times are determined, to a large extent, by the residual – or estuarine – circulation. Hence, classifications based on estuarine circulation or directly on residence times should be particularly relevant in the present context.

Like any model, classification schemes should be validated. This validation should verify whether all estuaries in the same class do indeed present similar behaviors. Yet, efforts to develop classifications

have seldom been followed by detailed validations. For instance, the classification of Hansen and Rattray (1966) was extensively used for several decades, and only recently were its limitations exposed (Rockwell and MacCready, 2014). This lack of validation may question the use of many classification schemes. Detailed estuarine studies could be used to provide the data required to validate classifications.

Classification systems are often developed in the scope of studies that aim at characterizing, in a simplified way, a large number of estuaries. Usually, this development occurs in the scope of nation-wide studies: examples include the U.S. (Engle *et al.*, 2007), New Zealand (Hume *et al.*, 2007) and South Korea (Jang and Hwang, 2013). In this scope, classifying the Tagus and Ria Formosa in some of these classification systems may foster a broader use and dissemination of our findings, and provide the required information to support an eventual validation of the classifications.

7.3 Physical classification

7.3.1 Literature review

A literature review was performed to summarize both classical and new classification metrics.

General classifications

Engle *et al.* (2007) developed a classification of estuaries based on 12 characteristics (e.g., volume, surface area, tidal prism, river flow, etc). A clustering analysis applied to 138 US estuaries highlights the existence of nine distinct classes. However, the possibility of using this classification to infer similar behaviors within a given class is unclear.

Hume *et al.* (2007) proposed a hierarchical classification of estuaries and applied it to New Zealand estuaries. The first level of the classification is associated to the location (latitude, ocean basin and land masses), following Bailey (1988). The paper focuses on levels 2 and 3 of the classification scheme. Level 2 categories are determined by basin morphometry and river and ocean forcings, while level 3 categories are determined by land cover and geology, which control the sediment and chemical inputs to the estuary. Level 4 aims at distinguishing different parts of the same estuary and is not addressed in the paper. This classification was later expanded by Jang and Hwang (2013) to account for wave effects and artificial structures.

These general classifications provide a very rough description of estuaries. It seems unlikely that climate change would affect the classification of an individual estuary. Also, these classifications use broad characteristics, and should not be significantly affected by seasonal or climate changes. Still, these classifications could be useful to help describing our systems and possibly extrapolating our results to other estuarine systems. Regarding the classification of Hume *et al.* (2007), the Ria Formosa seems to fit in Category E, tidal lagoon or barrier-enclosed lagoon, while the Tagus estuary is close to Category F – drowned valleys. However, some indices would have to be computed to verify this preliminary conclusion.

Classifications based on estuarine circulation

One of the most adopted conventional classifications of estuaries was proposed by Hansen and Rattray (1966). This approach described the low-frequency motion and salt distribution in an estuary as a balance between a near-bottom upstream flow forced by baroclinic pressure, and a near-surface downstream flow forced by river flow and barotropic pressure. Other effects, including the tidal motion, were wrapped-up in a diffusion-like term. As the understanding of estuarine physics evolved over the next 50 years, it became apparent that the conceptual model of Hansen and Rattray (1966) was overly simplistic.

Jay and Smith (1988) proposed an alternative classification scheme based on two numbers: an internal Froude number, which measures baroclinic residual circulation, and a ratio of tidal range to depth.

Geyer and MacCready (2014) proposed a more detailed model of estuarine circulation, and developed a more comprehensive classification diagram, also based on two dimensionless numbers:

- The mixing number M: $M^2 = \frac{C_D U_T^2}{\omega N_0 H^2}$, where C_D is a dimensionless friction coefficient, U_T is the amplitude of the depth-averaged tidal velocity, ω is the tidal frequency, H is the water depth and $N_0 = (\beta g s_{ocean}/H)^{0.5}$ is the buoyancy frequency for maximum top-to-bottom salinity variation in an estuary.
- The freshwater Froude number Fr_f : $Fr_f = \frac{U_R}{(\beta g s_{ocean} H)^{0.5}}$, where U_R is the river velocity, g is gravity and s_{ocean} is the ocean salinity.

Placing an estuary on this diagram indicates in which stratification class or classes the estuary falls.

The Geyer and MacCready (2014) classification scheme has both strengths and weaknesses. On the negative side, the authors do not provide any validation. Also, there are ambiguities on its application. For instance, it is unclear how the width of multi-inlet systems such as the Ria Formosa should be defined. Similarly, lateral bays, which are common in estuaries, affect estuarine circulation and are not taken into account. An application of this scheme in the scope of a modeling study (Karna and Baptista, 2016) provides an example of how to overcome some of the ambiguities, although in a geometrically simple estuary. Finally, this classification scheme does not provide any information on relevant descriptors such as temperature or light availability. On the positive side, this classification scheme is well anchored on the present understanding of estuarine circulation and is consistent with empirical observations. It provides a rich, yet simple, classification of estuaries.

Classifications based on residence times

Residence times have been suggested as a key descriptor for classification schemes (Jay *et al.*, 2000). Recently, Jones *et al.* (2017) developed a classification scheme based on residence times. However, the scheme targets freshwater systems and appears too simplistic to apply in estuaries.

7.3.2 Application to the Tagus estuary and the Ria Formosa

Based on the review a set of metrics was selected to classify the Tagus estuary and the Ria Formosa using an integrated data-modelling approach. The selected metrics were:

- the classification proposed by Geyer and MacCready (2014) to assess the circulation and the mixing conditions
- the Venice system (after Carriker, 1967).

Geyer and MacCready (2014) developed a classification diagram based on two dimensionless numbers, the mixing number and the freshwater Froude number. Based on the values of those numbers the system can be classified as "Fjord", "Bay", "SIPS - strain induced periodic stratification", "Strongly stratified", "Partly mixed", "Well mixed", "Salt wedge" or "Time-dependent salt wedge". This classification was applied to the Tagus estuary and the Ria Formosa. Results showed that the Tagus estuary is typically well mixed for mean river flows and partially mixed for higher river flows (> 1500 m3/s) - Figure 7.1. The Ria Formosa is consistently well-mixed (Figure 7.2). The Geyer and MacCready indicator is also automatically computed daily, using a Python script, based on the water levels and velocities forecasts for a given coastal system.



Figure 7.1 – Classification of the Tagus estuary based on Geyer and MacCready (2014)



Figure 7.2 – Classification of the Ria Formosa based on Geyer and MacCready (2014)

The Venice system (after Carriker 1967) is often used to classify waters with respect to the salinity (e.g. Fortunato *et al.*, 2002). This system considers six classes: limnetic (freshwater, <0.5), oligohaline (0.5-5), mesohaline (5-18), polyhaline (middle area, 18-25; lower area, 25-30), and euhaline (30-35). To evaluate the role of the freshwater discharge in the salinity distribution in the Tagus estuary two scenarios were established. These scenarios were based on two distinct periods, which were chosen due to their extreme characteristics regarding river discharge: July 2005 (low river discharge scenario) and February 1979 (high river discharge scenario). The estimated average Tagus river flow was 22 m³/s in July 2005 (estimation based on Macedo, 2006), although some uncertainty remains since no observations are available. In contrast, in February 1979 the average river flow was 5464 m³/s at Ómnias (near the Tagus riverine boundary of the model) (Macedo, 2006). Results show a pronounced progression of the saltwater upstream for low river discharges and a contrasting situation for high river discharges (Figure 7.3). Further details can be found in Rodrigues and Fortunato (2017).

0.0 0.5 5.0 18.0 25.0 30.0 Salinity 0.0 0.5 5.0 18.0 25.0 30.0

Figure 7.3 – Tagus estuary salinity classification for extreme river discharges using the Venice system: high river discharge scenario (A) and low river discharge scenario (B). Classification refers to mean salinity over a 30-days period

7.4 Water quality classification

Similarly to the physical classification, a literature review was also performed for the water quality indicators. Based on that review, a set of indicators, described below, was also selected to assess the water quality, in particular regarding the nutrients status, the chlorophyll *a* status and the trophic status. The following indicators covering both national and international metrics were select:

- nutrients status based on the benchmarks defined by Caetano *et al.* (2016) for the Portuguese transitional waters;
- chlorophyll a status based on the benchmarks defined by Brito et al. (2012a) for the Portuguese transitional waters;
- chlorophyll a status based on the benchmarks defined by Brito et al. (2012b) for the Portuguese coastal waters;
- the trophic index TRIX (Vollenweider et al., 1998).

Regarding the nutrients status, Caetano *et al.* (2016) established a methodology to classify the Portuguese transitional waters regarding the chemical status of nutrients. This approach defines nutrient benchmark values based on the 90th percentile of nutrients data collected in 12 Portuguese estuaries (Table 2). For each sample the [nutrient/benchmark] ratio was calculated. Ratios \leq 1.0 are classified as "High" quality, ratios]1.0, 2.0] are classified as "Medium" quality and ratios > 2.0 are classified as "Low" quality. The 90th percentile of all ratios for a given nutrient is then calculated and the final classification given by the worst score.

Nutrient	Salinity: < 1	Salinity: 1-35
NH4 ⁺ (μM)	18	18
NO3 ⁻ + NO2 ⁻ (μM)	89	47
PO4 ³⁻ (μM)	2.8	3.4

Table 7.1 – Nutrients benchmark values proposed by Caetano et al. (2016) for the Portuguese transitional waters

Brito *et al.* (2012a,b) proposed a methodology to assess the ecological quality in Portuguese transitional waters and adjacent coastal waters, using phytoplankton as a biological indicator and combining both the chlorophyll *a* concentrations (as a proxy for phytoplankton biomass) and single taxa cell elevated counts at the level of species or genus (blooms). In the present study, we use the proposed methodology to assess the Tagus estuary and the Ria Formosa status regarding the chlorophyll *a* concentrations. The proposed chlorophyll *a* reference conditions and boundary concentrations are presented in Table 7.2 and Table 7.3 for transitional waters and coastal waters, respectively. To assess the chlorophyll *a* status the 90th percentile of the chlorophyll *a* concentrations was used and compared against the boundary concentrations.

	Chlorophyll a (µg/L)			
	Salinity: ≤ 5	Salinity: > 5 - 25	Salinity: > 25	
Reference	8	8	6.67	
High/Good	12	12	10	
Good/Moderate	18	18	15	
Moderate/Poor	26.67	26.67	22	
Poor/Bad	40	40	33.5	

Table 7.2 – Chlorophyll *a* reference conditions and boundary values proposed by Brito *et al.* (2012a) for the Southwide typology Portuguese transitional waters

Table 7.3 – Chlorophyll *a* reference conditions and boundary values proposed by Brito *et al.* (2012b) for adjacent coastal waters (CW) and in southern coastal lagoons (CW-Ls)

	Chlorophyll a (µg/L)
Reference condition in adjacent CWs	4
Reference condition in southern CW-Ls	5.5
High/Good Boundary in southern CW-Ls	8
Good/Moderate Boundary in southern CW-Ls	12

The trophic index TRIX was used to aggregate the information of four key water quality variables using the following equation (Vollenweider *et al.*, 1998):

$TRIX = [Log(Chla \times |100 - \%D0| \times DIN \times SRP) - (-1.5)]/1.2$

where *Chla* is the chlorophyll *a* concentration (μ g/L), |100-%*DO*| is the absolute percentage deviation from oxygen saturation (%), *DIN* is the dissolved inorganic nitrogen (μ g/L, given by the sum of ammonium, nitrate and nitrite) and *SRP* is the soluble reactive phosphorus (μ g/L). The index was calculated using the data for each station for the overall sampling period. The classification of "High" – [0–4[, "Good" – [4–5[, "Moderate" – [5–6[and "Poor" – [6–10] quality was set (Giovanardi and Vollenweider, 2004; Penna *et al.*, 2004).

7.4.1 Tagus estuary

The water quality in the Tagus estuary was classified based on the data collected during the three main field campaigns performed in 2018 (section 4.2.1) and an assessment of the long-term evolution of the water quality in this estuary was also done using both historical and recent data (section 3.2).

Regarding the nutrients classification (Figure 7.4), results suggest that the upstream water body is at risk (WB4 presented "Medium" status). The middle and downstream water bodies (TE-WB1 and TE-WB2) presented a "High" status, with the exception of TE-WB3 (middle-right margin) that is also at risk ("Medium" status). The assessment of the historical data suggests that high loads of nutrients have been reaching the Tagus estuary over time, with a decreasing trend in the recent years. TRIX (Figure 7.5) suggests a "Moderate" trophic status in the middle and upstream of the estuary (TE-WB2 and TE-W4). A "Poor" classification was obtained for TE-WB3, mainly due to ammonium concentrations, suggesting a more intense anthropogenic pressure than at the other water bodies. Similarly to the nutrients status classification, TRIX suggests an improvement of the water quality in the Tagus estuary in recent years compared to the 1980s (Table 7.4). The results of nutrients status and TRIX classifications are available in the web portal (section 3.4, Figure 3.11, Figure 7.5). TRIX was also computed based on the results of the scenarios simulations, as mentioned above (section 6.3), and the resulting maps are also available on the web portal.

Results suggest a "High/Good" classification regarding the chlorophyll *a* concentrations at all the sampling stations located in the Tagus estuary, with exception of TE-WB4 ("Moderate-Low").

Further details can be found in Rodrigues et al. (2020).



Figure 7.4 – Nutrients status in the Tagus estuary based in the 2018 dataset using the methodology proposed by Caetano *et al.* (2016)



Figure 7.5 – TRIX in the Tagus estuary based in the 2018 dataset – as available in the UBEST observatory web portal

Table 7.4 – TRIX (H – High, G – Good, M – Moderate, P – Poor) in the Tagus estuary: comparison between datasets from three distinct periods

	TE-WB1	TE-WB2	TE-WB3	TE-WB4
1980s	Р	Р	Р	Р
2010	G	G	G	Р
2018	G/M	М	Р	М

7.4.2 Ria Formosa

The water quality in the Ria Formosa was classified based on the data collected during the four field campaigns performed in 2017 and 2019 (section 4.2.2) and are presented in Figure 7.6 and Figure 7.7. The TRIX results show that globally the trophic status of the Ria Formosa water bodies is classified as "High" (oligotrophic state), except for the WB5, that presented a classification of "Good" (mesotrophic state). BS showed the lowest TRIX classification showing the best water quality. In relation to the chlorophyll *a* status, based on the benchmarks defined by Brito *et al.* (2012b) for southern coastal lagoons the results indicate a "High/Good" classification at all the sampling stations located in the Ria Formosa.



Figure 7.6 – TRIX in the Ria Formosa based in the 2017 dataset – as available in the UBEST observatory web portal

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Figure 7.7 – Chlorophyll *a* status in the Ria Formosa based in the 2017 and 2019 dataset using the benchmarks proposed by Brito *et al.* (2012b)

8 | Task 6: Management and knowledge transfer

8.1 Overview

The main objectives of this task were to ensure the achievement of the project results and to provide the measures that guarantee the effective dissemination of the project outcomes.

The main results, described below, were:

- a wide dissemination of the project at both national and international levels;
- the realization of the final workshop;
- the progress and final reports of the project.

8.2 Dissemination

The dissemination of the project outcomes to the research and end-users communities was performed through the usual channels, such as reports, peer-reviewed papers and appropriate conferences. Section 10 provides the list of publications of the project and allows the overview of the objectives achieved regarding dissemination.

The bridge to the end-uses (e.g. National Environment Agency, Regional Coordination Commissions, Harbor Authorities) was performed through specific meetings.

A dedicated webpage in Portuguese and English was developed and maintained (http://ubest.lnec.pt) and dissemination materials were produced (Annex I).

A final workshop was also held on December 13, 2020 in the University of Algarve that allowed the dissemination of project outcomes for both the scientific community and the local authorities and managers (Figure 8.1). The workshop had about 20 participants from different institutions, including the Agência Portuguesa do Ambiente – ARH Algarve, the Águas do Algarve and the University of Algarve, among others. During the workshop a presentation was made by Prof. António Melo Baptista (advisory of the project). The agenda of the workshop is presented in Annex III.

The project was invited for two public sessions, namely the "2° Seminário: Estudo dos Cnidários, as ferramentas disponíveis" (Lisboa, 15 de novembro de 2017) and the "Jornadas Tecnológicas 2018, Engenharia do Ambiente" (Caparica, 6 de fevereiro de 2018).

In addition, the project was also invited to participate in the Workshop of the project MyCoast, that was held on December 10, 2019, envisioning the building of an "Observatório do Tejo e do Sado". This workshop had the participation of several institutions, including the Instituto Superior Técnico (Organizer) and the Faculdade de Ciências da Universidade de Lisboa, the Agência Portuguesa do Ambiente, among others. The building of this observatory is an ongoing initiative for which the results of the project, in particular for the Tagus estuary, will contribute.

<image>

Figure 8.1 – Final workshop of the project UBEST – University of Algarve, December 13, 2020

The lack of funding for the "Our Virtual Global Estuary" initiative prevented the linkage between the two projects. The participation of Prof. António Melo Baptista as consultant of UBEST was however maintained throughout the project through several remote meetings. In addition,

Within the project advanced training was achieved through an ongoing PhD thesis, M.Sc theses and several other opportunities at lower academic level, listed in Section 9.

8.3 Management

The functioning and coordination of the team was ensured by the Principal Investigator (PI), assisted by the coordinators of the work packages (Table 2.1), in order to ensure the fulfillment of the project program and the technical coordination. General and sectorial team meetings were frequent and fundamental to promote the collaboration in task execution and the good communication within the team and with the project consultant. Several remote meetings took place with the project advisor Prof. António Melo Baptista. Four general project team meetings took place (07/07/2016, 04/10/2017, 24/01/2019, 12/12/2019). Two annual scientific progress reports were submitted to FCT.

9 | Advanced training

9.1 PhD Theses

[1] **Rui Cereja** (October 2017-ongoing), PhD in Earthsystems, Faculdade de Ciência da Universidade de Lisboa, "Development of environmental quality indexes for estuaries: assessment of the temporal and spatial variability in the phytoplankton community". Supervised by Vanda Brotas (FCUL), Ana Brito (FCUL) and Marta Rodrigues (LNEC).

9.2 Master Theses

[1] **Sara Mendes** (September 2016-September 2017), Ms.C in Ecologia e Gestão Ambiental, Faculdade de Ciência da Universidade de Lisboa, "Influência da sedimentação de sólidos em suspensão na dinâmica da contaminação fecal no estuário do Tejo". Supervised by Maria Filomena de Magalhães (FCUL), Marta Rodrigues (LNEC) and Elsa Mesquita (LNEC).

[2] **Paolo Tufoni** (2019-ongoing). Ms.C in Sistemas Marinhos e Costeiros, Universidade do Algarve, "Temporal variability of physico-chemical parameters acquired in a real-time monitoring station in an inner area of Ria Formosa (ongoing)". Supervised by Alexandra Cravo (UAlg) and José Jacob (UAlg).

9.3 Others

[1] **Davinia Luzardo** (September-December 2017), Internship of the programme ERASMUS+, Universida de Las Palmas de Gran Canaria– integrated in the project UBEST (Task 1 and Task 5). Supervised by Marta Rodrigues (LNEC) and André B. Fortunato (LNEC).

[2] Romain Deburghgraeve (January-May 2018), Internship in the scope of the "Stage ingénieur", École Centrale de Lyon – collaboration in the development of the low-cost sensor for water levels. Supervised by João Rogeiro (LNEC).

[3] **Diana Silva** (2018). Technical-Cientific project for the Degree in Biologia Marinha, Universidade do Algarve, "Comparação da qualidade da água entre as extremidades da Ria Formosa (Praia de Faro e Cacela) e a Barra Faro-Olhão". Supervised by Alexandra Cravo (UAlg).

10 | Publications

10.1 Book chapters

[1] Oliveira A, Rodrigues M, Rogeiro J, Fortunato AB (2019). OPENCoastS: An open-access app for sharing coastal prediction information for management and recreation. In: Rodrigues J *et al.* (Eds) Computational Science – ICCS 2019. ICCS 2019. Lecture Notes in Computer Science, 11540, 794-807. https://doi.org/10.1007/978-3-030-22750-0_80

[2] Martins R, Rogeiro J, Rodrigues M, Fortunato AB, Oliveira A, Azevedo A (2019). Highperformance computing applied to numerical models in UBEST. In: Abramowicz W, Paschke A (Eds), BIS 2018 International Workshops, LNBIP 339, 507-516. https://doi.org/10.1007/978-3-030-04849-5_44

10.2 Papers in international journals

[1] Rodrigues M, Martins R, Rogeiro J, Fortunato AB, Oliveira A, Cravo A, Jacob J, Rosa A, Azevedo A, Freire P (2020, submmited). A web-based observatory for biogeochemical assessment in coastal regions. *Journal of Environmental Informatics*.

[2] Rodrigues M, Cravo A, Freire P, Rosa A, Santos D. (2020). Temporal assessment of the water quality along an urban estuary (Tagus estuary, Portugal). *Marine Chemistry,* in press, https://doi.org/10.1016/j.marchem.2020.103824

 [3] Cravo A, Rosa A, Jacob J, Correia C (2020). Dissolved oxygen dynamics in Ria Formosa lagoon a real time monitoring station observatory. *Marine Chemistry*, 223, https://doi.org/10.1016/j.marchem.2020.103806

[4] Oliveira A, Fortunato AB, Rogeiro J., Teixeira J, Azevedo A, Lavaud L, Bertin A, Gomes J, David M, Pina J, Rodrigues M, Lopes P (2020). OPENCoastS: An open-access service for the automatic generation of coastal forecast systems. *Environmental Modelling & Software*, 124, 104585. https://doi.org/10.1016/j.envsoft.2019.104585

[5] Rodrigues M, Fortunato AB, Freire P (2019). Saltwater intrusion in the upper Tagus estuary during droughts. Geosciences. 9(9), 400. https://doi.org/10.3390/geosciences9090400.

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In submission

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11 | Collaborations and acknowledgments

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- EPAL Empresa Portuguesa das Águas Livres
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- Águas do Algarve

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- Universidade do Algarve Cátia Correia and João Cunha
- Faculdade de Ciências da Universidade de Lisboa Joana Cruz, Juan Barcelo, Rui Cereja and Teresa Camelo

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- APS Administração do Porto de Sines
- Marina do Parque das Nações
- Marina de Cascais
- APL Administração do Porto de Lisboa
- Staal (formely SenZ2)
- S::CAN

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- project H2020 BINGO (Grant Agreement No. 641739) through the development of the hydrodynamics model of the Tagus estuary and the maintenance of the monitoring network in the Tagus estuary
- project FCT AQUAMON (PTDC/CCI-COM/30142/2017) through the maintenance of the monitoring network in the Tagus estuary

12 | Main results and critical appraisal

The proposed project scientific objectives were clearly achieved. The project contributed to improve the knowledge on the biogeochemical dynamics in estuaries and coastal lagoons, and in particular the Tagus estuary and the Ria Formosa. In particular, the project contributed with a detailed characterization of the current water quality and biogeochemical dynamics in these systems and provided further insights about their response to climate change and anthropogenic pressures. The use of an integrated approach, combining field observations and numerical modelling, was fundamental as it allowed to effectively cover the relevant temporal (past-present-future) and spatial scales (entire coverage of the water bodies). The main deliverable of the project was an innovative coastal observatory, denoted UBEST coastal observatory, to support the water quality management in transitional and coastal systems taking into account different levels of information. This observatory aggregates all the main results of the project as layers of information with different levels of aggregation. The results of the project also contributed to the capacity-building of the participant institutions through the availability of information and the improvement of tools (e.g., numerical modelling, real-time monitoring, real-time forecast system).

The main project results are:

- an improved understanding of the past physical, chemical and biological evolution in the Tagus estuary and the Ria Formosa coastal lagoon and its relation to climatic and anthropogenic drivers;
- a new data repository that stores the historical data compiled and the data acquired during the project;
- acquisition of complementary physical, chemical and biological data in the Tagus estuary and Ria Formosa coastal lagoon trough conventional field campaigns;
- the deployment of a state-of-the-art biogeochemical online probe and maintenance of realtime monitoring stations;
- online acquisition of real-time data and uploading to the data repository;
- conception, assembling and testing of a low-cost sensor for water levels;
- validated three-dimensional baroclinic hydrodynamics and biogeochemical models of the Tagus estuary and of the Ria Formosa
- extension of the Water Information and Forecast Framework to provide forecasts of physical, chemical and biological variables and the automatic comparison with online data for the Tagus estuary and Ria Formosa;
- estimation of the Net Ecosystem Metabolism (NEM) for the Ria Formosa for one year from continuous observations;
- database of physical, chemical and biological variables information for anthropogenic-induced and climate change scenarios for each system;

- assessment and quantification of anthropogenic-induced and climate change impacts and an improved understanding of the Tagus estuary and the Ria Formosa biogeochemical response to increased nutrients loads, sea level rise, changes in the hydrological regimes and in the air temperature;
- the classification of the Tagus estuary and Ria Formosa from physical metrics;
- the classification of the Tagus estuary and Ria Formosa from different water quality metrics trophic status;
- setting the relative positioning of the Tagus estuary and the Ria Formosa physical and trophic conditions at a global scale;
- an innovative web portal and associated services that provides access to all the information gathered and produced during the project to the users (http://portal-ubest.lnec.pt).

Globally, the biogeochemical dynamics of both systems presents seasonal patterns typical of temperate systems. In the Ria Formosa, the water characteristics depend strongly, not only on the seasonal variability but also on tidal mixing, which is reflected in both spatial and short-term temporal dimensions of the physical-chemical and biological water quality. Tides are also an important driver of the biogeochemical dynamics in the Tagus estuary, but the freshwater input also plays an important role in this system in controlling its dynamics.

Anthropogenic pressures affecting the nitrogen and phosphorus loads are typically of the same type in the Tagus estuary and the Ria Formosa, including the discharge of urban and industrial effluents and agriculture practices. However, remarkable differences are found between the Ria Formosa and the Tagus estuary on the estimated magnitudes of the nutrient loads. These loads are about two orders of magnitude higher in the Tagus estuary, highlighting the larger anthropogenic pressures in this system.

In the Tagus estuary 2018 data suggest that the upper estuary is at risk regarding the nutrients classification with a "Medium" status. The middle and downstream areas presented a "High" status, with the exception of the middle-right margin that is also at risk ("Medium" status). TRIX suggests a "Moderate" trophic status in the middle and upstream areas of the estuary. As for nutrients, a "Low" classification was obtained in the middle-right margin of the estuary, mainly due to ammonium concentrations, confirming an intensification of anthropogenic pressure at this site. The historical data suggest that high loads of nutrients have been reaching the Tagus estuary over time, with a decreasing trend in recent years, mostly related with reductions of the nitrogen and phosphorus loads. These reductions could be associated to the improvement/upgrade of the wastewater treatment systems or of the agricultural practices.

In the Ria Formosa (2017 and 2019 data), TRIX shows that globally the trophic status of the Ria Formosa water bodies is "High" (oligotrophic state), except for the WB5 area, that presented a classification of "Good" (mesotrophic state). Concerning the chlorophyll *a* status, a "High/Good" classification was obtained at all the sampling stations located in the Ria Formosa. Results of nutrients and chlorophyll *a* concentrations have shown a decreasing trend over the past 40 years (related with the improvement and/or upgrade of wastewater treatment systems, lower loads of fertilizers applied on

agriculture fields and increased circulation at certain inlets and channels). As a result, the water quality of Ria Formosa has been improving.

Future scenarios provided further insights into the systems' response to climate change and anthropogenic pressures. For the Tagus estuary, results suggest that for the evaluated scenarios changes in the sea level and river flow have a larger influence in the circulation and water quality dynamics compared to the changes in the nutrient loads at the riverine boundaries. Sea level rise and the decrease in river flow increase the salinity and decrease nutrients and chlorophyll *a* concentrations in the upper estuary. In the Ria Formosa, results suggest that sea level rise increases the salinity mainly in the vicinity of the wastewater treatment plants and that an increase of the air temperatures of about 1.7°C leads increases of the water temperature in the lagoon of about 0-1°C. Minimal differences were observed between the simulated scenarios regarding chlorophyll *a* concentrations.

The team dynamics led to a wider dissemination of the project results than expected at the time of the proposal.

The expected output indicators were in general exceeded (section 6): 2 papers in book chapters (0 proposed); 6 (+1 in submission) papers in international journals (4 proposed); 2 papers in national journals (0 proposed); 14 (+2 submitted for 2020) communications in international conferences (4 proposed); 11 (+2 submitted for 2020 and 2021) communications in national conferences (2 proposed); 12 reports (8 proposed); 1 organizations of seminars and conferences (1 proposed); 1 PhD thesis (ongoing) (1 proposed); 1 Master thesis (+1 ongoing) (0 proposed); 3 advanced training at lower academic level (0 proposed); 2 models (2 proposed); 3 software, namely the data repository, the forecast engine and the UBEST web portal (2 proposed); 2 pilot plants for water quality monitoring (2 proposed); and 1 prototype for water levels monitoring (0 proposed). Exception to the complete achieving of the output indicators was the advanced training of a PhD student. A PhD is ongoing but was not concluded. Within the project, advanced training was also achieved through a M.Sc thesis and several other opportunities at lower academic level.

Description	Proposed	Achieved
A – Publications Books chapters Papers in international journals Papers in national journals	0 4 0	2 6 2
 B – Communications Communications in international meetings Communications in national meetings 	4 2	14 11
C – Reports (including the Guidelines for Actors)	8	12
D – Organization of seminars and conferences	1	1
E – Advanced training PhD theses Master theses Others	1 0 0	1 (ongoing) 1 (+1 ongoing) 3
F – Models	2	2
G – Software	2	3
H - Pilot plants	2	2
I – Prototypes J – Patents L – Other Webpage	0 0 0	1 0 1

Table 12.1 – Expected and accomplished output indicators

Lisbon, LNEC, May 2020

APPROVED

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Annexes

ANNEX I Abstract for publication and dissemination

Final Report



Understanding the biogeochemical buffering capacity of estuaries relative to climate change and anthropogenic inputs

UBEST aims at improving the global understanding of the biogeochemical buffering capacity of estuaries and its susceptibility to future scenarios of anthropogenic inputs and climate change. UBEST will effectively support the short and long-term management of these systems. This goal will be achieved by deploying "observatories", which are emerging tools that integrate process-based numerical models and their results, and in-situ observations. To promote the generalization of the conclusions, two Portuguese estuaries with very distinct characteristics will be assessed, the Ria Formosa and the Tagus estuary.

The specific objectives of UBEST are i) the deployment of a monitoring network for biological and chemical parameters (e.g. chlorophyll-a, dissolved oxygen and nutrients) that will include an online biogeochemical station and a set of conventional stations; ii) the implementation/improvement and validation of state-of-the-art, process-based, coupled hydrodynamic-biogeochemical models in each system; iii) the quantification of the biogeochemical buffering capacity of each estuary under present conditions and for projected scenarios of sea level rise, changes in the hydrological regimes, air temperature and nutrients loads; and iv) the assessment of the estuarine physical and trophic conditions of the two estuaries under global classification metrics, and their comprehensive comparison with other estuaries worldwide.

By integrating online and conventional data with results of high-resolution numerical simulations to evaluate both the anthropogenic and climate change effects in the estuarine dynamics, UBEST will cover all the spatial and temporal scales in an effective manner and provide a long-term (past-present-future) analysis of the systems. Exploratory eutrophication and hypoxia analyses will be performed. Budgets of carbon, nitrogen, phosphorous and silica will be estimated and related with relevant metrics to evaluate the system's biogeochemical status, including the Net Ecosystem Metabolism. Both conventional and new classification systems, mechanistically related to the estuary's physical regimes, will be used to perform local and global comprehensive estuarine comparisons. This classification will be used as a stepping stone towards generalization of the conclusions driven from the Tagus and Ria Formosa systems. The estuarine case studies of UBEST are integrated in the international effort "Our Virtual Global Estuary", which envisions a global comprehensive comparison of the biogeochemical status and susceptibility of the estuaries worldwide.

To achieve the proposed goals, UBEST will involve a multidisciplinary team from LNEC and UALG-CIMA, with complementary expertise in the fields of numerical modelling, insitu data acquisition, laboratorial analyses and online data-model deployments.

http://ubest.lnec.pt/



Partners INIVERSIDADE DO ALGARVE

Funding FCT Fundação para a Ciência e a Tecnologia MINISTÉRIO DA CIÊNCIA, TECNOLOGIA E ENSINO SUPERIOR

ANNEX II Project meetings



Reunião de Lançamento

07 de julho de 2016 Laboratório Nacional de Engenharia Civil

Agenda

14:00-14:30	Visão geral do projeto
14:30-15:00	Contratação de bolseiros
15:00-15:20	Aquisição de equipamento
15:20-16:10	Preparação das campanhas de campo e instalação de equipamento
16:10-16:40	Requisitos da interface: observações, simulações e classificação
16:40-17:00	Outros assuntos

 UBEST - Understanding the biogeochemical buffering capacity of estuaries relative to climate change and anthropogenic input







Reunião de Progresso

04 de outubro de 2017 Laboratório Nacional de Engenharia Civil Sala de Reuniões do DHA

Agenda

10:30-10:40	Boas-vindas e agenda
10:40-11:20	Progresso das atividades técnico-científicas no 1º ano do projeto (MR)
11:20-13:00	Apresentação de desenvolvimentos do projeto
11:20-11:50	Monitorização na Ria Formosa (AC/JJ/AR)
11:50-12:10	Repositório de dados (JR/MR)
12:10-12:40	Plataforma WebSIG (RM/AO)
12:40-13:00	Discussão – Acesso e disponibilização de dados na plataforma
13:00-14:30	Almoço
14:30-15:00	Situação financeira (MR)
15:00-16:40	Preparação do 2º ano do projeto (tópicos para discussão) <i>Tarefa 2 - Monitorização</i>
	Tarefa 3 – Modelação hidrodinâmica-biogeoquímica e previsão
	Tarefa 4 – Cenários
	Tarefa 5 – Classificação e indicadores
	Tarefa 6 – Disseminação e ligação ao OGE
16:40-17:00	Outros assuntos

 UBEST - Understanding the biogeochemical buffering capacity of estuaries relative to climate change and anthropogenic input







Reunião de Progresso

24 de janeiro de 2019

Laboratório Nacional de Engenharia Civil e Universidade do Algarve

Videoconferência

Agenda

09:30-09:40	Boas-vindas e agenda
09:40-10:00	Progresso das atividades técnico-científicas no 2º ano do projeto (MR)
10:00-12:15	Apresentação de desenvolvimentos do projeto e preparação das próximas tarefas
10:00-10:15	Tarefa 2 - Monitorização
10:15-10:45	Tarefa 3 – Modelação hidrodinâmica-biogeoquímica e previsão
10:45-11:00	Tarefa 4 – Cenários
11:00-11:30	Tarefa 5 – Classificação
11:30-12:00	Plataforma de acesso aos resultados
12:00-12:15	Tarefa 6 – Disseminação
12:15-12:45	Situação financeira (MR)
12:45-13:00	Outros assuntos

 UBEST - Understanding the biogeochemical buffering capacity of estuaries relative to climate change and anthropogenic input







Reunião de Final

12 de dezembro de 2019 Universidade do Algarve Edifício 1 FCT / Sala 010

Agenda

14:00-14:15	Boas-vindas e informações gerais
14:15-15:55	Ponto de situação das tarefas e discussão das tarefas a finalizar até ao final do projeto
15:55-16:30	Discussão sobre aspetos relevantes de preparação do workshop
16:30-17:00	Disseminação do projeto
17:00-17:30	Situação financeira
17:30-17:45	Outros assuntos

 UBEST - Understanding the biogeochemical buffering capacity of estuaries relative to climate change and anthropogenic input





ANNEX III Agenda of the workshop

Final Report

Compreensão da capacidade de regulação biogeoquímica dos estuários num contexto de alterações climáticas e das fontes antropogénicas



Workshop - Projeto UBEST Observatórios costeiros: ferramentas de apoio à gestão

Universidade do Algarve, Campus de Gambelas, Edifício 1 FCT / Sala 010, 13/12/2019

Agenda

13:45-14:00 - Recepção de participantes
14:00-14:10 - Boas vindas
14:10-15:00 - Apresentação do Prof. António Melo Baptista (OHSU/EUA): "Um quarto de século depois, sabemos tanto e tão pouco sobre o estuário do Rio Columbia"
15:00-15:10 - O projeto UBEST
15:10-15:40 - Monitorização a diferentes escalas temporais: Ria Formosa e estuário do Tejo
15:40-16:10 - Previsão diária e efeitos das alterações climáticas e ações antropogénicas na hidrodinâmica e na qualidade da água
16:10-16:30 - Coffee-break
16:30-17:10 - UBEST app: Observatórios estuarinos em ambiente WebSIG
17:10-17:30 - Lições e perspetivas/Discussão
17:30-17:40 - Encerramento
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