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REALQUAL: TOWARDS REAL-TIME HIGH-RESOLUTION MONITORING AND PREDICTION OF WATER QUALITY IN ESTUARIES AND COASTAL AREAS

Final Report

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Título

REALQUAL: TOWARDS REAL-TIME HIGH-RESOLUTION MONITORING AND PREDICTION OF WATER QUALITY IN ESTUARIES AND COASTAL AREAS
Final Report

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REALQUAL: TOWARDS REAL-TIME HIGH-RESOLUTION MONITORING AND PREDICTION OF WATER QUALITY IN ESTUARIES AND COASTAL AREAS

Final Report

Abstract

This report presents the main activities and results of the project *RealQual: Towards real-time high-resolution monitoring and prediction of water quality in estuaries and coastal areas*, a collaborative project of the FLAD / NSF 2013, Portugal - U.S. Research Networks Program. RealQual aimed at developing the foundations of a quality-controlled network for real-time, high-resolution monitoring and prediction of the water quality in estuaries and coastal areas.

Regarding the real-time monitoring component, an online monitoring station for water quality was maintained operational in the Tagus estuary. Several procedures were tested for data quality control using the data from the SATURN OHSU-CMOP (Oregon Health & Science University – Center for Coastal Margin Observation and Prediction) network and will be extrapolated to the monitoring network of the Tagus estuary.

The numerical modelling system for water quality ECO-SELFE was extended to improve its flexibility. A preliminary application of the coupled hydrodynamics and biogeochemical model was performed in the Tagus estuary, based on the improvements made to the horizontal grid and bathymetry. Tests to the computational times showed that the use of the biogeochemical model in real-time is possible and a set of requirements were established towards this deployment within the Water Information and Forecasting System (WIFF).

A dedicated operational Web-based platform was developed for the project, providing access to the real-time data and forecasts of the hydrodynamics and fecal contamination in the Tagus estuary.

Keywords: Online monitoring, Data quality control, Water quality forecasts, Operational Web-based platforms, Tagus estuary

REALQUAL: TOWARDS REAL-TIME HIGH-RESOLUTION MONITORING AND PREDICTION OF WATER QUALITY IN ESTUARIES AND COASTAL AREAS

Relatório Final

Resumo

O presente relatório apresenta as principais atividades e resultados do projeto *RealQual: Towards real-time high-resolution monitoring and prediction of water quality in estuaries and coastal areas*, um projeto colaborativo do programa FLAD / NSF 2013, Portugal - U.S. Research Networks Program. O projeto RealQual visou o desenvolvimento das bases com a vista à implementação de um sistema de monitorização e previsão da qualidade da água em estuários e zonas costeiras, de elevada resolução e baseado no controlo de qualidade da informação.

Na componente de monitorização em tempo real, a estação de monitorização da qualidade da água instalada no estuário do Tejo, em Alcântara, foi mantida em funcionamento operacional. Foram ainda testados vários procedimentos de controlo de qualidade dos dados, utilizando a informação disponível na rede SATURN da OHSU-CMOP (Oregon Health & Science University – Center for Coastal Margin Observation and Prediction), os quais serão extrapolados para a rede de monitorização do estuário do Tejo.

O sistema de modelação numérica da qualidade da água ECO-SELFE foi melhorado, visando o aumento da sua flexibilidade para diferentes aplicações. O modelo acoplado hidrodinâmico e biogeoquímico foi implementado preliminarmente no estuário do Tejo, tendo por base as melhorias realizadas na malha de cálculo horizontal e na batimetria. Foram realizados testes de eficiência computacional, os quais mostraram ser possível a utilização do modelo para a previsão em tempo real da qualidade da água. Neste sentido, foram estabelecidos os requisitos para a implementação deste modelo em tempo real na plataforma operacional Water Information and Forecasting System (WIFF).

Adicionalmente, foi desenvolvida uma plataforma operacional baseada numa aplicação Web, a qual permite o acesso em tempo real aos dados e às previsões hidrodinâmicas e de contaminação fecal no estuário do Tejo.

Palavras-chave: Monitorização em tempo real, Controlo de qualidade dos dados, Previsão da qualidade da água, Plataformas operacionais, Estuário do Tejo

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Acknowledgments

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1 | Introduction

This report presents the main activities developed in the scope of the project *RealQual: Towards real-time high-resolution monitoring and prediction of water quality in estuaries and coastal areas*.

RealQual is a collaborative project of the FLAD / NSF 2013, Portugal - U.S. Research Networks Program developed by the Laboratório Nacional de Engenharia Civil (LNEC) in collaboration with the Oregon Health & Science University, Center for Coastal Margin Observation and Prediction (OHSU-CMOP, USA), led by Prof. António Melo Baptista, and with the consultancy of Prof. Alexandra Cravo from the University of Algarve, Centre for Marine and Environmental Research (UALG-CIMA). RealQual was coordinated at LNEC by Dr. Marta Rodrigues, from the Estuaries and Coastal Zones Division. The project aimed at the development of the foundations towards a quality-controlled network for real-time high-resolution monitoring and prediction of the water quality in estuaries and coastal areas. RealQual started in June 1, 2013 and has been ongoing since then.

The report is organized in 10 sections. Section 2 presents a general overview of the project. Section 3 describes the main results related to the observational network. Section 4 presents the main results related to the water quality numerical modelling system. Section 5 presents the developments of the operational platform. Section 6 provides a general overview of the short-term internships at CMOP. Section 7 presents the main dissemination actions. Section 8 provides an overview of the main initiatives undertaken for future collaborations between RealQual partners. A brief summary of the budget is presented in Section 9. The final remarks are presented in Section 10.

2 | RealQual: Project Overview

RealQual: Towards real-time high-resolution monitoring and prediction of water quality in estuaries and coastal areas aimed at developing the foundations of a quality-controlled network for real-time high-resolution monitoring and prediction of the water quality in estuaries and coastal areas, in particular to anticipate potential eutrophication events.

The main goals of the project were:

i) to transfer OHSU's knowledge on real-time sophisticated observation networks for water quality to the Portuguese team, and to integrate it with LNEC's strategies for quality controlled monitoring;
ii) to develop a highly effective predictive numerical modeling system for water quality, exploring strategies that leverage the hierarchical use of models of different complexity and computational cost;
iii) to improve an operational platform for automated management of the monitoring and predicting water quality network;
iv) to develop a pilot demonstration of the real-time water quality network in the Tagus estuary (Portugal).

RealQual was developed in five main activities:

- Activity 1: Observational network knowledge and technology transfer from OHSU's and implementation of the real-time monitoring network at the demonstration site (Tagus estuary, Portugal);
- Activity 2: Implementation of an effective nowcast-forecast modeling system for water quality;
- Activity 3: Improvement of the operational platform for automated management of the monitoring and predicting water quality network;
- Activity 4: Demonstration in the Tagus estuary;
- Activity 5: Identification of long-term common research goals and funding mechanisms to support the long-term relationship between the involved institutions.

The team of the project was:

- from LNEC, Marta Rodrigues (PI), Anabela Oliveira (co-PI), André B. Fortunato, Gonçalo Jesus, João L. Gomes and João Rogeiro; the project also had the collaboration of LNEC's technicians to support the maintenance of the online observation network and the implementation of the operational platform, Luís S. Pedro, Fernando Brito, Ana Mendes and Américo Louro;
- from OHSU-CMOP, António M. Baptista (PI), Tuomas Karna, Clara Llebot, Pat Welle, Jesse Lopez, Michael Wilkin, and Yvette Spitz;

- consultant from UALG/CIMA, Alexandra Cravo.

The total expected duration of the project was one year. However, the project has been ongoing since its beginning in June 1, 2013, and a real-time observatory for the water quality in Tagus estuary is maintained operational by LNEC. The implementation and maintenance of this network was made possible by the synergies between RealQual and other recent research projects developed at LNEC, namely PREPARED (FP7-ENV-2009-1, Grant agreement 244234, http://www.prepared-fp7.eu/), SPRES (EFDR-EU (SPRES-2011-1/168), http://spres.ihcantabria.com/), SI-GeA (PORLisboa/QREN/FEDER, Project n. 23053, http://www.lnec.pt/organizacao/dha/gti/estudos_id/SI-GeA) projects, which enhanced the achievements of the various projects with positive feedbacks between them. The activities of the project were also integrated in the post-doctoral research of the PI, entitled “Real-time prediction of the microbiological conditions in estuarine and coastal areas in the context of the uncertainty of the models and its forcings”, supervised by Dr. André Fortunato and Dr. José Menaia. The work developed in the data quality control (section 3.2) is also integrated in the Ph.D. program in Computer Science of the University of Lisbon/Faculty of Sciences of Gonçalo de Jesus, supervised by Prof. António Casimiro and Dr. Anabela Oliveira.

3 | Observational Network

3.1 Real-time Monitoring Network in the Tagus Estuary

The real-time monitoring network was deployed in the Tagus estuary in the vicinity of the discharge of the Alcântara outfall (Figure 3.1), which is the largest urban discharge within the estuary including both treated effluents from the Alcântara wastewater treatment plant (WWTP) and combined sewer overflows discharges. A set of criteria was used for site selection [1].

Figure 3.1 – General overview of the Tagus estuary, and location of the Alcântara outfall discharge and of the real-time monitoring network (Source: GoogleEarth).

This monitoring station includes a set of sensors, acquired by LNEC in the scope of the project PREPARED (Figure 3.2): UV-Vis spectrophotometric probe (5 mm optical window), spectro::lyser S::CAN, with municipal WWTP effluent calibration (TSS, COD, soluble COD and nitrates); ammonium and nitrates probe, ammo::lyser S::CAN (ammonium, nitrates, pH, temperature); conductivity and temperature probe, condu::lyser S::CAN (conductivity, temperature, salinity); dissolved oxygen probe, oxi::lyser S::CAN (dissolved oxygen, temperature). The monitoring sensors are controlled on-line using the Con::cube S::CAN controller, which communicates with the operational platform (Figure 3.2; Chapter 5; e.g. [2] [3]).

Figure 3.2 – Sensors installed at the Tagus estuary online monitoring station and Con::cube S::CAN controller: spectro::lyser S::CAN (UV-Vis spectrophotometric probe calibrated for COD, TSS and nitrates), ammo::lyser S::CAN (ammonium, nitrates, pH, temperature), condu::lyser S::CAN (conductivity, temperature, salinity) and oxi::lyser S::CAN (dissolved oxygen, temperature).

The design of the online monitoring station took into account the conditions at the implementation site. An innovative supporting structure was designed and built to support and protect the sensors, taking into account the bidirectional flows due to tides in the estuary [1]. An overview of the deployed monitoring station is presented in Figure 3.3. This station is in operation since October 2013 and data are measured continuously. A set of maintenance procedures was implemented in order to guarantee the quality of the data and the safety of the sensors. These procedures were improved through time, based on the knowledge transfer between LNEC and OHSU-CMOP. Three levels of maintenance procedures are considered:

- Automated cleaning – automated cleaning is promoted using air compressors to clean the sensors (Figure 3.3);
- Periodic cleaning and inspection – procedures of manual cleaning of the equipment and probes, and visual inspections of the infrastructures (e.g. status of the cables, corroded parts) are performed on a weekly basis (Figure 3.4). Checklists are used for this purpose, to guarantee that all the relevant components of the monitoring installation are verified and that a registry of inspections and failures is maintained (Figure 3.5);

- Out-of-schedule cleaning – supplementary procedures for cleaning the sensors may be undertaken when needed (e.g. after severe rain events, trash may accumulate in the supporting structures and needs to be removed – Figure 3.4).

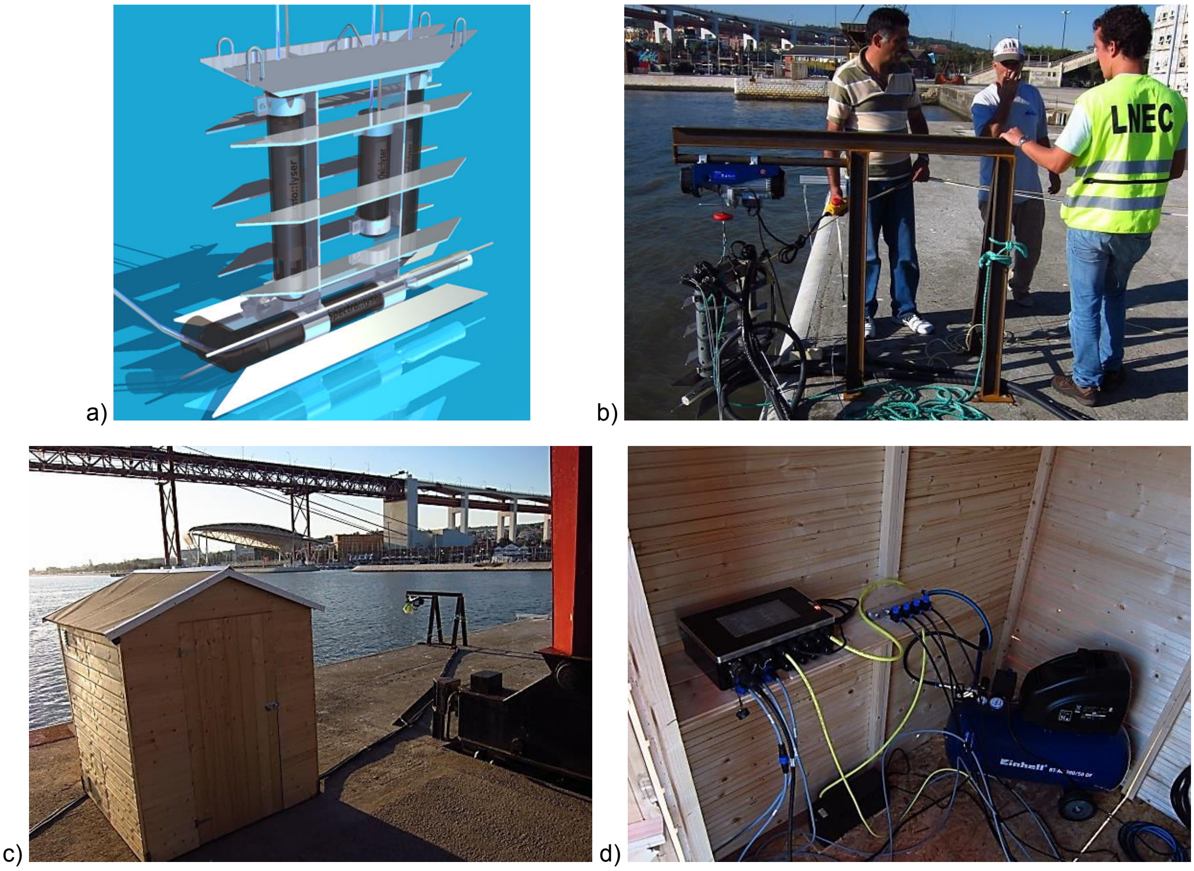

Figure 3.3 – Conceptual design of the support structures of the sensors (a) and Tagus estuary online monitoring station: detail of the supporting structure of the sensors and hoist (b), environmental shelter and supporting structures (c), and Con::cube S::CAN controller and air compressor installed inside the environmental shelter (d).

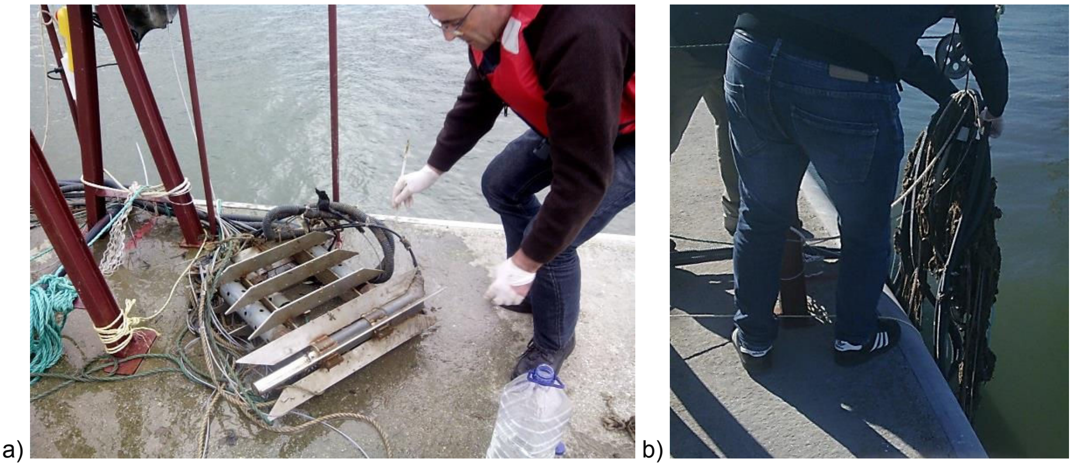

Figure 3.4 – Periodic cleaning and inspection (a, January 14, 2014) and out-of-schedule cleaning after an extreme rain event (b, November 30, 2013).

Sistema de Monitorização em Tempo Real

Folha de Registo de Manutenção Periódica

Local: Cais de Alcântara

Data	**Estruturas Exteriores - Verificação**			**Sondas - Limpeza**					**Abrigo - Verificação**			**Observações**	**Responsável**
	Cabos	Estruturas de Suporte	Outro Material	Remoção de Detritos	Célula Óptica Spectro	Ammo	Condu	Oxi	Estado Geral	Compressor	Cabos Interiores		

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Figure 3.5 – Example of the checklist used in the periodic cleaning and inspection of the receiving waters on-line monitoring station (in Portuguese).

Measured raw data are transmitted using GSM/GPRS and stored in SQL databases (Figure 3.6). Data can be accessed online through the operational platform (Chapter 5). A set of procedures are being developed for the automated quality-control of raw data as described in next section.

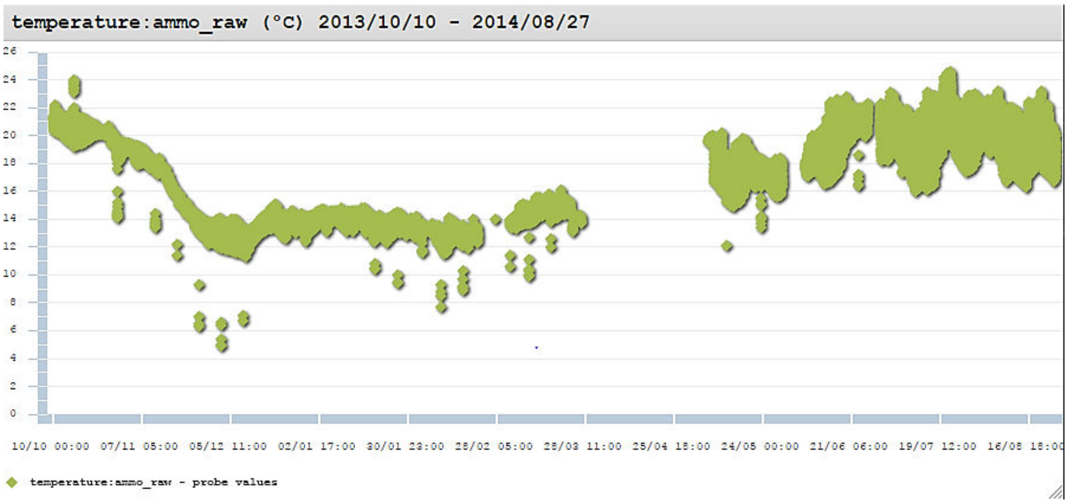


Figure 3.6 – Raw water temperature data acquired between October 10, 2013 and August 27, 2014. Some of the maintenance periods are well identified in the data, characterized by a sharp decrease in a short period of the water temperature.

3.2 Data Quality Control

In water emergency systems, inaccurate information in aquatic monitoring may not be critical for safety within the time frame of other types of monitoring, such as aeronautics, but a possibility of an incorrect forecast may lead to the issuing of false warnings or not issuing real warnings in damaging situations (for instance pollution events).

Existing solutions for aquatic monitoring are composed by a set of heterogeneous sensors [4] most of which vulnerable to the unpredictable natural conditions of a harsh environment. It is important to realize that due to many plausible reasons water-related sensors are unable to always ensure dependable measurements. Dependability of sensor is taken here as a high probability of sensors behaving according the requirements.

The notion of dependability introduced by [5] declares that it is “the measure in which reliance can justifiably be placed on the service delivered by a system”. So, in order to understand if a system is dependable one must learn about the potential reasons for imprecise actions and what are the means to overcome it. The goal is to establish a way to state the level of dependability desired and evaluate if it was achieved.

In order to achieve dependability one should sever the chain that goes from a fault to a failure. To do so, dependable systems use strategies that include fault removal, fault forecasting, fault prevention and/or fault treatment schemes. These strategies are either for stopping fault events from happening or, despite the occurrence of one or more faults, to block their effect (failures), thus making the system fault-tolerant.

The design of a fault-tolerant framework requires an analysis and classification of typical aquatic sensor failures. This step is necessary to determine an effective fault detection strategy identifying its causes and the properties of the failure types. When designing a sensor the optimal strategy would be to detect and correct the fault events at its origins (transducer or software components). But when designing a framework to deal with the failures of commercial, heterogeneous and/or already deployed aquatic sensors one has to analyse how sensor faults affect its measurements and what are the main external disturbances that cause the fault events.

In the previous section, the monitoring network consisting of multiple sensors that communicate using wireless technologies was described. Wireless sensor networks have been the origin to several studies of monitoring failures and causes, especially when addressing harsh situations such as the aquatic environment, where even the most robust sensors are subject to operational faults. Most of the dependability approaches for robustness is to create partial functional redundancy among the sensor nodes in the network.

Herein, the application of a statistical approach in the aquatic monitoring network is introduced, in order to: i) detect outliers or anomalous measurements ii) infer on future measurements. In this strategy it is considered that in the sensor network some neighbouring nodes measure local environments that are temporally and spatially correlated [6].

Several strategies have been proposed that utilize statistical models to summarize data in sensor networks and reconstruct missing or erroneous measurements [7]. A method based on the statistics of differences between sensor measurements was applied [8]. The goal here is to perform automatic event detection and data quality assurance, based on the statistical distributions of the differences between a sensor measurements and those of its neighbors, and also between the same sensor but at different times.

There are two main assumptions required for the method to work: 1) the observed phenomena are spatiotemporally coherent, so that not only readings from neighboring sensors but also from the same sensor over time, present mutual information; 2) the probability density of the differences has a peak near the mean and tails that taper as differences deviate away from it (as in the normal distribution function). The second assumption may be relaxed, but the first is crucial and it is verifiable in our application.

In this project, the data from extensive monitoring network held by CMOP (SATURN – http://www.stccmop.org/datamart/observation_network, Figure 3.7) was used to perform the outlier detection and future measurements estimation. The Science and Technology University Research Network (SATURN) Collaboratory is an interdisciplinary, river-to-shelf observational network. SATURN includes tidal freshwater stations, ocean gliders, autonomous underwater vehicles (AUVs), and estuarine and plume stations measuring everything from salinity and temperature to biogeochemistry and bacterial diversity on a 24/7 basis. The data collected from SATURN feeds the Virtual Columbia River, a skill-assessed modeling system that offers multiple representations of processes, variability and change across river-to-ocean scales. A human-based quality control procedure is available for all datasets, providing a ground-truth for comparison with the automatic quality control proposed herein.

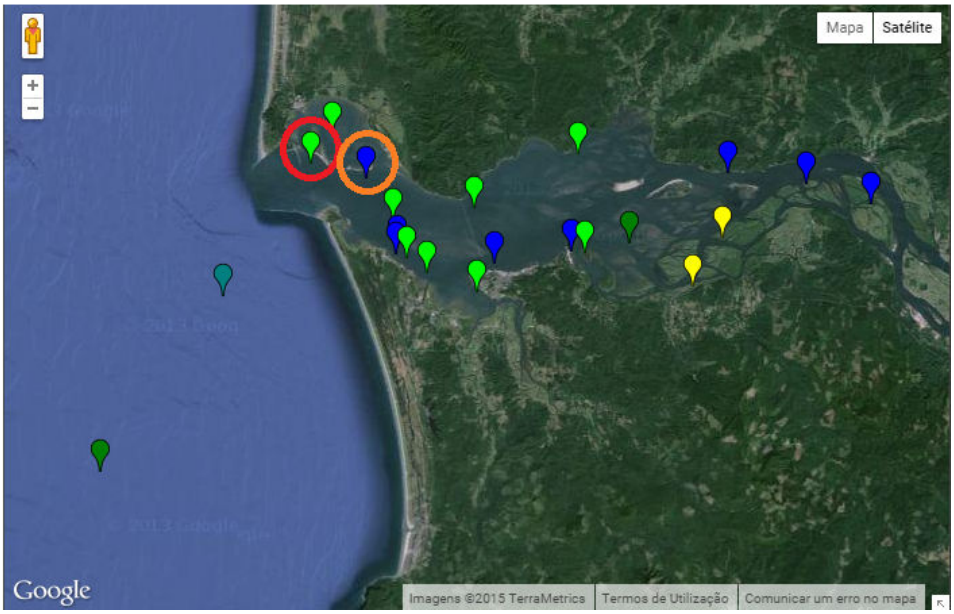


Figure 3.7 – CMOP's Saturn observation network with JettyA and SandI sensors signaled in red and orange respectively.

Stations JettyA (Figure 3.7, in the red circle) and Lower Sand Island light (Figure 3.7, in the orange circle) were selected due to having in common several variables (temperature, elevation and salinity) and were measuring at the same period of time and approximate depths. For this first application of the method the variable salinity was chosen, due to the sensor high sensitivity to changes in the environment.

To set the notation for the applied method, the Lower Sand Island light (SandI) salinity sensor was considered as the object of this method, thus being Φ the sensor's reading, Φ_0 the previous measurement, and Φ_1 the reading of its neighbour (JettyA salinity sensor). At each SandI new reading, the difference between its current reading and its previous measurement and between its reading and the reading of JettyA, $d_i = \Phi - \Phi_i$, $i = 0,1$, were compute. So, given the distribution of the differences each new reading can be tested for errors. It should be noted that the d_0 distribution represents the temporal correlation and that d_1 distribution represents the spatial correlation. Figure 3.8 and Figure 3.9 present an example of both distributions, respectively, the temporal correlation best fit is a Logistic distribution function whereas the spatial correlation is a t-location-scale function (normal distribution could be considered as a substitute when the fitting does not converge).

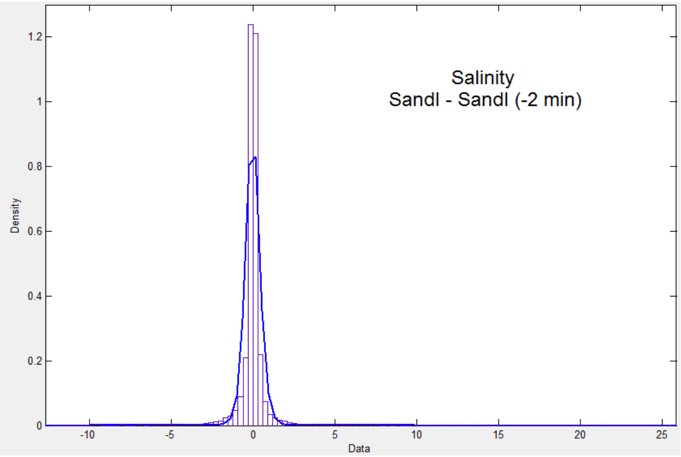


Figure 3.8 – Logistic distribution density of the differences between the actual reading and the previous one.

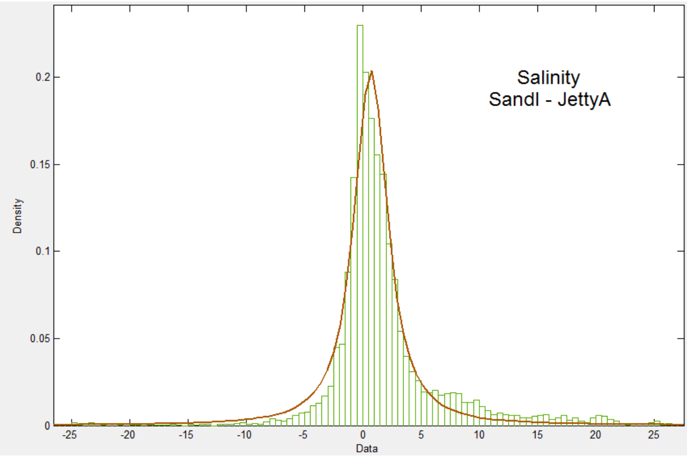


Figure 3.9 – t-location-scale distribution density of the differences between the SandI previous measurement and the actual reading of the JettyA.

Each probability distribution P(*d*) is learned from observed differences. The most natural estimator of a sensor's missing or incorrect reading by the method of differences is through the mean differences:

$$\hat{\phi} = \frac{1}{k+1}\sum_{i=0}^{k}(\phi_i + \mu_i) \qquad (1)$$

where *Φ* estimated is the reading estimate and μ_i is the mean difference relative to the ith neighbour, or if i=0, Φ_0 is the previous reading and μ_0 is the mean difference between the current and previous measurements. A weighted average based on a measure of mutual information between the sensors could also be adopted, but this is the simplest scheme. Knowing the distribution class, μ_i is a stored value, calculated from a previous set of measurements.

A batch of runs with different periods of measurements was performed, based on the major tidal constituents affecting the circulation of Columbia, M2 (half M2 period was also tested) and K1. The method was tested for larger (Mf) periods, but the mean square error increased relative to smaller periods. The minimum mean square error was obtained with a period of M2, MSE = 1.1435, for the same dataset (Figure 3.10).

As for outlier and anomalous detection (filtering), a simple p-value test was adopted, to determine if a new measurement difference is significant. If the new difference fails the significance test it is flagged as an outlier or anomaly, which indicates a single point failure in the sensor. In this case, we will observe that this anomaly translates both in time (previous measurement) and space (neighbour measurement), failing the according *p*-value test ($p_0 < \alpha$ and $p_1 < \alpha$, being α the significance level). The detection of anomalies was performed in the same batch of runs of the inference of missing readings, previously presented, with three levels of significance. α = 0.01 representing significant readings, α = 0.005 for highly significant readings and α = 0.001 for very high significance.

As shown in Figure 3.11 and Figure 3.12, the choice of the significance level will influence on the number of anomalous readings or outliers. For the same run, using α = 0.001, there was not any outlier detected. In conclusion, this method enables to detect not only anomalous reading but also abrupt changes in the phenomena behaviour using higher values of α, and with lower values of α will narrow the results to real outliers (compared to noise).

The present analysis will be extrapolated later to the monitoring network available for the Tagus estuary.

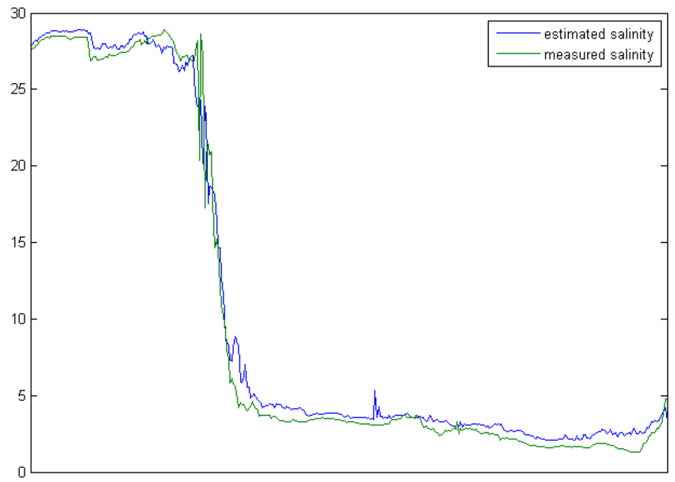


Figure 3.10 – A comparison between the estimator and the actual reading of the salinity sensor Sandl for M2 period.

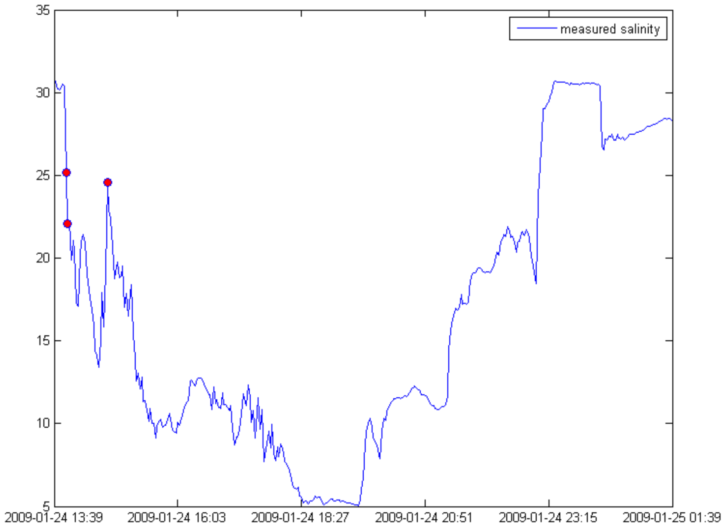


Figure 3.11 – Anomalous readings detected in red, with the filtering method using α = 0.01.

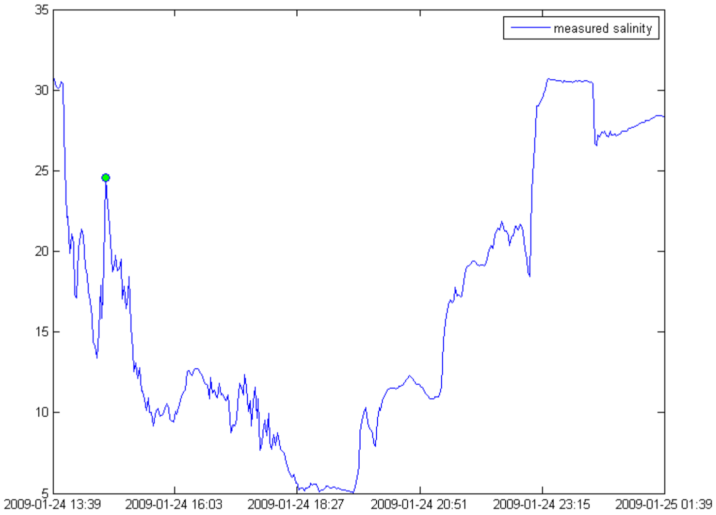


Figure 3.12 – Anomalous readings detected in green, with the filtering method using α = 0.005.

4 | Water Quality Numerical Modeling System

4.1 ECO-SELFE Model Developments

ECO-SELFE is an open-source, three-dimensional, fully coupled hydrodynamic and water quality model [9] [10] [11], which couples the hydrodynamic model SELFE [12] and water quality models for biogeochemical and fecal contamination processes. The model is fully parallelized with Message Passing Interface (MPI) which improves the computational times [13]. The coupled model was developed in the scope of previous collaborations between LNEC and OHSU-CMOP. In RealQual several developments were performed in both the biogeochemical and fecal bacteria models increasing ECO-SELFE's flexibility for different applications. In particular, options to use models with different levels of complexity to simulate the biogeochemical processes were implemented, allowing the user to explore both the accuracy of the predictions and the computational efficiency for a given application.

4.1.1 Fecal Bacteria Model

The fecal bacteria model allows the simulation of two fecal bacteria (fecal coliforms, *Escherichia coli* (*E. coli*) or enterococcus), considering the die-off and sedimentation processes as sink terms. Two options were available for the definition of the die-off rate: a user-defined constant coefficient and the formulation proposed by [14], which presents a direct relation between the die-off rate and the environmental conditions (irradiation, salinity and temperature). The model was further extended to include an additional formulation to simulate the die-off rate of fecal coliforms dependent on water temperature [15] [16] [17]:

$$k_d = k_{20} \frac{\exp\left(-\frac{(T-25)^2}{400}\right)}{\exp\left(\frac{25}{400}\right)} \qquad (2)$$

where k_D is the die-off rate (s^{-1}), k_{20} is the die-off rate at 20 ºC (1.25×10^{-5} s^{-1}) and T is the water temperature (ºC).

4.1.2 Biogeochemical Model

The biogeochemical model formulation was extended from EcoSim 2.0 [18] to simulate zooplankton and the oxygen cycle [9] [11] [19]. ECO-SELFE includes the carbon, nitrogen, phosphorus, silica, oxygen and iron cycles and simulates several ecological tracers (Figure 4.1), and was successfully applied to the Aveiro lagoon [20].

Several options were already implemented within the model allowing the user to select the relevant variables for a given application. These options allowed the user to simulate a minimum of 25 ecological tracers for the carbon, nitrogen, phosphorous and silica cycles, namely: one zooplankton group (expressed in carbon, nitrogen and phosphorous), one phytoplankton group (expressed in carbon, nitrogen, phosphorous and silica), chlorophyll a, bacterioplankton (expressed in carbon, nitrogen and phosphorous), dissolved organic carbon, dissolved organic nitrogen, dissolved organic phosphorous, particulate organic carbon, particulate organic nitrogen, particulate organic phosphorous, particulate organic silica, ammonium, nitrate, phosphate, silicate, dissolved inorganic carbon, dissolved oxygen and chemical oxygen demand.

The model was further extended to allow the simulation of carbon and nitrogen cycles only, considering 15 ecological tracers (Figure 4.2): one zooplankton group (expressed in carbon and nitrogen), one phytoplankton group (expressed in carbon and nitrogen), chlorophyll a, bacterioplankton (expressed in carbon and nitrogen), dissolved organic carbon, dissolved organic nitrogen, particulate organic carbon, particulate organic nitrogen, ammonium, nitrate, dissolved inorganic carbon and dissolved oxygen.

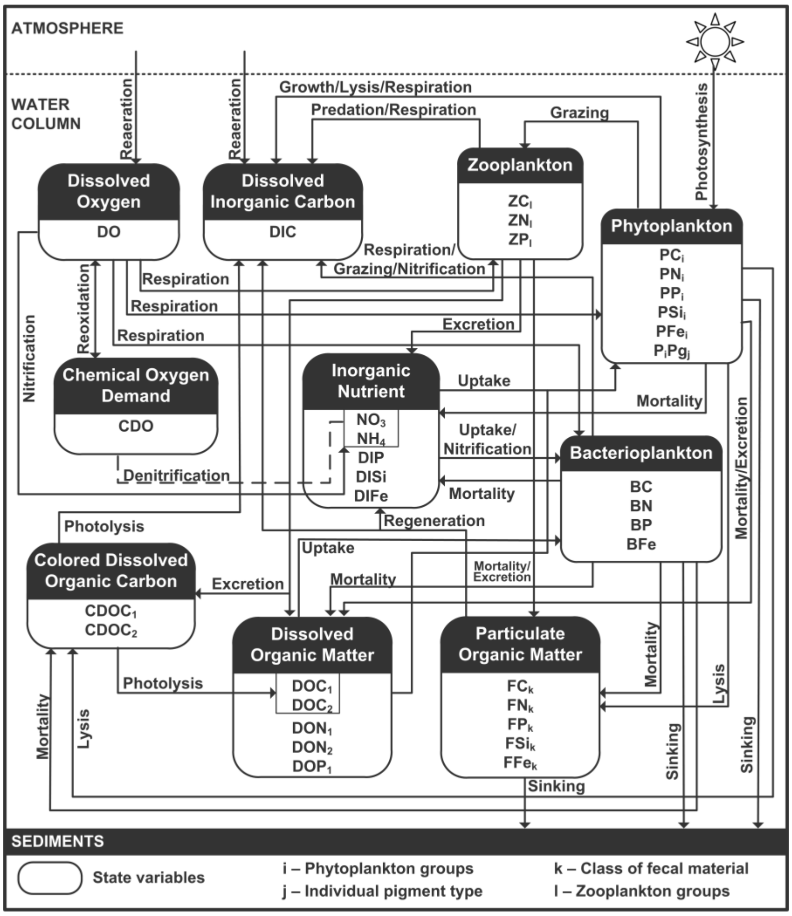


Figure 4.1 – Source and sink terms of the whole biogeochemical model. C – Carbon, N – Nitrogen, P – Phosphorous, Si – Silica, Fe – Iron.

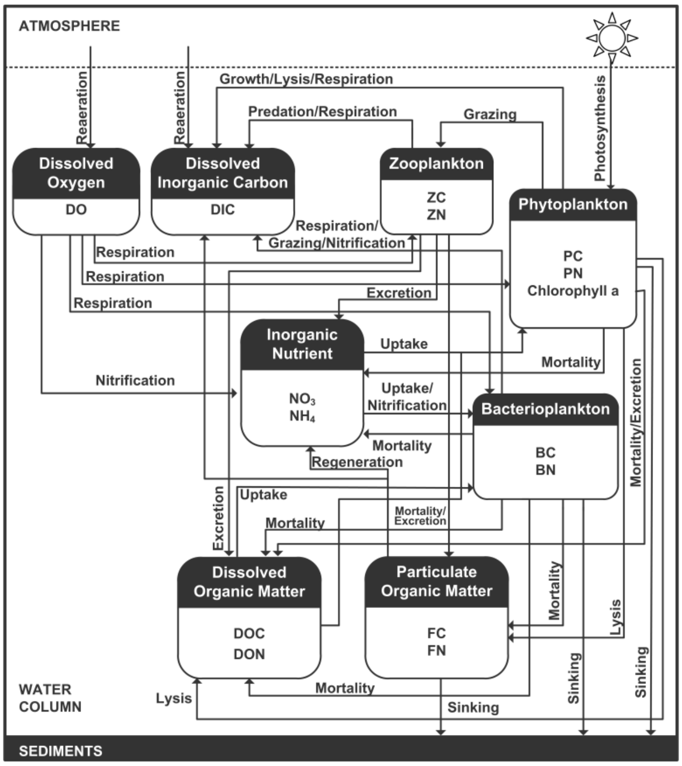


Figure 4.2 – Source and sink terms of the biogeochemical model considering the carbon and nitrogen cycles only and 15 ecological tracers. C – Carbon, N – Nitrogen.

The water quality numerical modelling system was also extended to include an additional simpler biogeochemical model with only 3 ecological tracers. The NPZ (Nitrogen-Phytoplankton-Zooplankton) model of [21] was chosen, following an approach similar to the one used at OHSU-CMOP, where this model is one of the biological models available within the water quality box model developed by OHSU-CMOP (Clara Lebot, CMOP internal report). The model simulates 3 ecological tracers: zooplankton (expressed in nitrogen), phytoplankton (expressed in nitrogen) and dissolved inorganic nitrogen (DIN) – Figure 4.3. The equations that represent the sources and sinks of the ecological tracers are:

$$Q_{\lim} = \frac{DIN}{DIN + K_s} \tag{3}$$

$$I_{\lim} = \frac{\alpha I_0}{\sqrt{V_m^2 + (\alpha I_0)^2}} \tag{4}$$

$$T_{\lim} = \exp\left(\frac{-(T - T_{opt})^2}{dT^2} \right) \tag{5}$$

$$\frac{\partial P}{\partial t} = V_m T_{\lim} I_{\lim} Q_{\lim} P - m_P - R_m (1 - \exp(-\lambda P))Z - \upsilon_P Z \tag{6}$$

$$\frac{\partial Z}{\partial t} = \gamma R_m(1-\exp(-\lambda P))Z - m_Z Z \quad (7)$$

$$\frac{\partial DIN}{\partial t} = -V_m T_{\text{lim}} I_{\text{lim}} Q_{\text{lim}} P + m_P + (1-\gamma)R_m(1-\exp(-\lambda P))Z + m_Z Z \quad (8)$$

where P is the phytoplankton (mmol N m^{-3}), Z is the zooplankton (mmol N m^{-3}), DIN is the dissolved inorganic nitrogen (mmol N m^{-3}), T_{lim} is the temperature-limited growth, I_{lim} is the light-limited growth, Q_{lim} is the nitrogen-limited growth, T is the water temperature (ºC), I_0 is the light intensity (W m^{-2}), V_m is the phytoplankton maximum growth rate (day^{-1}), K_s is the half saturation constant for DIN uptake (mmol N m^{-3}), α is the slope of the light saturation curve (day^{-1} W^{-1} m^2), T_{opt} is the optimal temperature growth of phytoplankton (ºC), dT is the optimal temperature range for phytoplankton (ºC), m_P is the mortality rate of phytoplankton (day^{-1}), v_P is the sinking rate of phytoplankton (day^{-1}), R_m is the zooplankton maximum grazing rate (day-*1*), λ is the Ivlev parameter (m^3 mmol N^{-1}), γ is the efficiency of zooplankton grazing (%/100), and m_Z is the mortality of zooplankton (day^{-1}).

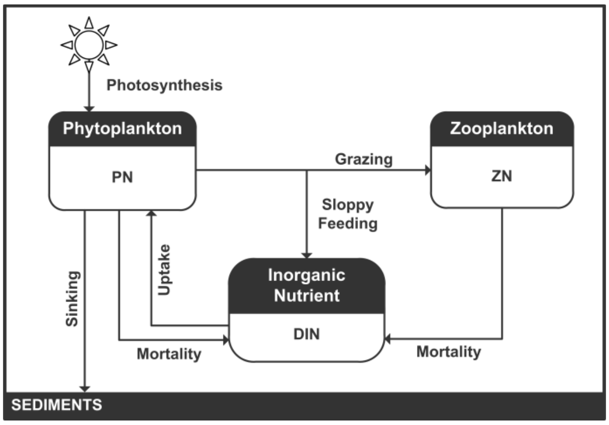


Figure 4.3 – Source and sink terms of the biogeochemical model with 3 ecological tracers (NPZ model based in [21]). N – Nitrogen, DIN – Dissolved Inorganic Nitrogen.

The changes made in the ECO-SELFE source code were validated using the BioToy test case [19]. A very small grid, with 49 nodes (600 m x 600 m) and 11 *S* vertical levels was used. All boundaries were closed. Simulations were performed considering 25 ecological tracers (carbon, nitrogen, phosphorous and silica), 15 ecological tracers (carbon and nitrogen cycles only) and 3 ecological tracers (NPZ model). Initial conditions were set using the analytical initial conditions option. For purposes of comparison between the results of the 25 and 15 ecological tracers' applications, phosphorous and silica were considered in excess, providing that there is no uptake of these nutrients by phytoplankton. Results show the expected correlations between phytoplankton and zooplankton growth, with the zooplankton spikes occurring after the phytoplankton spikes (Figure 4.4 and Figure 4.5).

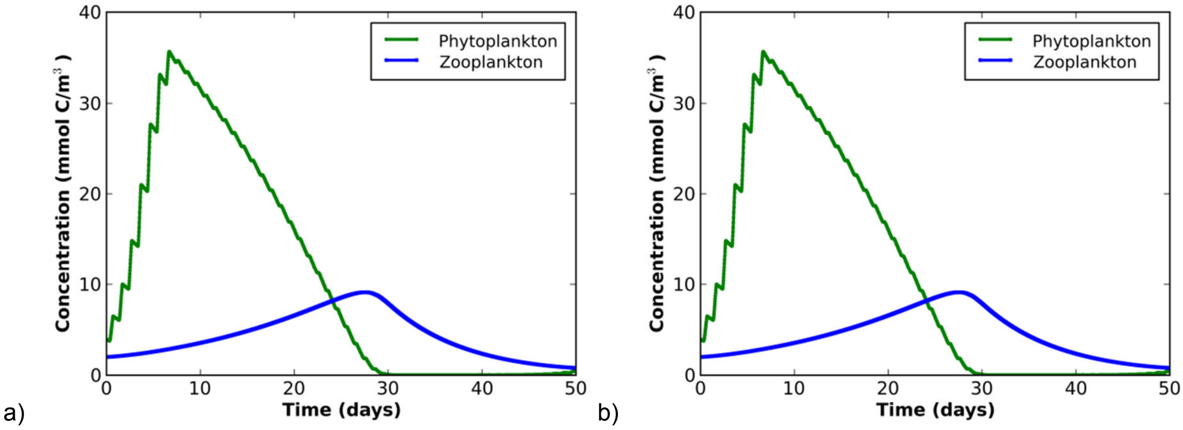


Figure 4.4 – BioToy test case: phytoplankton and zooplankton concentration in the 25 ecological tracers (a) and 15 ecological tracers (b) applications.

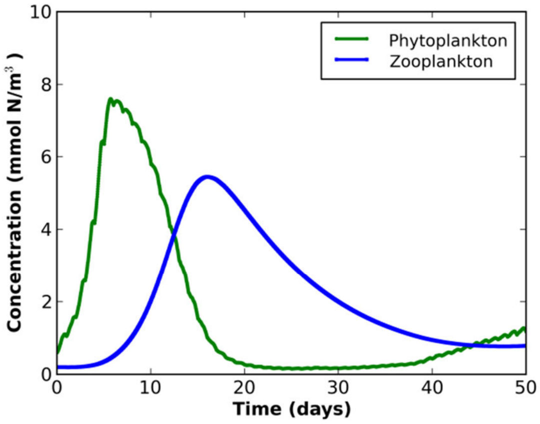


Figure 4.5 – BioToy test case: phytoplankton and zooplankton concentration in the 3 ecological tracers (NPZ model option) application.

4.2 Tagus Estuary Model Improvements

The Tagus estuary hydrodynamics and water quality are simulated using ECO-SELFE 3.1d, considering the simulation of two fecal bacteria tracers: *Escherichia coli* (*E. coli*) and fecal coliforms.

The model setup derived from the application of [22]. A detailed description of the Tagus estuary hydrodynamics and fecal contamination model setup, calibration and validation can be found in [23]. The Tagus estuary model was further extended from this application to account for the relevant urban discharges in the waterfront Algés-Alcântara-Terreiro do Paço and the horizontal grid was improved for a detailed representation of this area. The bathymetry was also updated with the most recent data sets available.

The new domain is discretized with a horizontal grid with about 54000 elements and 29000 nodes (Figure 4.6) and a vertical grid with 20 SZ levels (15 S levels and 5 Z levels). The spatial resolution of the horizontal grid varies from about 1-2 m in the discharges' areas (Figure 4.6) to 2 km in the oceanic area.

The model bathymetry (Figure 4.6) was built from several tens of different data sets. The only available bathymetry that covers the whole estuary, dating from 1964-67, was taken as the baseline and updated wherever more recent data were available. These updates cover the majority of the estuary, so most of the model domain has bathymetric data from the 21st century. Bathymetric data from the Lisbon Harbor Authority cover all the navigable routes and the estuary mouth and sandbanks, typically with resolutions between 3 and 20 m. Along the closed boundaries, two alternative sources of data were used. LIDAR data from 2013 cover all the coastline and part of the northern shore of the estuary; elsewhere, topographic data from the Direção Geral do Território dating from 2008 were used. Both datasets have a resolution of the order of 2 m. One of the major lateral bays, the Seixal Bay, is covered by a bathymetric survey from 2009 with a resolution of 25 m. The major limitation of the model bathymetry occurs in the riverine part of the domain, upstream of Vila Franca de Xira, where only bathymetric cross-sections from 1978, about 2.5 km apart, were available.

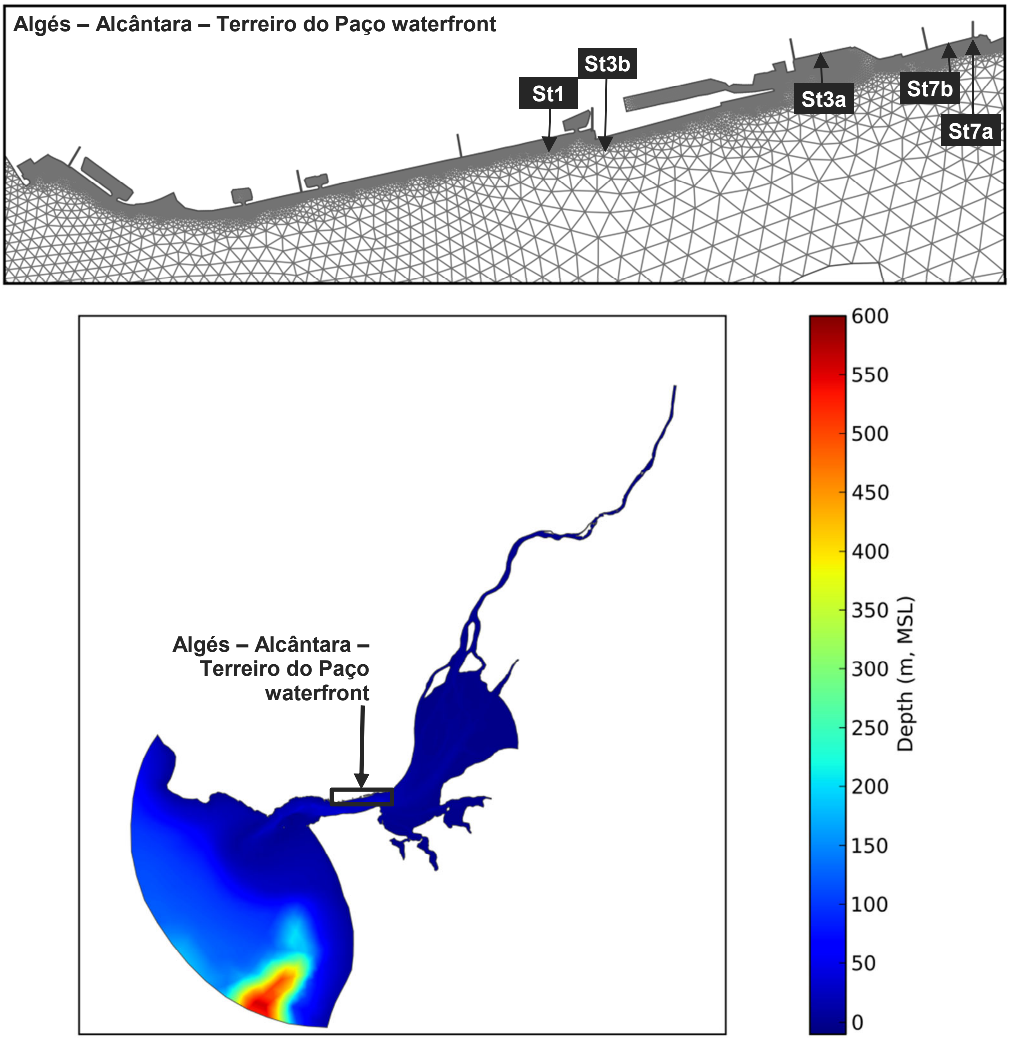


Figure 4.6 – Tagus estuary horizontal grid with the updated bathymetry and detailed view of the updated grid in the Algés – Alcântara – Terreiro do Paço waterfront. Location of the sampling stations is presented.

The updated model was compared against field data. Simulations were performed for the same period that was used to calibrate and validate the previous version of the model [23], between July 2011 and September 2011, during which two field surveys (July 15 and September 6) were undertaken in the scope of the project PREPARED (see [24] for details). The die-off rate of the fecal bacteria tracers was simulated using the new formulation implemented in the water quality model (section 4.1.1). Nine open boundaries were considered: the Atlantic Ocean, the Tagus river, the Alcântara outfall and six additional urban discharges in the waterfront Algés-Alcântara-Terreiro do Paço. These oceanic, riverine and Alcântara outfall boundaries were forced with the conditions considered by [23]. At the additional urban boundaries (defined in the scope of the SI-GeA project) the freshwater flow was set to 0 m^3/s, since simulations correspond to a dry period where no discharges occur at these points. Atmospheric forcing was also considered equal to [23]. The time step was set to 30 seconds. Results show that the updated model is able to represent the main patterns observed (Figure 4.7 and Figure 4.8), and some improvements are observed for some variables when compared with the results obtained with the previous bathymetric data (Figure 4.7).

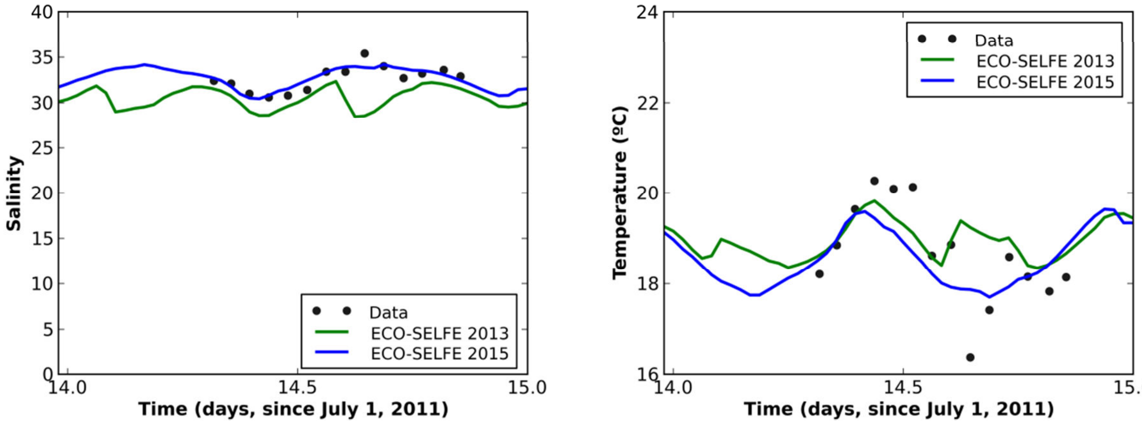


Figure 4.7 – Salinity and water temperature data-model comparisons at station 1 for the previous model application (ECO-SELFE 2013, [23]) and the updated model application (ECO-SELFE 2015).

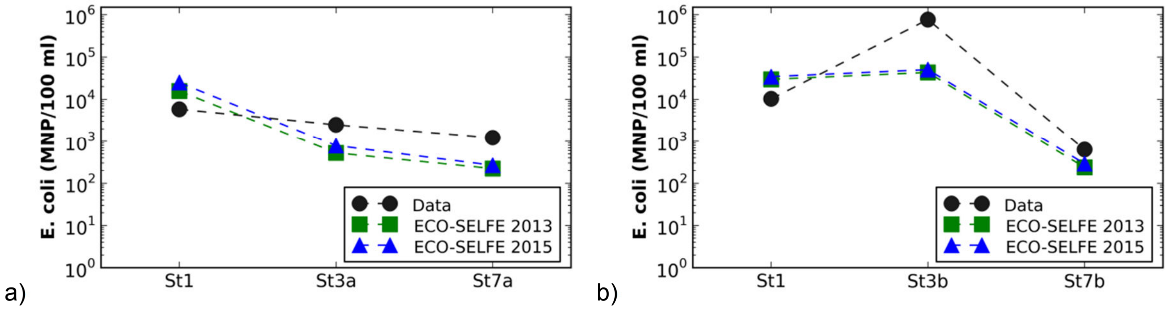


Figure 4.8 – Comparison between data and model spatial variation of average concentrations of *E. coli* on July 15, 2011 (a) and September 6, 2011 (b) for the previous model application (ECO-SELFE 2013, [23]) and the updated model application (ECO-SELFE 2015).

The Tagus estuary model is operational within the Water Information and Forecast Framework (WIFF, [25]), providing daily 24-hours forecasts of water levels, velocities, salinity, temperature, fecal coliforms and *E. coli* (Chapter 5).

4.3 Biogeochemical Model Preliminary Implementation in the Tagus Estuary and Computational Times Evaluation

The computational efficiency is one of the major limitations in the usage of high-resolution water quality models in nowcast-forecast systems. The recent advances in high-performance computing, such as the ones achieved with the LNEC's cluster MEDUSA [26], provide the means for a timely and adequate real-time response to pollution events.

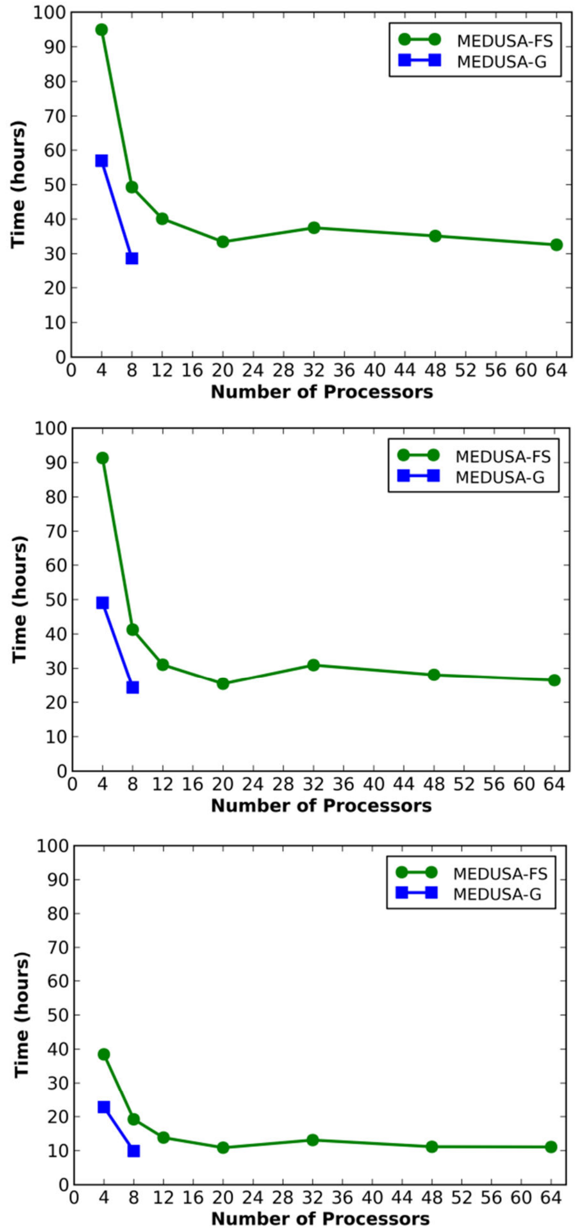
MEDUSA is one of the clusters integrated in the Portuguese Science Foundation Digital Research Infrastructures Roadmap and the Portuguese Grid network. The computational resources of this cluster include:

- MEDUSA – FUJITSU SIEMENS – 67 servers Fujitsu Siemens PRIMERGYRX220, Ethernet (1 Gbit/s), 268 cores, 1 GB RAM per core (4 GB RAM per server);
- MEDUSA – TYAN – 1 server Tyan FT48B8812, Ethernet (1 Gbit/s), 32 cores, 8 GB RAM per core (256 GB RAM per server);
- MEDUSA – GATEWAY – 1 server Gateway GR380 F2, Ethernet (1 Gbit/s), 12 cores, 4 GB RAM per core (32 GB RAM per server).

In order to optimize the use of computational resources within the MEDUSA cluster, a computational analysis was performed for a preliminary implementation of the biogeochemical models described in section 4.1.2 in the Tagus estuary, using the improved setup described in the previous section. Three levels of complexity were considered for the biogeochemical models: 25 ecological tracers, 15 ecological tracers and 3 ecological tracers.

Initial and boundary conditions were set for the summer period. For the ecological tracers where field data were available, the initial and boundary conditions were set based on that data. These tracers include: chlorophyll a, dissolved organic carbon, ammonium, nitrate, phosphate, silicate and dissolved oxygen [24] [27] [28] [29]. The phytoplankton values were determined based on the ratio to chlorophyll *a* proposed by [30]: 60 mg C/mg chlorophyll a. For the variables where data are not available, the initial and boundary conditions were estimated based on analytical initial conditions of the EcoSim 2.0 model or other modeling applications in the Tagus estuary (e.g. [31]), using a similar approach to the one described in [9]. The input parameters for the 25 ecological tracers and 15 ecological tracers models were set as defined in [9] [11], while for the 3 ecological tracers model the input parameters were set as defined by Lebot (CMOP internal report). A period of 4 days was simulated.

Simulations were performed using both the MEDUSA – FUJITSU SIEMENS and the MEDUSA – GATEWAY resources. Results show an optimal performance around the 20 processors for the FUJITSU SIEMENS servers, for all the biogeochemical models evaluated (Figure 4.9), with computational times of about 8 hours per day simulated for the 25 tracers ecological model. These times are equivalent to the GATEWAY servers computational times for 8 processors. Results also suggest a linear trend between the number of tracers simulated and the computational times (Figure 4.10). Overall results show that the use of the biogeochemical model of the Tagus estuary in nowcast-forecast systems is possible. The preliminary implementation of the biogeochemical model in the Tagus estuary should be further calibrated and validated by comparison with historical data prior to its deployment in forecast mode (Figure 4.11).



a)

b)

c)

Figure 4.9 – Computational times of the ECO-SELFE model applied to the Tagus estuary, using the MEDUSA – FUJITSU SIEMENS (MEDUSA-FS) and the MEDUSA – GATEWAY (MEDUSA-G) resources and considering three levels of complexity for the biogeochemical model: 25 ecological tracers (a), 15 ecological tracers (b) and 3 ecological tracers (c)

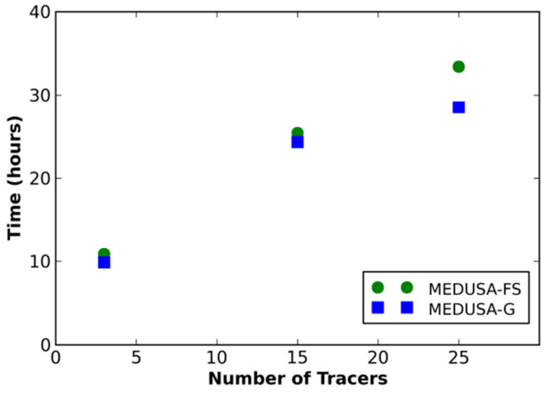


Figure 4.10 – Relationship between the number of ecological tracers and the computational times using 20 processors (servers FUJITSU SIEMENS) and 8 processors (server GATEWAY).

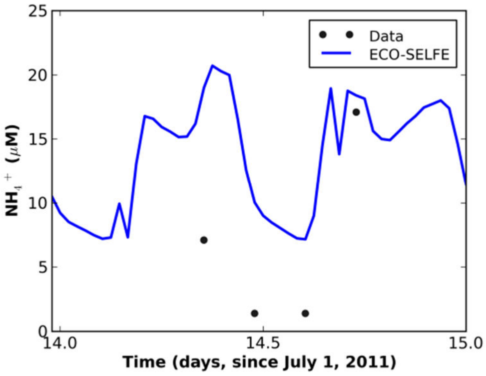


Figure 4.11 – Ammonium (NH4+) preliminary data-model comparisons at station 1 for July 15, 2011.

4.4 Requirements for the Operational Biogeochemical Model of the Tagus Estuary

The deployment of the biogeochemical model of the Tagus estuary in operational mode must attend to a set of requirements, namely the definition of the oceanic, riverine and atmospheric forcings, which were established.

For the circulation forcing, a similar approach to the one already in use for the hydrodynamics and fecal contamination operational model [1] [23] will be used to force the model:

- River boundary – extrapolations from real-time river flow data from SNIRH (snirh.pt) and water temperature climatology based on SNIRH’s database;
- Ocean boundary – forecasts of water levels, salinity and water temperature from the regional ocean model of MyOcean (www.myocean.eu.org/);
- Urban boundaries – forecasts from the urban drainage model [33].

In case of failure of these sources, redundancy schemes will be implemented in the system: river flow climatology and/or tidal elevations from harmonic synthesis are used in alternative to force the river and the oceanic boundary, respectively.

For the atmospheric forcings, atmospheric forecasts from WRF 9 km will be used for wind, air temperature, sea level pressure and specific humidity (available at http://www.windguru.cz), while for shortwave and longwave radiation GFS 25 km forecasts will be used (available at http://nomads.ncep.noaa.gov/model), based on the already implemented operational model [1] [23].

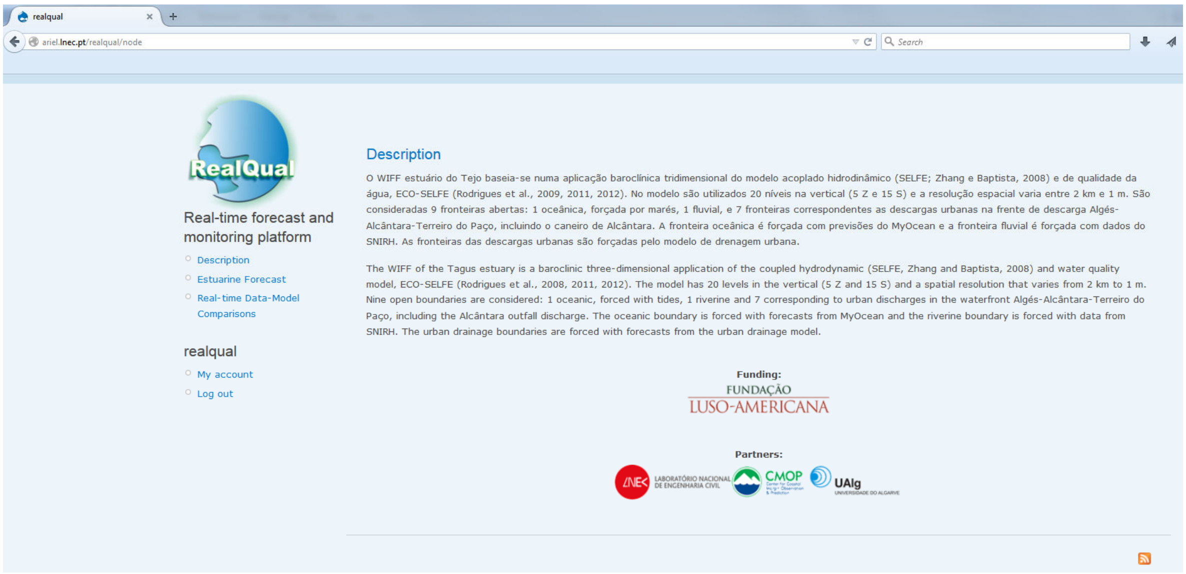
For the ecological tracers forcing, climatology will be used at the riverine boundary based on the analysis of available data, including the SNIRH’s database. At the oceanic boundary several sources may be considered, including both climatology and forecasts, namely:

- Atlantic-Iberian Biscay Irish- Ocean Biogeochemistry Non Assimilative Hindcast (2002-2011), which provides three-dimensional monthly fields for several biogeochemical variables, including chlorophyll a, nitrate, ammonium, dissolved oxygen, phosphate, silicate, and phytoplankton for the period between 2002-2011 (available at www.myocean.eu.org/);
- Global Ocean Biogeochemistry Analysis, which provides 3D global ocean biogeochemical weekly mean analysis for the past 2 years updated every week, including nitrate, chlorophyll a, phosphate, silicate, dissolved oxygen, and phytoplankton concentrations (available at www.myocean.eu.org/);
- Operational Modelling for the Portuguese Coast (PCOMS), which provides forecasts for zooplankton, chlorophyll a, nitrate, phosphate and dissolved oxygen (available at http://forecast.maretec.org/maps_pcoms.asp);

Regional model for the Iberian Margin, which provides forecasts of chlorophyll a (available at http://climetua.fis.ua.pt/fields/oceanoAtlantic/templ1).

5 | Operational Platform

The outcomes of RealQual were made available through a new WebGIS observatory platform, tailored for risk assessment and emergency preparation and response in coastal areas. A dedicated platform was developed for the project – ariel.lnec.pt/realqual (Figure 5.1), which is available by password request.



Description

O WIFF estuário do Tejo baseia-se numa aplicação baroclínica tridimensional do modelo acoplado hidrodinâmico (SELFE; Zhang e Baptista, 2008) e de qualidade da água, ECO-SELFE (Rodrigues et al., 2009, 2011, 2012). No modelo são utilizados 20 níveis na vertical (5 Z e 15 S) e a resolução espacial varia entre 2 km e 1 m. São consideradas 9 fronteiras abertas: 1 oceânica, forçada por marés, 1 fluvial, e 7 fronteiras correspondentes as descargas urbanas na frente de descarga Algés-Alcântara-Terreiro do Paço, incluindo o caneiro de Alcântara. A fronteira oceânica é forçada com previsões do MyOcean e a fronteira fluvial é forçada com dados do SNIRH. As fronteiras das descargas urbanas são forçadas pelo modelo de drenagem urbana.

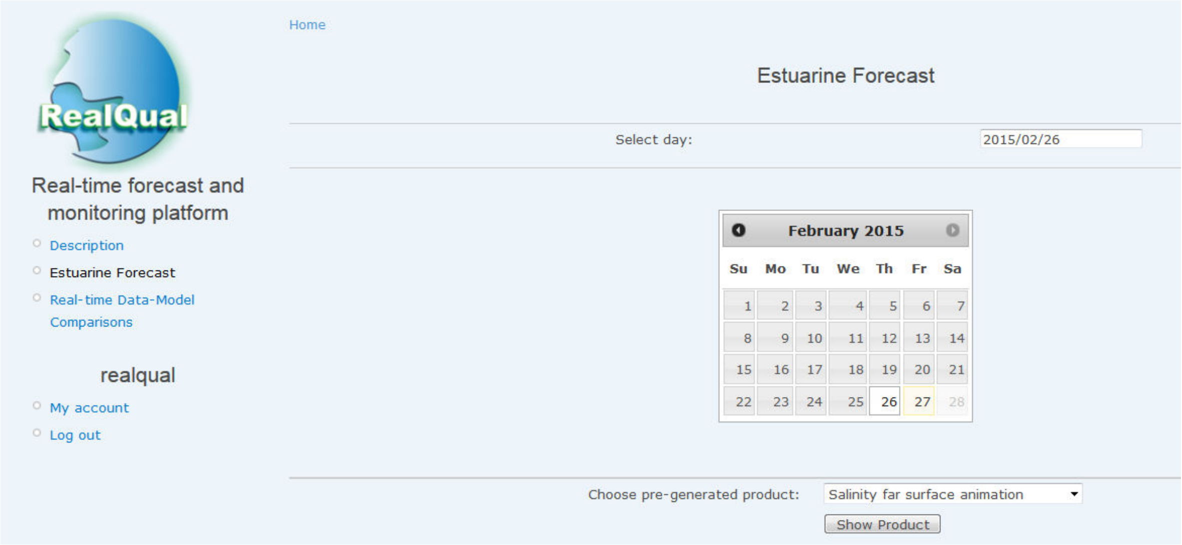
The WIFF of the Tagus estuary is a baroclinic three-dimensional application of the coupled hydrodynamic (SELFE, Zhang and Baptista, 2008) and water quality model, ECO-SELFE (Rodrigues et al., 2008, 2011, 2012). The model has 20 levels in the vertical (5 Z and 15 S) and a spatial resolution that varies from 2 km to 1 m. Nine open boundaries are considered: 1 oceanic, forced with tides, 1 riverine and 7 corresponding to urban discharges in the waterfront Algés-Alcântara-Terreiro do Paço, including the Alcântara outfall discharge. The oceanic boundary is forced with forecasts from MyOcean and the riverine boundary is forced with data from SNIRH. The urban drainage boundaries are forced with forecasts from the urban drainage model.

Figure 5.1 – General overview of the RealQual operational platform.

At the back-end, this tool combines a sophisticated forecast modeling system for multi-scale analysis of water bodies, including waves, hydrodynamics and water quality prediction, with real-time monitoring networks for forcing and continuous validation purposes. Tailor-made visualization and analysis products, conceptualized for multiple uses through a service-oriented framework, provide an easy and interactive access to both data and predictions. The system was customized for hydrodynamics and biogeochemical assessment, and applied to the Tagus estuary.

The enhanced interface is based on a previous deployment using Drupal, a PHP-based Content Management System (CMS) used to access model metadata, status and products. To allow for geospatial placement of monitoring and forecast products, as well as model output query capabilities, map server support (Geoserver) providing Web Map Services (WMS) have been added to the RDFS-PT. A WebGIS was developed in Flex, using the OpenScales library to handle geospatial information. This WebGIS is being built in a modular and generic way, to allow future inclusions of new models, sensor networks and services required by coastal authorities and emergency agents.

The platform is conceived in a user's service-oriented architecture, providing an on-line access to both real-time model predictions (Figure 5.2) and data-derived products, at different levels of detail and complexity. In both cases data are stored in the filesystem via NETCDF standard format, allowing future use in other models. A set of webservices is provided at the RealQual website, through an alpha-numeric webservice to scope time series from the data outputs in user-specific points of the model grid (Figure 5.3). The interface also grants access to the historic of simulations from past days.

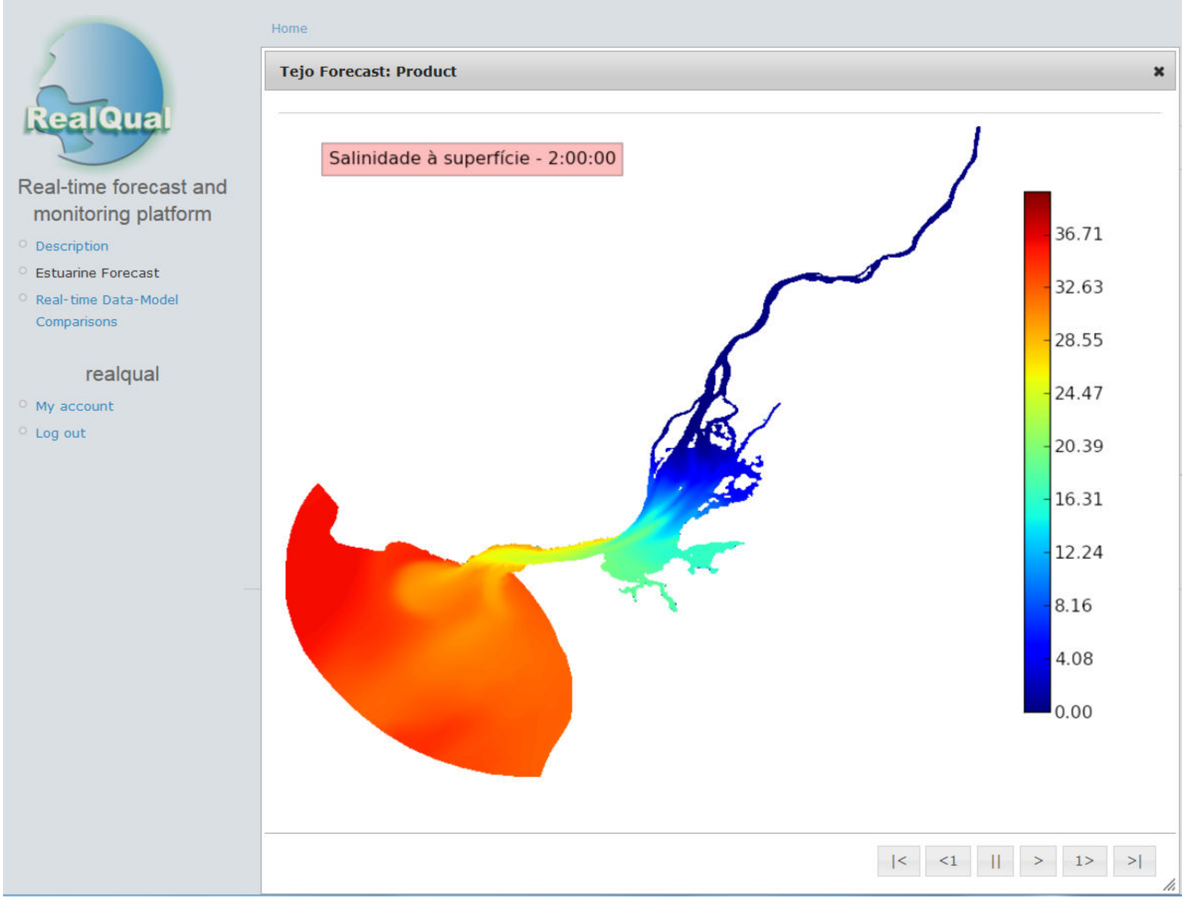


Estuarine Forecast

Select day: 2015/02/26

Choose pre-generated product: Salinity far surface animation

a)



Tejo Forecast: Product

Salinidade à superfície - 2:00:00

b)

Figure 5.2 – Overview of the RealQual forecast products. Top panel: forecast day and variable selection (a); Bottom panel: sample salinity field for the selected day (b).

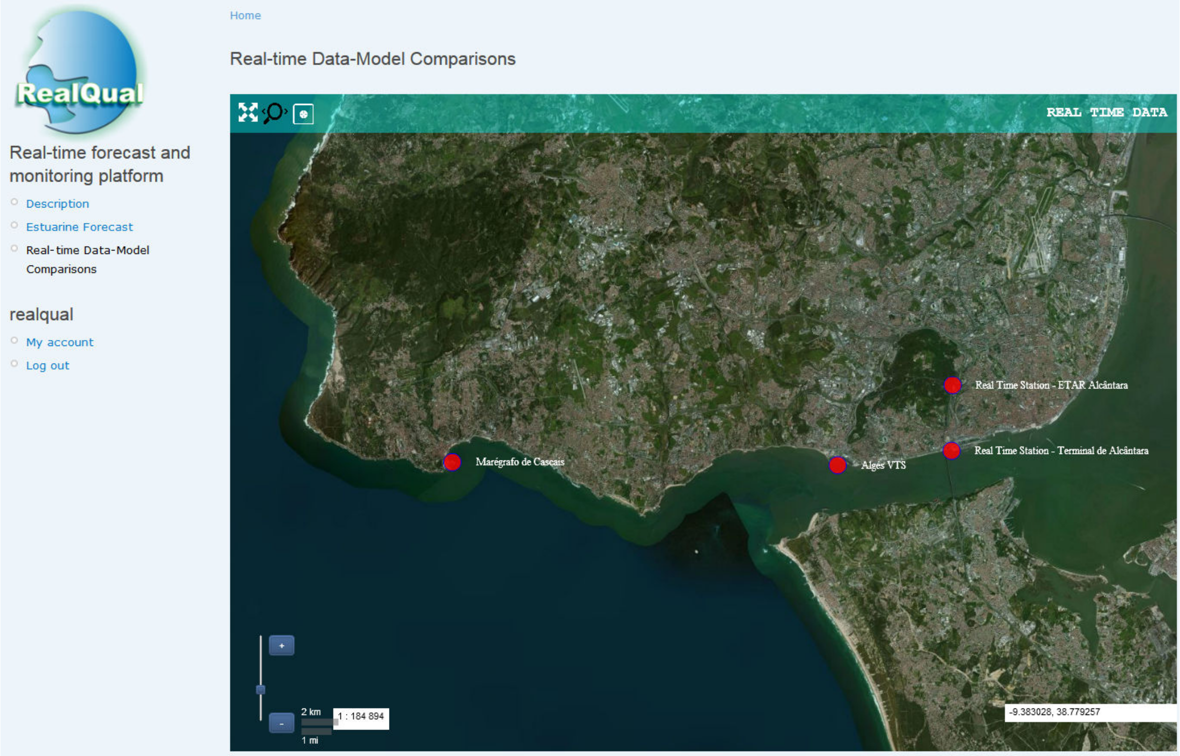
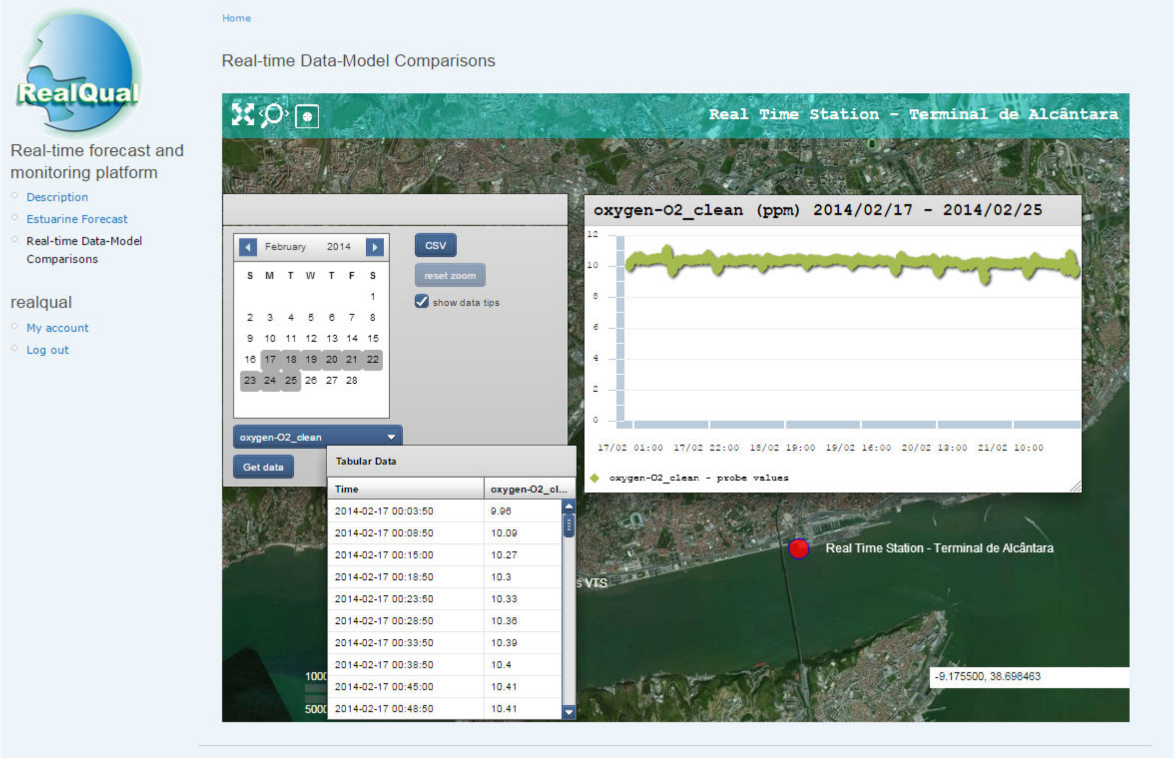


Figure 5.3 – Overview of the RealQual data products.



February 2014: 17–25 selected

oxygen-O2_clean

☑ show data tips

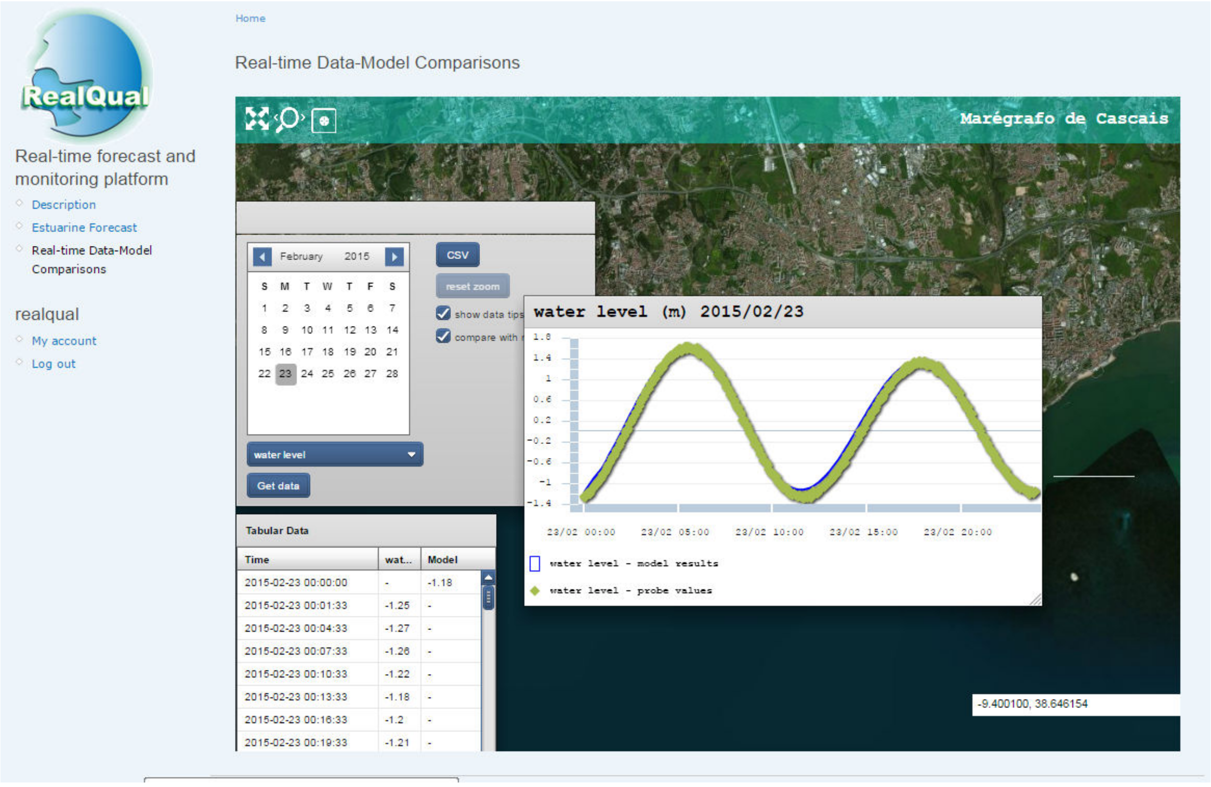
Tabular Data

Time	oxygen-O2_cl...
2014-02-17 00:03:50	9.96
2014-02-17 00:08:50	10.09
2014-02-17 00:15:00	10.27
2014-02-17 00:18:50	10.3
2014-02-17 00:23:50	10.33
2014-02-17 00:28:50	10.36
2014-02-17 00:33:50	10.39
2014-02-17 00:38:50	10.4
2014-02-17 00:45:00	10.41
2014-02-17 00:48:50	10.41

Figure 5.4 – Sample time series from the Terminal de Alcântara station.

LNEC’s monitoring platform is composed of several sensors, managed online by Con::cube S::CAN controllers (section 3.1) that also maintain the communication with the real-time platform. These controllers measure data continuously, with 5 minutes intervals and transmit it to LNEC’s servers every hour. This transmission is performed using GSM/GPRS communications directly to a central server where they are parsed and stored in PostgreSQL databases. This process allows the data to be available for easy visualization in the WebGIS platform (Figure 5.4).

In RealQual, the platform includes quasi-real time access to both LNEC’s and public data streams (Figure 5.3), providing also automated data-model comparisons Figure 5.5. LNEC's continuous data stream is gathered from the project monitoring network and, as referred before, supports the forecasting and early-warning platform. Public data streams include water levels measured by tide gauges located in Cascais and Algés



Tabular Data

Time	wat...	Model
2015-02-23 00:00:00	-	-1.18
2015-02-23 00:01:33	-1.25	-
2015-02-23 00:04:33	-1.27	-
2015-02-23 00:07:33	-1.26	-
2015-02-23 00:10:33	-1.22	-
2015-02-23 00:13:33	-1.18	-
2015-02-23 00:16:33	-1.2	-
2015-02-23 00:19:33	-1.21	-

Figure 5.5 – Sample of data-model comparisons for water levels at Cascais.

6 | Short-term Research Internships

LNEC's team members Marta Rodrigues and Gonçalo Jesus visited at OHSU-CMOP between June 23 and June 26, 2014, in the scope of two short-term research internships. During this period, the project consultant Prof. Alexandra Cravo was also present at OHSU-CMOP. The agenda of these short-term internships is presented in Table 1.

Table 6.1. Agenda of the short-term internships at OHSU-CMOP.

Day 1 *June 23, 2014*	- Logistics - Introduction to CMOP's team - Meeting with Prof. António Melo Baptista *(agenda setup)* - Introduction to SATURN observation network
Day 2 *June 24, 2014*	- Modelling team meeting - *LNEC's team presentation* (*Developing and implementing biogeochemical models in estuaries and coastal areas,* MR) - Halve-baked talk – *Rolling out "Data Near Here" tool on CMOP website*, Veronika Megler, Portland State University - Meeting with António Melo Baptista, Yvette Spitz, Alexandra Cravo, Clara Lebot; first steps to implement CMOP biogeochemical model in the Aveiro lagoon - Meeting with Paul Turner (GJ)
Day 3 *June 25, 2014*	- Visit to Astoria – monitoring network
Day 4 *June 26, 2014*	- Meeting with Charles Seaton (GJ) - Meeting with Tuomas Karna (MR) - Meeting with Alexandra Cravo (MR) – *Box models* - Implementation of CMOP biogeochemical model in the Aveiro lagoon - continued
Day 5 *June 27, 2014*	- Meeting with Jesse Lopez (MR) - Meeting with Charles Seaton (GJ) - CMOP team meeting - Coordinators team meeting - Cyberinfrastructure team meeting – *LNEC's team presentations* (*Towards real-time monitoring and prediction of water quality in estuaries and coastal zones*, MR/GJ; *Towards reliable measurements in remote aquatic sensor networks*, GJ)

MR – Marta Rodrigues; GJ – Gonçalo Jesus

These internships promoted the knowledge transfer between the partners, in particular on the themes related to numerical modelling and in-situ monitoring of the water quality in estuaries and coastal zones, and to the implementation and use of these tools in real-time, automated, quality-controlled nowcast-forecast and online monitoring systems.

Regular OHSU-CMOP meetings were held during this period, including the modelling team meeting and the cyberinfrastructure team meeting, during which LNEC's team members presented the ongoing research activities at LNEC in the areas mentioned above:

- "Developing and implementing biogeochemical models in estuaries and coastal areas" (Marta Rodrigues);
- "Towards real-time monitoring and prediction of water quality in estuaries and coastal zones" (Marta Rodrigues, Gonçalo Jesus);
- "Towards reliable measurements in remote aquatic sensor networks" (Gonçalo Jesus).

Several specific meetings were also held between the team members, which allowed sharing detailed knowledge in the areas of interest. In particular, a preliminary implementation of the biogeochemical model developed by OHSU-CMOP was performed for the application developed by LNEC for the Aveiro lagoon, aiming to explore the behavior of the model in wetting and drying areas. The developments performed by OHSU-CMOP team within the hydrodynamic model SELFE were also shared between the team.

A visit to the MERTS (Marine and Environmental Research and Training Station) Campus of the OHSU-CMOP, located in the Clatsop Community College in Astoria (Oregon, USA), , was held on June 25, 2014. The MERTS supports the monitoring network operating in the Columbia river (Figure 6.1, Figure 6.2). The visit was led by Dr. Michael Wilkin (OHSU-CMOP) and had also the participation of Prof. Alexandra Cravo. Two online monitoring stations of the Columbia river, SATURN 03 and SATURN 04, were also visited (Figure 6.2).

Finally, several interactions were performed aiming the collaboration between the partners in future research initiatives (Chapter 8).

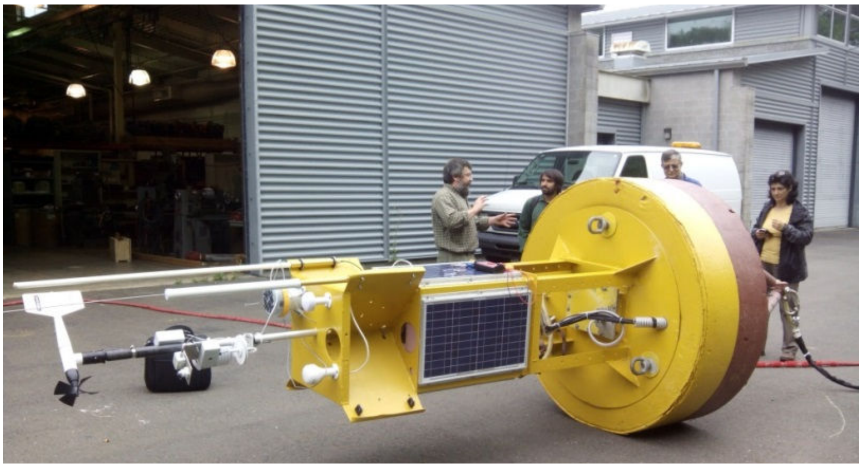


Figure 6.1 – Visit to the MERTS Campus, OHSU in Astoria during the short-term research internships, June 25, 2014.

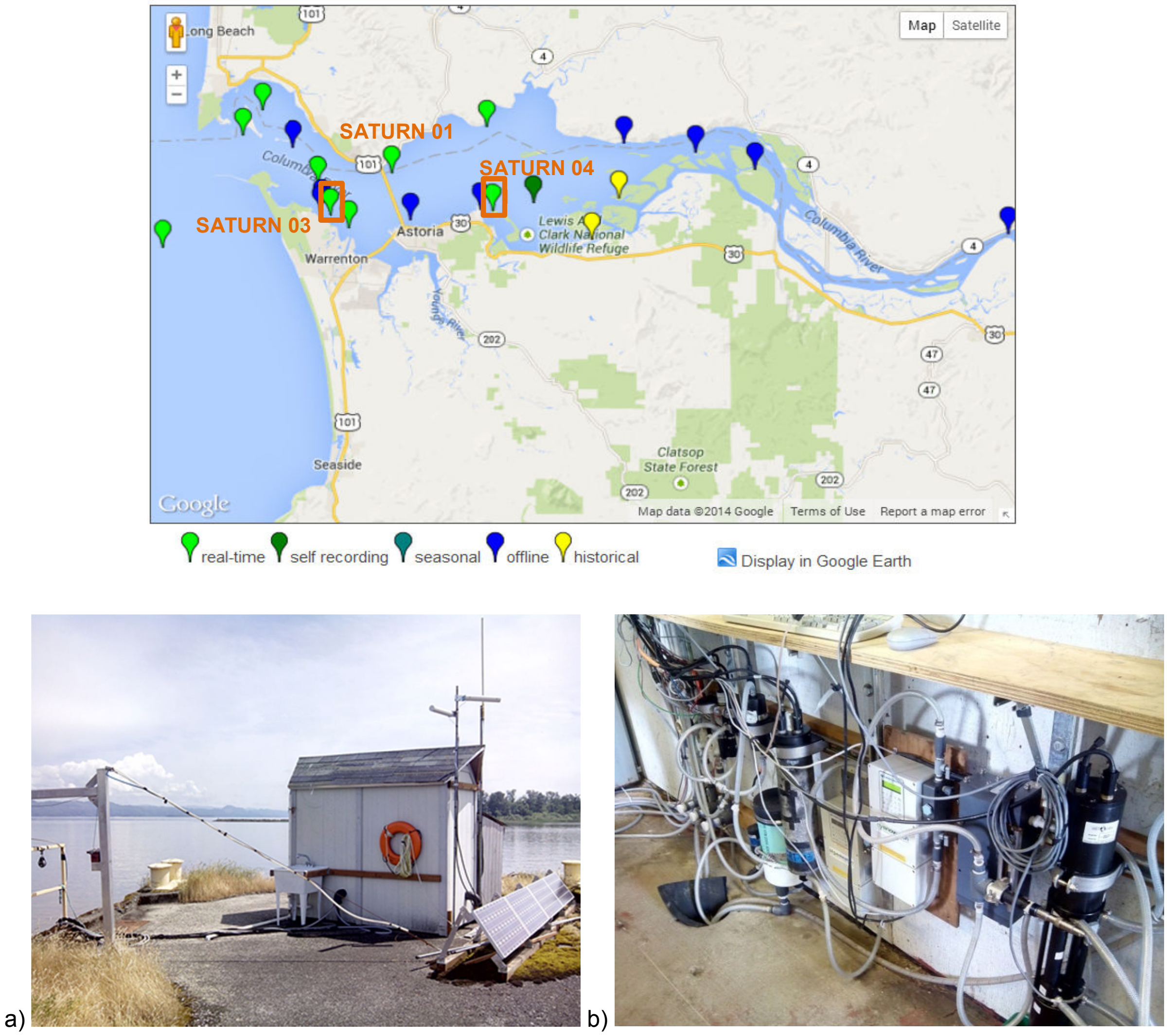


Figure 6.2 – Online monitoring stations at the Columbia river visited during the short-term research internships: SATURN 04 (a) and SATURN 03 (b), June 25, 2014.

7 | Dissemination

The project outcomes were disseminated in several scientific meetings, through oral presentations and papers:

- ECSA 54 Conference – Coastal systems under change: tuning assessment and management tools (Sesimbra, Portugal, May 12-16, 2014)

  Rodrigues M., Oliveira A., Fortunato A.B., Queiroga H., David L.M., Brotas V., Costa J., Rogeiro J., Jesus G., Gomes J., Azevedo A. (2014). Management of estuarine and coastal ecosystems: observatories as effective tools to predict and anticipate changes. Book of Abstracts of the ECSA 54 Conference – Coastal systems under change: tuning assessment and management tools (Sesimbra, Portugal), p. 82;

- IMUM 2014 – 13th International workshop on Multiscale (Un)-structured mesh numerical Modeling for coastal shelf and global ocean dynamics (Lisbon, Portugal, August 25-27, 2014)

  Rodrigues M., Oliveira A., Fortunato A.B., Costa J., Rogeiro J., Costa R., David L.M., Gomes J.L., Jesus G. (2014). A real-time water quality model of the Tagus estuary. Proceedings of the 13th International Workshop on Multiscale (Un)-structured mesh numerical ocean modelling – IMUM 2014 (Lisbon, Portugal), 2 pp;

- 7th EuroGOOS Conference – Operational Oceanography for Sustainable Blue Growth (Lisbon, Portugal, October 28-30, 2014)

  Rodrigues M., Oliveira A., David L.M., Fortunato A.B., Costa J., Rogeiro J., Gomes J.L., Jesus G., Mota T., Póvoa P., David C., Ferreira F., Matos R., Matos J.S., Santos J., Matos R.S. (in press). Real-time observatory of the water quality in the Tagus estuary. Book of Proceedings of the 7th EuroGOOS Conference (Lisbon, Portugal), 5 pp.

A particular mention should be made to the IMUM 2014 conference which was organized in LNEC by Dr. André Fortunato, Dr. Marta Rodrigues and Dr. Alberto Azevedo (LNEC) – http://imum2014.lnec.pt/. This conference focused on the several fields of multiscale unstructured grids modeling. Prof. António Melo Baptista presented a keynote talk during the conference entitled “Lessons learned from pushing a circulation model to the brink”. The participation of Prof. António Melo Baptista in this conference as a keynote speaker was supported by FLAD. Dr. Tuomas Karna (OHSU-CMOP) also participated in the conference. The SELFE Developer’s Meeting 2015 was also organized as a side event to the IMUM 2014 conference. This meeting was led by Prof. António Melo Baptista and Prof. Joseph Zhang (Virginia Institute of Marine Sciences, USA), and allowed the discussion of the current and future developments related to the community model SELFE.

8 | Future Research: Common Goals

The common ground on the long-term goals of the partners and the extension of the partnership to other institutions was sought along the project. Several proposals have already been submitted or are under preparation aiming at supporting the long-term of the collaboration of the partners in future research projects and the enhanced and continuous improvement of the results achieved towards the state-of-the-art in real-time monitoring and prediction of the water quality in estuaries and coastal areas.

Among the submitted proposals, the "Our Virtual Global Estuary" proposal is one of the major initiatives envisioning the future collaboration among LNEC, OHSU-CMOP and UALG-CIMA. "Our Virtual Global Estuary" is led by Prof. António Melo Baptista and was submitted to the Partnerships for International Research and Education (PIRE) – NSF Program (NSF 14-587). This proposal involves 14 partners from 6 countries (USA, Portugal, China, Brazil, India and Spain). The project will anchor in 6 estuaries (Tier 1) and others will be will be engaged over the lifetime of the project. Among the Tier 1 estuaries are the Tagus estuary and the Ria Formosa. The pre-proposal "Our virtual Global Estuary" was recently approved and the preparation of the proposal is underway.

Several research proposals were submitted to the 2014 Call for SR&TD Project Grants promoted by Fundação para a Ciência e Tecnologia (FCT):

- UBEST – Understanding the biogeochemical buffering capacity of estuaries relative to climate change and anthropogenic inputs, coordinated by LNEC (PI: Marta Rodrigues). UALG-CIMA is a partner in the project and Prof. António Melo Baptista is the project consultant;
- iCOAST – Integration of artificial intelligence methods and process-based models for the enhanced forecast of coastal hydrodynamics, coordinated by LNEC (PI: André B. Fortunato). University of Lisbon/Faculty of Sciences (FCUL) is a partner in the project and Prof. António Melo Baptista is the project consultant;
- DOWSE – Dependable monitoring with wireless sensor networks in water environments, coordinated by FCUL (PI: António Casimiro). LNEC is one of the partners of the project and Prof. António Melo Baptista is one of the project consultants;
- ESTOPINHAS – Improved understanding of estuaries role on coastal margins: Observation and Prediction of environmental changes – case study South Portugal, coordinated by UALG-CIMA (PI: Alexandra Cravo). LNEC is a partner in the project.

Finally, a proposal is envisioned to be submitted to PRACE (Partnership for Advanced Computing in Europe) Infrastructure, coordinated by LNEC. Prof. António Melo Baptista and Prof. Joseph Zhang will be project advisors.

9 | Final Remarks

RealQual, a collaboratory project between LNEC, OHSU-CMOP and UALG-CIMA, aimed at developing the foundations of a quality-controlled network for real-time, high-resolution monitoring and prediction of the water quality in estuaries and coastal areas. Overall the main objectives of the project were achieved.

Regarding the real-time monitoring component, an online monitoring station for water quality was maintained operational in the Tagus estuary. This deployment includes a set of sensors for salinity, water temperature, dissolved oxygen, pH, ammonium, nitrates and a spectrophotometer. The data are transmitted using GSM/GPRS and stored in databases, being easily accessed through the operational platform and allowing the timely identification of faults and their fast correction. Several procedures were already tested for data quality control using the data from the SATURN OHSU-CMOP network and will be extrapolated to the monitoring network of the Tagus estuary.

The numerical modelling system for water quality ECO-SELFE was extended to improve its flexibility. In particular, options to use models with different levels of complexity to simulate the biogeochemical processes were implemented. A preliminary application of the coupled hydrodynamics and biogeochemical model was performed in the Tagus estuary. This application was based on the improvements made to the horizontal grid and bathymetry used in the Tagus estuary hydrodynamics and fecal contamination application. Tests to the computational times showed that the use of the biogeochemical model in real-time is possible even using a complex model with 25 ecological tracers and a set of requirements were established towards this deployment within the WIFF.

A dedicated operational Web-based platform was developed for the project, providing access to the real-time data and forecasts of the hydrodynamics and fecal contamination in the Tagus estuary.

The future scientific research collaboration between the partners is envisioned and several proposals were already submitted aiming to guarantee the prosecution of the cooperation.

Lisboa, LNEC, março de 2015

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