SMARTLAGOON

DELIVERABLE 3.2

Complete GOTM-WET model setup for Mar Menor

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101017861.

Innovative modelling approaches for predicting Socio-environMentAl evolution in highly anthRopized coasTal LAGOONs

Deliverable 3.2

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Abstract

This report presents the Deliverable 3.2 of Work Package 3 of the SMARTLAGOON project. Work Package 3 aims to develop innovative modelling strategies that can be applied to the Mar Menor lagoon and catchment, where Deliverable 3.2 covers the setup of an aquatic ecosystem model of the lagoon. This deliverable describes the model that was used (GOTM-WET), the data that was used to run the model, the choices that were made during the model configuration, the performance of the model, and how it couples to the other data sources and models within SMARTLAGOON. We also describe the calibration method that will be used to develop the final operational model and results from initial model calibrations. When developing the model setups, Lake Erken was first used as a pilot study site, and in this report both the Lake Erken and Mar Menor setups are described.

The one-dimensional GOTM model simulates lake and lagoon physics and it is coupled at runtime with the aquatic ecosystem model WET. We utilised the new hypsographic version of GOTM, meaning that the individual depth layers in Mar Menor are represented by their actual volumes, and also that the benthic depth contours and are represented individually, resulting in a pseudo two-dimensional approach. As inputs, the models require weather conditions and catchment boundary conditions (discharge and nutrient concentrations). In order to run short-term forecast or long-term future climate projections, weather data are retrieved from direct measurements, weather forecasts or global climate models, and catchment input data are acquired through the SWAT+ catchment model, which was described in Deliverable 3.1. The ultimate goal of the coupled SWAT+&GOTM-WET setup is incorporation into a real-time “digital twin” (Work Package 5).

In Lake Erken, the calibrated GOTM-WET model simulated lake dynamics well, including spring peaks in chlorophyll-a (indicative of phytoplankton blooms) and seasonal anoxia in the deeper water layers. Future climate simulations were used to predict Lake Erken water quality conditions until the end of the century. A manuscript is in preparation that will publish these results in a scientific journal. In the Mar Menor, a similar setup has been constructed, with the important addition of a representation of the exchange between the Mediterranean Sea and the lagoon. An initial, uncalibrated, model simulated observed patterns in water temperature, salinity, and chlorophyll, whereas patterns in nutrients and oxygen need further calibration. Short-term stratification events were also simulated, that are of crucial importance for the water quality in the Mar Menor. Therefore, the results confirm that the GOTM-WET model is capable of realistically simulating the water quality conditions in the Mar Menor, contributing significantly to increased understanding and forecasting capacity of the Mar Menor ecosystem.

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Table of Contents

List of tables

List of Figures

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101017861.

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1. Introduction

1.1. Motivation

Lakes, lagoons, and coastal areas are collection points of water from their surrounding catchments, and receive a variety of biogeochemical compounds from these areas. For this reason, these water bodies are seen as “sentinels” of climate change, where disparate signals of climatic change come together and become most apparent (Adrian et al., 2009). However, coupled modelling studies of both catchments and lakes are surprisingly few, despite the catchment providing essential boundary conditions in terms of water (Senent-Aparicio et al., 2021), heat (Olsson et al., 2022), and nutrient (Jeppesen et al., 2005; Radbourne et al., 2019) balances. This is especially apparent in the Mar Menor, where short-term and seasonal variation in evaporation and catchment runoff influence the water balance (Senent-Aparicio et al., 2021) and where the nutrient loads from the catchment are the primary cause of the water quality issues experienced in recent years (Fernandez-Alias et al., 2022; Lopez-Ballesteros et al., 2022). Therefore, in this deliverable, we describe the coupled hydrodynamic-ecosystem lake/lagoon model in conjunction with the model of the surrounding catchment (itself outlined in more detail in Deliverable 3.1).

A standing water body (ocean, lake, lagoon) has its own complex dynamics in terms of density stratification and mixing, also involving exchanges with the atmosphere, catchment, and sediment, which in turn affect the nutrient balances, biogeochemistry and ecology. All of these processes can be simulated with process-based models. In Work Package 3 of SMARTLAGOON, we want to simulate the water quality dynamics of the Mar Menor to be able to forecast these dynamics into the future, both for short-term forecasting and for scenario testing purposes. The GOTM-WET hydrodynamic-ecosystem model was chosen for the Mar Menor, fed with inflow discharge and nutrient loading data provided by the SWAT+ catchment model (see Deliverable 3.1). This is a one-dimensional (1D) model, which can capture important vertical heterogeneity due to density stratification. Although the Mar Menor is shallow, short-term stratification events likely occur and may play an important role in anoxia and fish-kill events. A three-dimensional (3D) model could give more information about horizontal gradients within the lagoon. However, the water quality measurements seem to be rather uniform in the horizontal dimension (Section 3.2.1, but also see Fernandez-Alias et al. 2022). These models are more complex, costly and time consuming to set up and increased dimensionality greatly increases the computational times of 3D models (e.g. Ishikawa et al., 2022), limiting their use for long-term and iterative forecasting studies. To avoid these limitations, we choose to use the 1D GOTM-WET model that is still able to account for important vertical variations in water quality, and has a hypsographic representation that also accounts for the relative importance of the differing vertical layer volumes as well as a pseudo 2D representation of bottom sediments. Use of 1D GOTM WET should provide an overall indication of changes in lagoon water quality, even though horizontal gradients will not be simulated.

Similar to the 3.1 Deliverable, we present results from both the Mar Menor and Lake Erken (see 1.3). The extensively monitored Lake Erken is used as a pilot training site in SMARTLAGOON, due to limited data availability and significant uncertainty in nutrient loading from the Mar Menor catchment. The Lake Erken test case showcased the potential of the approach and allowed us to test several methodologies before applying the optimal methods to the Mar Menor.

1.2. Goals

The aim of the GOTM-WET model in SMARTLAGOON is to simulate the dynamics of the following variables: water temperature, oxygen, salinity, nutrients (nitrogen, phosphorus, silicon), and chlorophyll. Especially chlorophyll and oxygen are of direct relevance to local authorities and water quality regulations (high algal biomass may lead to swimming bans and anoxia can cause fish kills), but all these variables are intrinsically linked to each other. For instance, vertical heterogeneity in water temperature and salinity may cause the water to stratify, which leads to a lack of oxygen near the sediment. The anoxia and stratification may promote a build-up of nutrients near the sediment, which, when finally mixed into the water column, can cause a phytoplankton bloom. The GOTM-WET model is capable of simulating these processes, and this and similar models have been applied successfully to a variety of water bodies (Nielsen et al., 2014; Luo et al., 2018; Chen et al., 2020; Schnedler-Meyer et al., 2022).

The ultimate goal of the GOTM-WET application within SMARTLAGOON is its inclusion in the digital twin (Work Package 5). Therefore, we train and test the model on observed data, with the goal in mind that the model can be used for short-term forecasting and scenario assessment studies. For the Mar Menor, we have therefore aligned the data used for training the model with the data source that will be used for generating the weather forecasts. We aim to create a model that is as good as possible with the current availability of data, but ensure that future data aggregation (e.g. data generated by the SMARTLAGOON buoy, Work Package 2) can improve the model further.

1.3. Study areas

1.3.1. Lake Erken

Lake Erken is a meso-eutrophic lake on the east coast of Sweden (Figure 1). It has an average depth of 9 m, maximum depth of 21 m, a surface area of 24 km^2, and a residence time of around 7 years. It is classified as a dimictic lake, meaning that it stratifies in summer and experiences ice cover in winter. Considering the size of the lake, the catchment is rather small (135 km^2), mostly covered by coniferous forest with some agricultural areas (Malmaeus and Håkanson, 2004). Roughly 50% of the discharge enters the lake at Kristineholm, at the western side of the lake (Figure 1).

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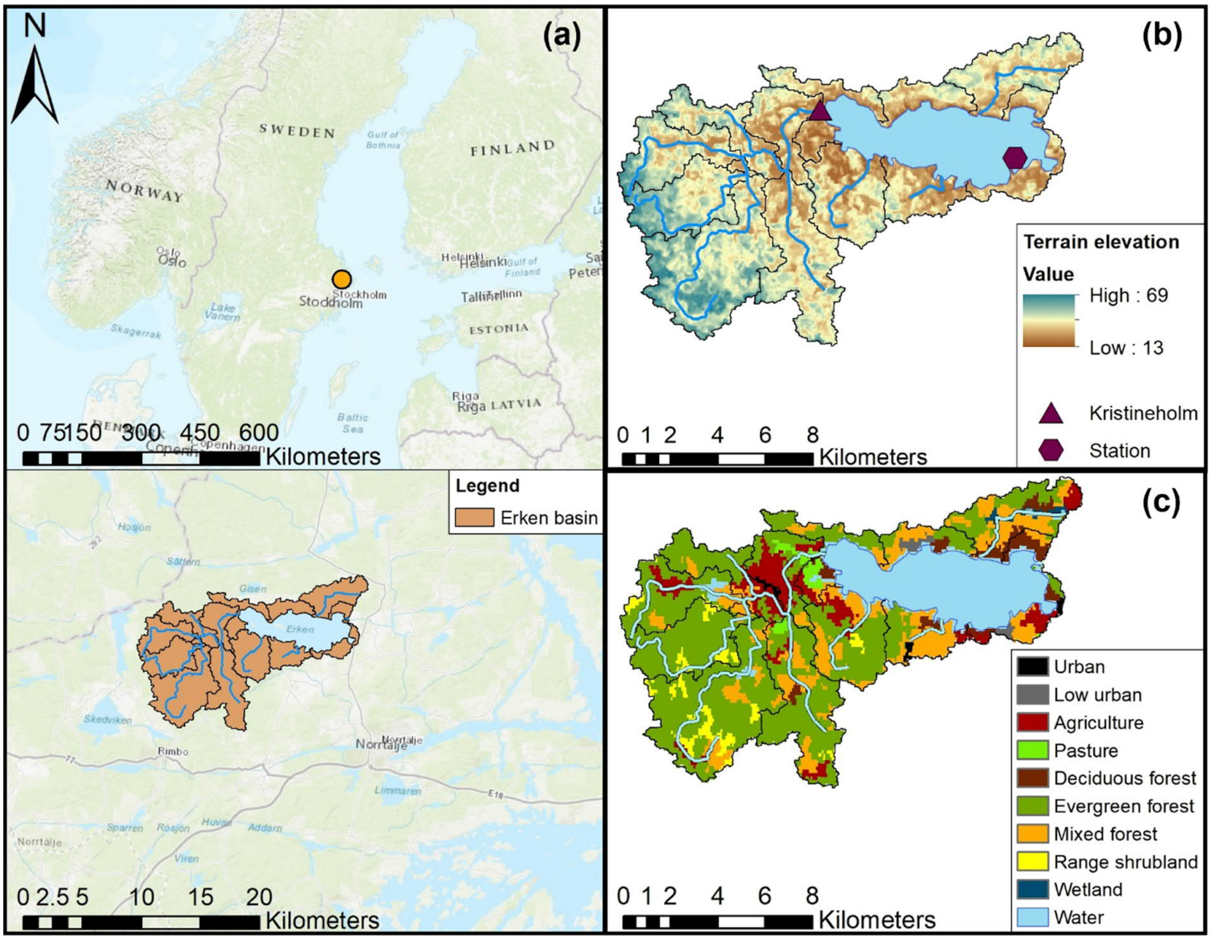

Figure 1. Map of Lake Erken and its catchment: (a) Lake Erken and its basin in the Scandinavian Peninsula; (b) digital elevation map of the Lake Erken basin and location of the Kristineholm inflow (triangle) and the weather station (hexagon) where temperature and the nutrients were measured; (c) land uses in the Lake Erken basin. Figure is from Jiménez-Navarro et al. (in preparation)

Lake Erken is exceptionally well monitored, with data records starting in the 1930s, although frequent and consistent monitoring efforts have been carried out since the early 1990s. In our study, data from 2000 onwards are used, including weather station measurements, temperature and oxygen profile measurements from automated sensors, and nutrient and chlorophyll data gained from weekly to biweekly samples. At the inflow, discharge, water temperature, and nutrient measurements were collected.

1.3.2. Mar Menor

The Mar Menor is a hypersaline lagoon located in southeastern Spain, bordering the Mediterranean Sea (Figure 2). It has a surface area of 135 km^2, a mean depth of 4.4 m and a maximum depth of 7 m (Umgiesser et al., 2014). The lagoon is separated from the sea by a narrow barrier island and water exchange between the lagoon and the sea occurs through three openings in this barrier island. Being a Ramsar international site and an EU special protected area, the lagoon used to have a good ecological condition, but with the intensification of agriculture in the catchment, water quality has deteriorated, with severe signs of eutrophication especially from around 2016 onwards

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(Marín et al., 2015; Pérez-Ruzafa et al., 2019). Recurrent fish kills and algal blooms formed a large part of the motivation for the SMARTLAGOON project.

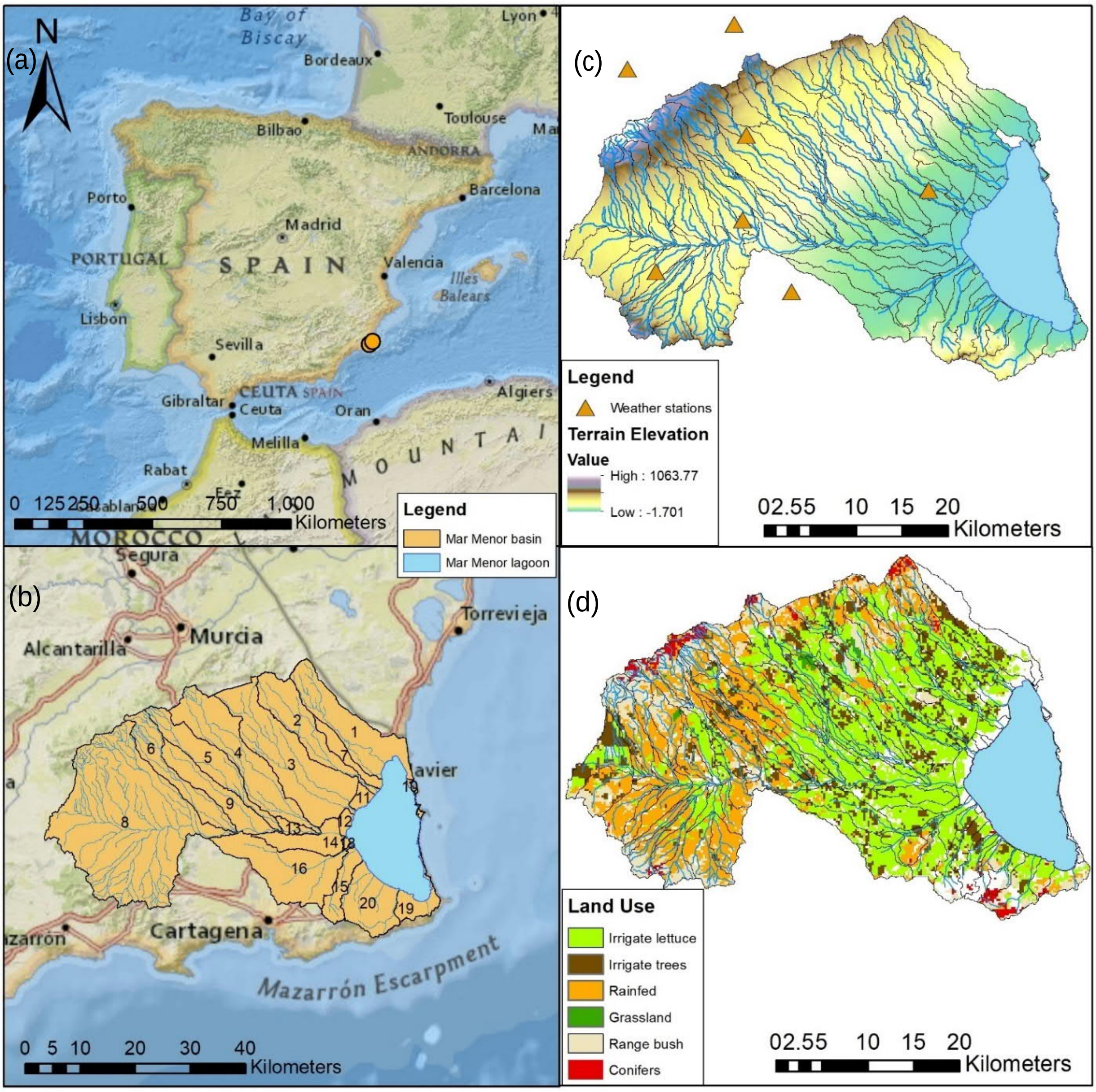

Figure 2. Map of the study area in Spain: (a) location of the Mar Menor and its basin in the Iberian Peninsula; (b) watershed of the Mar Menor divided in sub-basins by SWAT; (c) digital elevation map of the Mar Menor basin and location of the weather stations; (d) land uses in the Campo de Cartagena (figure from the 3.1 SMARTLAGOON Deliverable report).

The catchment of the Mar Menor, the Campo de Cartagena, has a long history of intensive agriculture, leading to a steady and severe increase in nutrient loading to the lagoon (e.g. Jiménez-Martínez et al., 2016). Due to the Mediterranean climate, average rainfall is low (around 300 mm/yr), but it tends to come in short and intense events (see Deliverable 3.1), during which large amounts of nutrients will be transferred to the lagoon. The exchange with the Mediterranean Sea forms another important part of the water, salt, and nutrient balance; due to the low rainfall and high evaporation rates, the net water movement is from the sea to the lagoon most of the year, apart from the winter months and during extreme rainfall events (Senent-Aparicio et al., 2021).

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Frequent data collection started in earnest in 2016, after the start of the most severe eutrophication issues, and it is therefore from this moment that we run our models. Weekly to monthly samples of temperature, salinity, oxygen, nutrients (ammonium, nitrate, phosphate, silicate), and chlorophyll have been collected by the Instituto Español de Oceanografía (IEO) and Dirección General del Mar Menor (CARM) and will be used for calibration and validation. The SMARTLAGOON buoy is now also collecting data, and these will additionally be used for further model validation as they become available. We additionally make use of CARM measurements of nutrient concentrations in the Albujón wadi, the main inflow into the lagoon.

Considering the use of Lake Erken as a data-rich pilot site before model application to the Mar Menor, we list here the major differences between Erken and the Mar Menor, from a modelling perspective, and how to deal with this. The GOTM-WET model is adapted to work for lakes, reservoirs, and lagoons of various depths, climatic regions, and trophic state, so, despite clear differences between Lake Erken and the Mar Menor, we do not foresee major problems regarding model application. As GOTM was originally designed for oceans (see 2.3.1), the effect of salinity on density is included in the model, but the effect of intense bursts of freshwater inflow into the hypersaline lagoon on short-term stratification could be challenging to simulate, especially if observations of these events are few. We plan to use high-frequency temperature, salinity, and oxygen observations, including those coming in from the new buoy, to detect short-term stratification and calibrate the model to capture these events. The exchange with the Mediterranean Sea is another important difference: this constitutes a significant source of water, with its own salinity and nutrients, for the Mar Menor. We use the results from the study by Senent-Aparicio et al. (2021) to estimate the magnitude and seasonality of the inflow, and realistic salinity and nutrient values for the Mediterranean seawater offshore of the Mar Menor. In section 3.2.1 we explain in detail how the sea-lagoon exchange was incorporated in our model setup.

2. Model descriptions and framework

2.1. Coupled catchment-lagoon model framework

The model framework has been visualised in Figure 3. The meteorological conditions act as the primary driver of both the catchment and the (lake and) lagoon model. Because the lagoon model also needs inputs from the catchment, the catchment model is run first, generating predictions of discharge. These outputs are then used as inputs in the lagoon model. The model is first applied by using reanalysis weather data and observed catchment data and calibrated (i.e. parameter values are changed to optimize the match between simulated and observed data). After model performance is assessed, the models can be driven instead by future weather conditions, and as such, forecasts of catchment and lake/lagoon conditions can be made.

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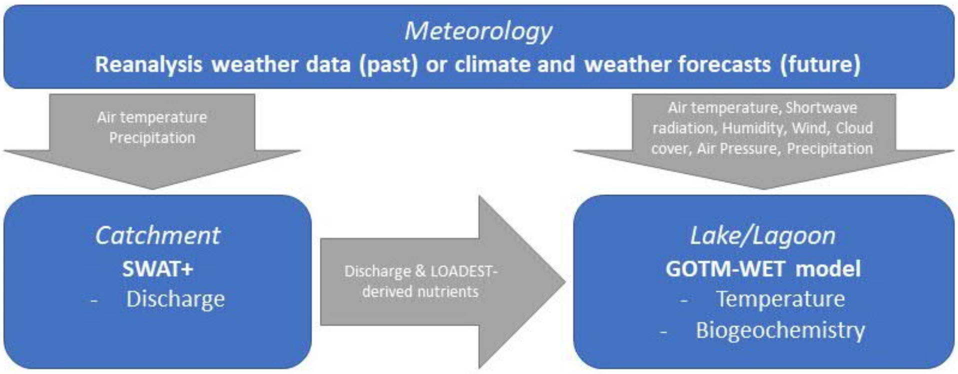

Figure 3. Schematic of the model framework to simulate catchment and lake/lagoon dynamics in Lake Erken and the Mar Menor. The models are set up and trained on reanalysis weather data and can then be applied when forced with predicted weather conditions, for example based on a weather forecast model or global climate models.

2.2. SWAT+ catchment model and simulation of stream temperature and nutrients

The SWAT+ model (Soil and Water Assessment Tool+, Bieger et al., 2017) was used to simulate discharge dynamics in the Lake Erken and Mar Menor catchments. SWAT+, an updated version of the SWAT model (Arnold et al., 1998), uses digital elevation, land use, and soil types to calculate the stream channel network and divide the landscape into hydrological response units. The model tracks most fundamental aspects of the catchment water balance (precipitation, evapotranspiration, surface runoff, lateral flow, groundwater flow, soil moisture, etc.) and calculates amongst others, channel flow out of the catchment (Arnold et al., 1998). The SWAT+ model application to the catchments of Lake Erken and the Mar Menor was the topic of the 3.1 Deliverable report, so we refer to that report for a more detailed explanation of the model.

Although SWAT+ is capable of simulating nutrient loads in addition to discharge, the performance of the model for simulated nutrient loads was not as good as that obtained when using the LOADEST (Load Estimator, Runkel et al., 2004) software to estimate nutrient loads from the catchment (as a function of SWAT+ simulated discharge), in the form of the R package rloadest (Runkel and De Cicco, 2017). Using this package, we tested multiple statistical relationships between the natural-log-transformed nutrient load and natural-log-transformed discharge that optionally could include a seasonal cycle. The best relation was then used to calculate nutrient loads from SWAT+-derived discharges.

The GOTM-WET model can also use stream temperature as an input. For Lake Erken, we used the air2stream software (Piccolroaz et al., 2016), a hybrid process-based and statistical model, to find a relation between discharge, air temperatures, and stream temperatures and extrapolate this to future conditions. In the Mar Menor, we lacked measured stream temperatures, so we assumed that the streams had the same temperatures as the lagoon's surface water temperature. However, this is unlikely to have a significant negative effect on the model performance, as in most lakes (except those with very high flushing rates), the advective heat flux is a negligible part of the

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heat budget (Imboden and Wüest, 1995) and the Mar Menor's shallow depth limits the extent of intrusion of sub-surface flows.

2.3. GOTM-WET lake/lagoon model

2.3.1. GOTM

The General Ocean Turbulence Model (GOTM, Umlauf et al., 2005) is a one-dimensional water column model, simulating aquatic physical processes. The model divides the water column into a grid of fixed vertical layers, that are forced by atmospheric and advective boundary conditions. GOTM then calculates turbulence and heat fluxes between the layers. Applications range from calculating effects of long-term climatic warming (Moras et al., 2019) to studies on sediment-induced stratification (Amoudry and Souza, 2011). As the name suggests, it was originally developed for oceans, but it has been adapted for use in lakes as well. The main difference between the ocean and lake applications, is the presence of a hypsographic representation of the individual layers and their sediment-water interface (i.e. surface area over depth) in the lake-version. Only Aveytua-Alcázar et al. (2008) have applied the GOTM model to a coastal lagoon before, but the use of GOTM in both ocean and lake settings gives confidence that GOTM can reproduce one-dimensional dynamics in the Mar Menor as well.

GOTM can be coupled to a biogeochemical model using the Framework for Aquatic Biogeochemical Models (FABM, Bruggeman and Bolding, 2014). In this framework, the equations of a biogeochemical model are applied to every layer in GOTM, while GOTM estimates changes in the vertical distribution of biogeochemical substances as well as density-dependent lateral inputs from watershed sources. The coupling is calculated at every model computational time step, so that feedbacks between biogeochemistry and physics (e.g. decreased light penetration due to phytoplankton biomass) can be included as well. In SMARTLAGOON, the GOTM model was coupled to the WET model using FABM.

2.3.2. WET

WET (Water Ecosystems Tool) is a modular aquatic ecosystem model that can simulate dynamics of oxygen, nutrients, and aquatic plants and organisms in the water column and sediments of water bodies (Schnedler-Meyer et al., 2022). It is a further development of the FABM-PCLake model (Hu et al., 2016), which was again an expansion of the established standalone PCLake model (Janse and van Liere, 1995). Its modular setup makes the model versatile, as simple or complex food webs can be created, based on the study site and available data. Moreover, the original PCLake model and WET also include macrophytes, which are also present in the Mar Menor and play an important role in nutrient uptake (Pérez-Ruzafa et al., 2019). The WET/FABM-PCLake model has been applied to several lakes, focusing on topics like eutrophication (Chou et al., 2021) and extreme weather events (Chen et al., 2020).

3. Model descriptions and framework

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First, we discuss the application of the model framework to Lake Erken. This application has been completed, including future climate simulations, and a manuscript is in preparation (Jiménez-Navarro et al., in preparation). Second, the progress in the model application to the Mar Menor is described, which has been set up completely, but will undergo additional calibration, as data keeps coming in from project activities including the recently deployed buoy. As the focus of this report, and SMARTLAGOON in general, is mostly on the Mar Menor, we describe the Mar Menor application in more detail.

3.1. Lake Erken

3.1.1. Input data and model setup

Weather data collected on and near the lake were used to drive both the SWAT+ and the GOTM-WET model, and observations of discharge and nutrients at the major inflow were used to drive the GOTM-WET model and calibrate/validate the SWAT+ model. The GOTM-WET model was calibrated and validated with water temperature and lake biogeochemical data collected by the Uppsala University Erken Laboratory. A model computational time step of one hour was used, although the forcing data was averaged to daily values, to coincide with the frequency of the future climate simulation data (see 3.1.3). We used four phytoplankton groups (diatoms, cyanobacteria, green algae, and flagellates), one macrophyte group, and one zooplankton group to represent the Lake Erken food web. We performed a literature search to find initial parameter values that were representative for Lake Erken.

Because GOTM-WET is a model with many parameters, we used the parsac software (Bruggeman and Bolding, 2020) to do a sensitivity analysis in order to reduce the number of parameters to calibrate from 275 to 165. The same software was then used to perform the calibration, where we optimised the model fit for water temperature and concentrations of oxygen, nitrate, ammonium, phosphate, silicate, total nitrogen, total phosphorus, and chlorophyll. The period 2000-2015 was used to calibrate and the period 2016-2021 was used to validate the model. A stepwise calibration approach was chosen, where parsac would optimise parameters for 30,000-70,000 iterations and based on plots of parameter performance, we adjusted parameter ranges and repeated the process. The calibration process has been outlined in more detail in the Deliverable 6.4 - Interim Progress Report.

3.1.2. Model performance

The SWAT+ and GOTM-WET models performed well in Lake Erken, capturing the seasonal dynamics of discharge and lake temperature, oxygen, nutrients, and chlorophyll (Table 1, Figure 4, Figure 5, Supplement A). As is common in modelling studies, physical variables are better simulated than chemical and biological variables, but the goodness-of-fit statistics are comparable with previous applications of physical-biogeochemical models in lakes (e.g. Ladwig et al., 2021; Mesman et al., 2022). The physical simulations (discharge and water temperature) did not show clear, systematic errors, but winter nutrient concentrations of nitrate and phosphate were underestimated by the model (Figure 5). Nevertheless, the timing and magnitude of the spring chlorophyll peak were

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accurate. In some summer blooms, the model underestimated chlorophyll levels, which may be due to a buoyant cyanobacteria species in Lake Erken, Gloeotrichia echinulata, that relies heavily on resting stages in the sediment (Karlsson-Elfgren et al., 2003). This is a process that is poorly understood and is not represented in WET, potentially explaining the mismatch between model and observations in some years.

Table 1. Model performance of SWAT+ (discharge) and GOTM-WET models for the calibration (2000-2015) and validation (2016-2021) periods. For a complete overview of the goodness-of-fit for all variables and all depths, see Supplement A.

		Calibration		Validation	
Variable	Depth (m)	RMSE	R^2	RMSE	R^2
Discharge (m^3/s)	-	0.31	0.63	0.27	0.63
Water temperature (°C)	3	0.80	0.99	0.69	0.99
Oxygen (mg/l)	15	2.07	0.77	2.08	0.79
Nitrate (mg/l)	3	0.041	0.64	0.048	0.48
Phosphate (mg/l)	3	0.013	0.41	0.011	0.29
Chlorophyll-a (mg/m^3)	3	4.89	0.35	6.81	0.16

The performance during the calibration and validation periods was similar for most variables, although nutrients and chlorophyll showed a weaker fit during validation. Visually (Figure 5), the model fit was not noticeably different from the calibration period, but the timing of the chlorophyll spring peak was a few weeks off, which can have a strong negative effect on goodness-of-fit (Elliott et al., 2000). Moreover, the 2019 summer bloom was exceptionally strong and also missed in a recent machine learning study in Lake Erken (Lin et al., under review). Therefore, we conclude that the model reproduced the lake dynamics to a reasonable extent, and that there is no strong evidence for overfitting.

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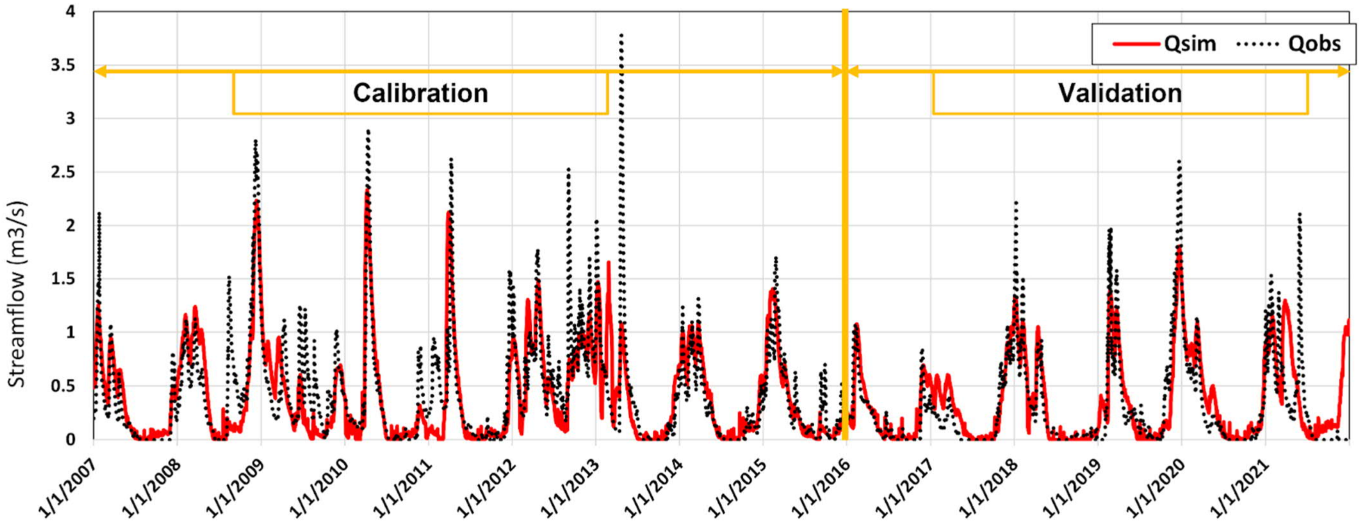

Figure 4. Observed (Qobs) and simulated (Qsim) discharge inflow in Lake Erken for the calibration and validation periods, simulated by SWAT+.

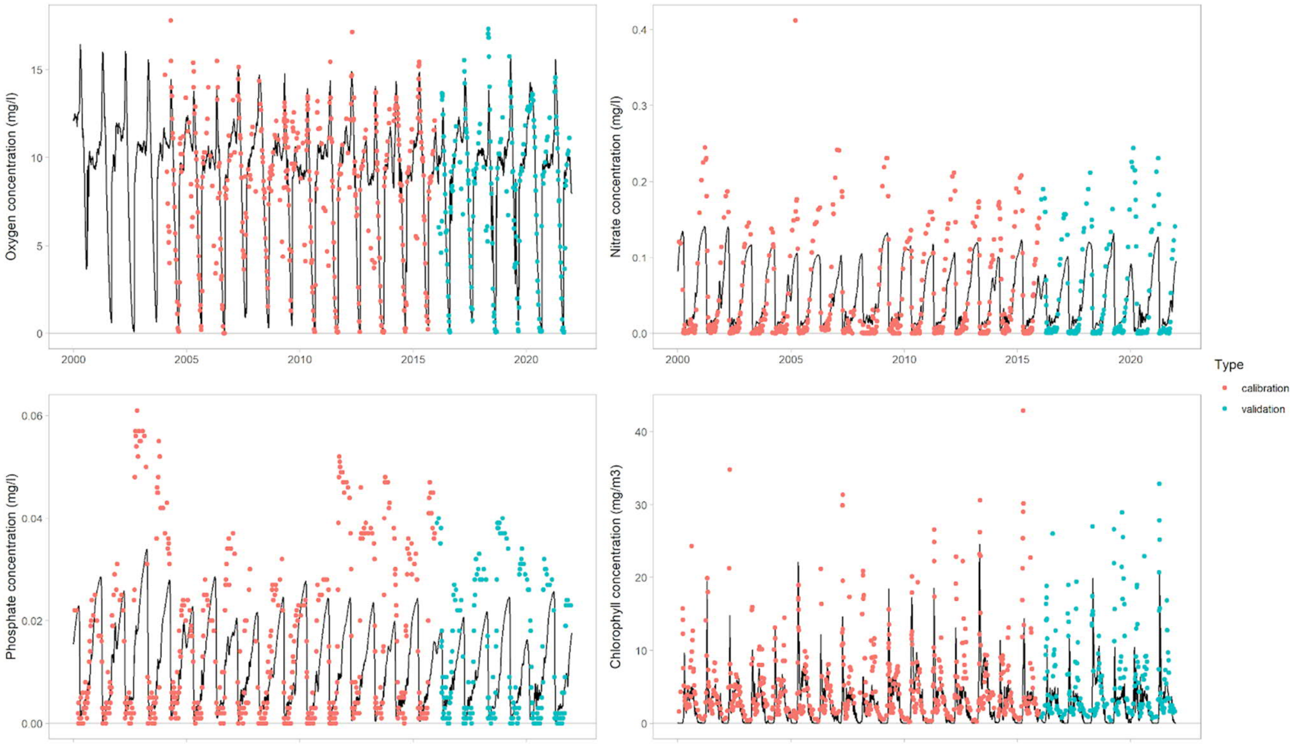

Figure 5. Concentrations of oxygen (mg/l, at 15 m depth), nitrate (mg/l, at 3 m depth), phosphate (mg/l, at 3 m depth), and chlorophyll (mg/m3, at 3 m depth) simulated by GOTM-WET (black line) compared to observations (dots). Red dots indicate the calibration period and blue dots the validation period.

The derivation of nutrient loads from discharge values using LOADEST resulted in an accurate simulation of loading dynamics (Supplement B), with R^2 values between 0.5 and 0.9 for all constituents. Although concentrations were not always simulated accurately by LOADEST, it was the discharge that controlled the largest variations in loading, which increases the reliability of LOADEST in future climate scenarios. Loadings were highest in winter and very low in summer. Lastly, the air2stream model also performed well, with R^2 values for simulated stream temperature higher than 0.95 (results not shown).

3.1.3. Future climate simulations

The calibrated GOTM-WET-SWAT+ setup was then forced with future climate data for the Lake Erken area, using outputs from five Global Climate Models (GCMs) from the CMIP6 project (O'Neill et al., 2016), in order to simulate future catchment and lake conditions. Two future climate scenarios were used; the SSP2-45 scenario, in which mitigation measures limit the intensity of climate warming, and the more pessimistic SSP5-85 scenario. Some striking results were a clear shift in the seasonality of discharge (with more discharge in winter and less in summer) and a strong decline in lake oxygen concentrations (mostly in the deeper water layers, but also decreases in the surface after autumn turnover). Changes were typically more severe in the SSP5-85 scenario compared to the SSP2-45 scenario.

The description of the GOTM-WET-SWAT+ setup in Lake Erken and the future climate scenarios will be the focus of the publication by Jiménez-Navarro et al. (in preparation).

3.2. Mar Menor

3.2.1. Input data and model setup

Lagoon water quality data provided by IEO and CARM were compiled into a consistent file format that can be read by GOTM and parsac. Monthly nutrient data from 3 -4 m depth and weekly chlorophyll, oxygen, salinity, and temperature profiles from 2016 are used. The nutrients data (Figure 6) suggested that the water quality is rather homogeneous in the horizontal dimension during most days, which adds credibility to the use of a 1D model.

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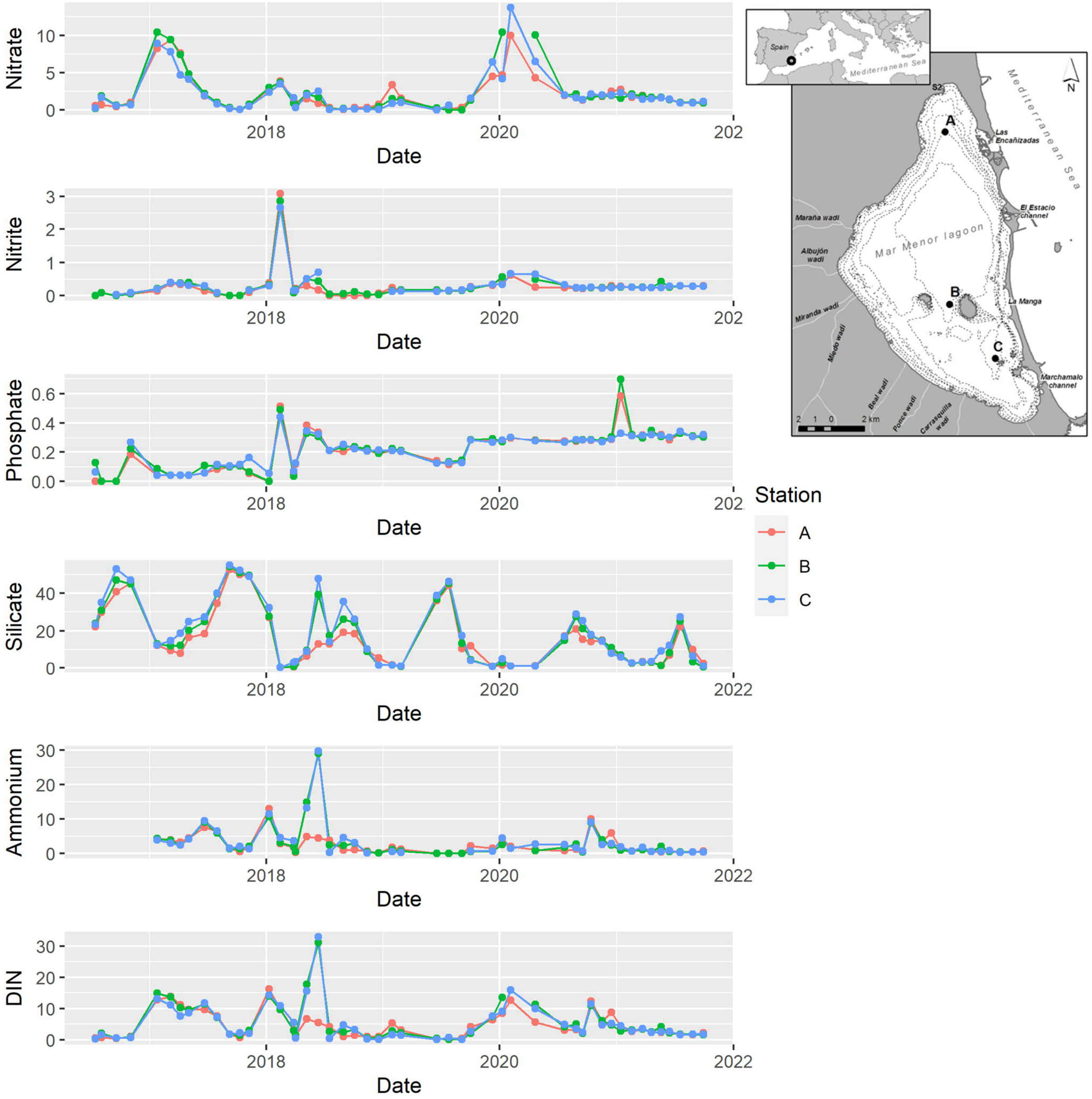

Figure 6. Time series of nutrient concentrations in the Mar Menor, based on data collected by the IEO. The colours indicate the different stations where the data were collected (see inset figure). All units are in mmol/m^3. DIN stands for dissolved inorganic nitrogen. Source of inset figure: IEO.

Although data are available from weather stations close to the Mar Menor, we made the conscious choice to use ERA5 (ECMWF atmospheric reanalysis, fifth generation) reanalysis data (Muñoz-Sabater et al., 2021) instead. The reason for this is that a combination of ERA5 data and weather forecasts based on the ECMWF model will be used in the digital twin. Therefore, we want to train the GOTM-WET model using weather data that is generated by a similar atmospheric model, in the hope that this would make the lagoon forecasts more reliable. The official ERA5 download portal and a web application developed by the WIT partner (http://test.asap-

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forecast.com:3000/, Last accessed: 2022-12-05) were used to download the ERA5 data for the location of the Mar Menor (latitude: 37.720, longitude: -0.784).

The major differences between the Erken and the Mar Menor sites are the temporal dynamics of salinity and the two-way exchange with the Mediterranean Sea in the case of the Mar Menor, and here we explain in detail how we dealt with this. As observed water level fluctuations in the Mar Menor are generally < 0.15 m (Umgiesser et al., 2014), we assumed a fixed water level in GOTM, and any imbalance in the water budget would be corrected by GOTM by the creation of an artificial outflow at the surface. We used the results of the Mar Menor water balance study by Senent-Aparicio et al. (2021) to fit a sine-relationship between day-of-the-year and net exchange between the lagoon and the Mediterranean Sea driven in part by seasonal changes in evaporation from the lagoon, and used this relationship to create a separate inflow file for the GOTM-WET setup. However, Senent-Aparicio et al. (2021) investigated only the net exchange, as the missing factor in the water balance, whereas there is also a “regular” two-way exchange between both water bodies, which, has a limited effect on water balance (Umgiesser et al., 2014), but is essential for determining nutrient and salt concentrations. In absence of measured data and a coupled hydrodynamic model between the lagoon and the sea, we assumed an additional constant (“offset”) rate in time for the “regular” exchange and used measured salinity in the lagoon as target variable to estimate this rate. Salt is a conservative substance, and is therefore ideal to estimate exchange rates. By increasing the “offset” value in the GOTM configuration file, we increased inflow from the Mediterranean until a reasonable value for salinity in the lagoon was achieved. This “offset” value will also be included in the final calibration. The salinity concentration in the Mediterranean was based on a Marine Copernicus product (E.U. Copernicus Marine Service Information; 10.48670/moi-00051), and so were the nutrient concentrations (with an added seasonal cycle, E.U. Copernicus Marine Service Information; 10.25423/cmcc/medsea_multiyear_bgc_006_008_medbfm3).

Inflow values from the catchment rely on a SWAT+ model, which is still undergoing calibration. And, since the calibration of the GOTM-WET model is expected to take several weeks, potentially months, for the initial calibration reported on here we are using the results of Senent-Aparicio et al. (2021) in combination with measured inflow nutrient concentrations by CARM to get preliminary watershed discharge and nutrient loads. Once the final input data is in place, the model should already perform close to optimal, so that only few additional calibration iterations will be needed. As for Lake Erken, we used LOADEST to estimate continuous nutrient concentrations in the catchment inflows.

The current WET food web model for the Mar Menor has one group each for macrophytes, phytoplankton, and zooplankton. We may extend this later to multiple groups for phytoplankton, as different groups are known to be responsible for bloom dynamics (Gilabert, 2001; Mercado et al., 2021). We are currently performing a literature search for parameter values in the Mar Menor. Compared to Lake Erken, we are finding less parameter values, but some examples are given in Table 2.

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Table 2. Examples of literature-based parameter values for the Mar Menor, compared to the example value from the Lake Ravn GOTM-WET test case. In case references gave different values, the average value was taken.

Parameter	Unit	Default	Mar Menor value	References
abiotic_water/tNDepoNO3	g/m2/d	0.0	0.0008	(Garcia-Gomez et al., 2014; Puertes et al., 2021)
abiotic_sediment/cCPerDWS	gC/gDW	0.4	0.58	(Pérez-Ruzafa et al., 2012)
abiotic_sediment/bPorS	m3/m3	0.85	0.67	(Baudron et al., 2015; Vallejo et al., 2021)

3.2.2. Model performance

The results shown here are before automated calibration; the plots therefore serve only to show that the model can reproduce the overall seasonal patterns of variation or if there are substantial issues that we need to address in the model code or calibration. These results should not be seen as a final product, but rather as an important step in the development of a complete model. All results are shown for 3.5 m depth (this was the depth around which the nutrient samples were collected), although at the end of this section we also show a plot of the differences between 1 and 6 m depth to visualise short-term stratification patterns.

Seasonal dynamics in water temperature and salinity were simulated accurately (Figure 7). The good fit for water temperature indicates that the ERA5 forcing can give a reasonably good representation of the weather conditions around the Mar Menor, which adds confidence to its use for forecasting in the digital twin. The temporal patterns in salinity were captured well, although summer salinity values were sometimes overestimated. This could mean that the exchange between the Mediterranean Sea and the lagoon needs to be optimised further, but the reproduction of the temporal patterns means that the hydrological inputs, both from the catchment and the Mediterranean, calculated by Senent-Aparicio et al. (2021) using SWAT, are of good quality.

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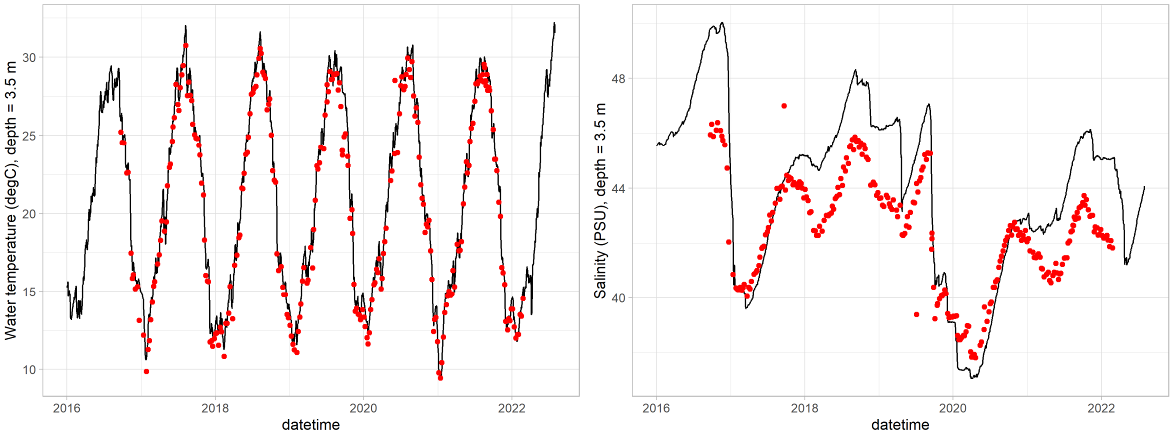

Figure 7. Simulated (black line) versus observed (red dots) water temperature (left) and salinity (right) values in the Mar Menor at 3.5 m depth. Pre-calibration.

The nutrients fitted worst of all variables, with the model clearly missing the observed dynamics (Figure 8). However, this pattern was observed at earlier stages in Lake Erken as well – the model assumes strong limitation of one nutrient (phosphate, in this case), leading to overestimated values of another nutrient. This is something that the automated calibration can usually optimise, and using multiple phytoplankton groups (with diverging affinities for different nutrients) may also lead to further improvements.

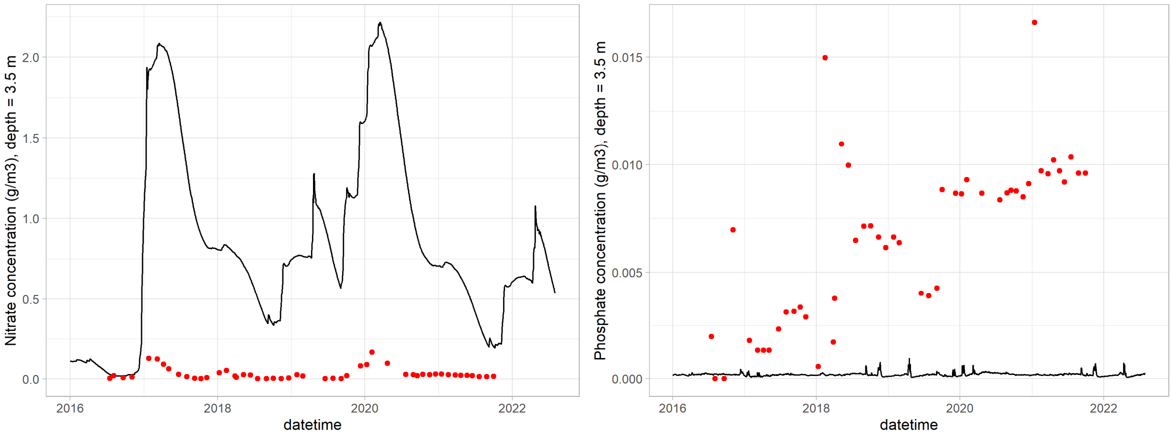

Figure 8. Simulated (black line) versus observed (red dots) nitrate (left) and phosphate (right) concentrations in the Mar Menor at 3.5 m depth. Pre-calibration.

A further sign that the above problem is indeed related to nutrient co-limitation is that the chlorophyll values were following observed values surprisingly closely, considering this is still an uncalibrated fit (Figure 9, left). Chlorophyll peaks, indicating blooms, in 2017, 2019, and 2021 were captured by the model, although the baseline concentration in the model was too high and the model simulated several peaks that were not represented in the data. Regardless, chlorophyll had been the primary challenge in the Lake Erken application, but in the Mar Menor the uncalibrated version of the model is much closer to reality than the uncalibrated model had been in Lake Erken. Further calibration is absolutely necessary, but the current simulation suggests that a good result can be obtained.

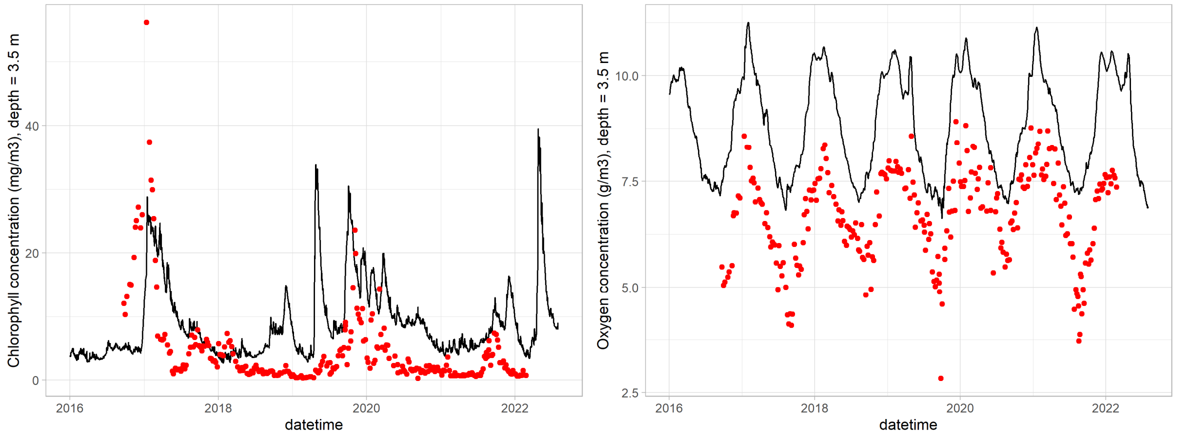

Figure 9. Simulated (black line) versus observed (red dots) chlorophyll (left) and oxygen (right) concentrations in the Mar Menor at 3.5 m depth. Pre-calibration.

Although the oxygen concentrations followed a correct seasonal cycle and the fit looked, at first glance, better than that of the nutrients, the model systematically overestimated oxygen concentrations (Figure 9, right), and this may point to a problem in the model code. The WET code takes into account the effect of salinity on oxygen saturation, but the simulation suggests that there is a distinct difference between the model and the situation in the Mar Menor that requires further investigation.

The frequency of the water quality measurements may not be sufficient to capture short-term stratification events, but an exceptional stratification event that occurred in the summer of 2019 was partially reproduced by the model (Figure 10). It seems that the uncalibrated model run overestimates strength of stratification, which is something that can probably be adjusted during the automated calibration. Due to the importance of short-term stratification and anoxia/phytoplankton blooms (compare the 2019 stratification event in Figure 10 and the chlorophyll-a and oxygen patterns in Figure 9), it is important that the model can reproduce these events. This will be challenging as many stratification events likely occur on time scales of one to a few days, and may be missed by the sampling campaign. However, the newly installed monitoring buoy (D2.1) will provide high frequency (hourly) data of water column temperature and surface and bottom oxygen that can be used to further improve model calibration. When using the historical data from manual sampling campaigns GOTM-WET shows that it is able to simulate such events, and reproduced the 2019 stratification event (Figure 10).

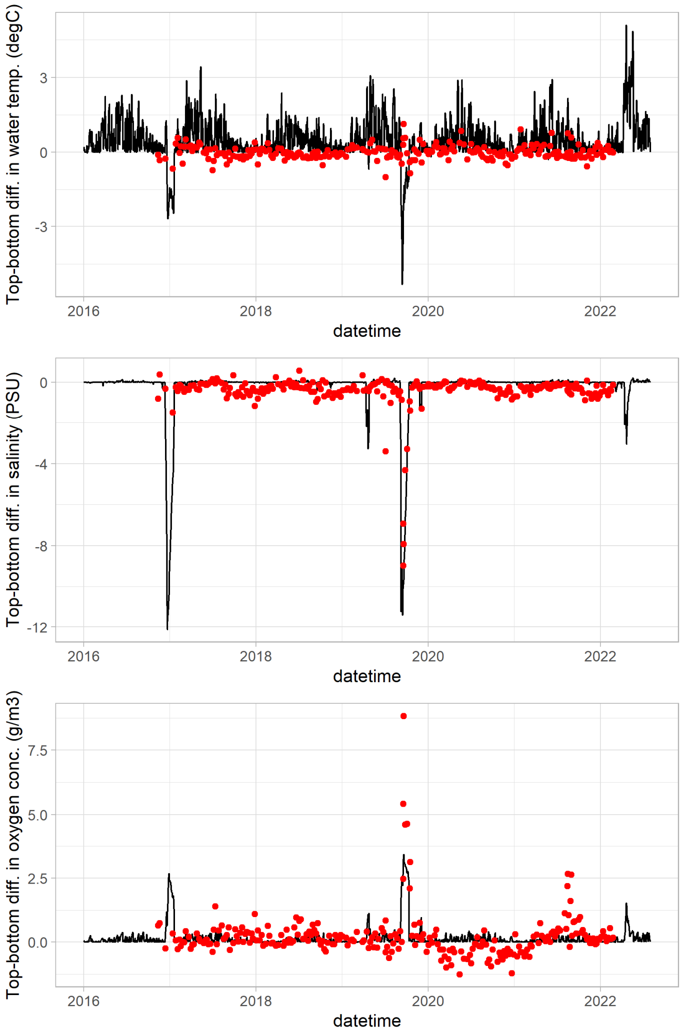

Figure 10. Difference between top (1 m depth) and bottom (5.5 m) values of water temperature, salinity, and oxygen concentration. The black line is the simulation and the red dots are observations. Note that the model simulations show daily mean values whereas the measurements are taken at a single moment. Pre-calibration.

3.2.3. Next steps

The literature search for parameter estimates for the Mar Menor are ongoing. Following this, we will perform a sensitivity analysis of the model, and, like in Lake Erken, use this to select the parameters that should be calibrated. We will then proceed with the automated calibration, using the same strategy as for Lake Erken: iterative calibration rounds and adjustment of parameter ranges based on plots (for more details, see Deliverable 6.4 - Interim Progress Report). We are on schedule to start the calibration before the end of 2022 and to finish in January/February 2023, although this may be repeated during the lifetime of the project, as more data is coming in from the buoy.

Following the final calibration, we will implement the coupled SWAT+-GOTM-WET model into the forecasting system, which is part of Work Package 5. The format of the model setup is such that it can be implemented in the ASAP portal directly.

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4. Conclusions

This report described the setup and initial calibration of the GOTM-WET model, coupled to SWAT+, for the Lake Erken and Mar Menor sites, including the input data that was used, the choices that were made in the model configuration, and the model performance. In Lake Erken, the calibrated GOTM-WET model simulated the lake dynamics accurately and when using future climate weather conditions, we could make projections of lake water quality conditions until the end of the century. In the Mar Menor, the model has been set up, and we can soon start the final calibration. Challenging aspects of the Mar Menor application included the data compilation, where data from multiple sources had to be standardised and put in the GOTM-WET format, and the parameterisation of the exchange between the lagoon and the Mediterranean Sea. The GOTM-WET model for the Mar Menor showed a promising first simulation, especially for the variables water temperature, salinity and chlorophyll, despite lack of automated calibration. The simulations of nutrients and oxygen will need to be improved during the final calibration phase, as expected.

The ultimate aim of the GOTM-WET model setup in the Mar Menor is its implementation into the digital twin, where it can be used for forecasting and scenario testing studies. Because the model showed a good replication of water temperatures using the ERA5 forcing data, it is likely that the model will perform well with the ECMWF weather forecasts used by the digital twin. Short-term runoff and stratification events are crucial determinants of water quality in the Mar Menor. Despite using an uncalibrated model and an older study for catchment runoff, the model showed a promising capacity to capture such events, as shown by reproduction of phytoplankton blooms and short-term density stratification. As such, the calibrated model will be a valuable part of the SMARTLAGOON digital twin and helpful to better understand and predict water quality issues in the Mar Menor lagoon.

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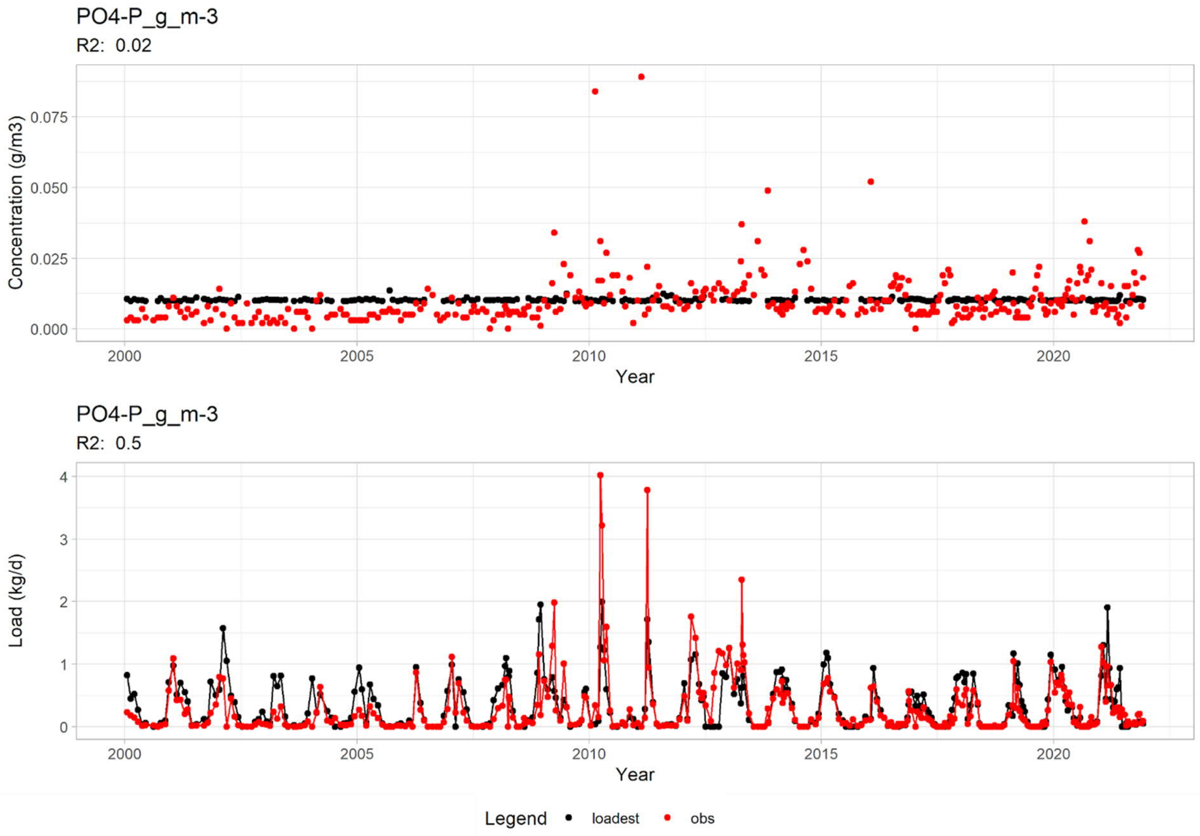
Supplementary material

Supplement A – Goodness-of-fit metrics of the GOTM-WET model application in Lake Erken (The units for RMSE are in mg/l, except for temperature (°C) and chlorophyll (mg/m^3)

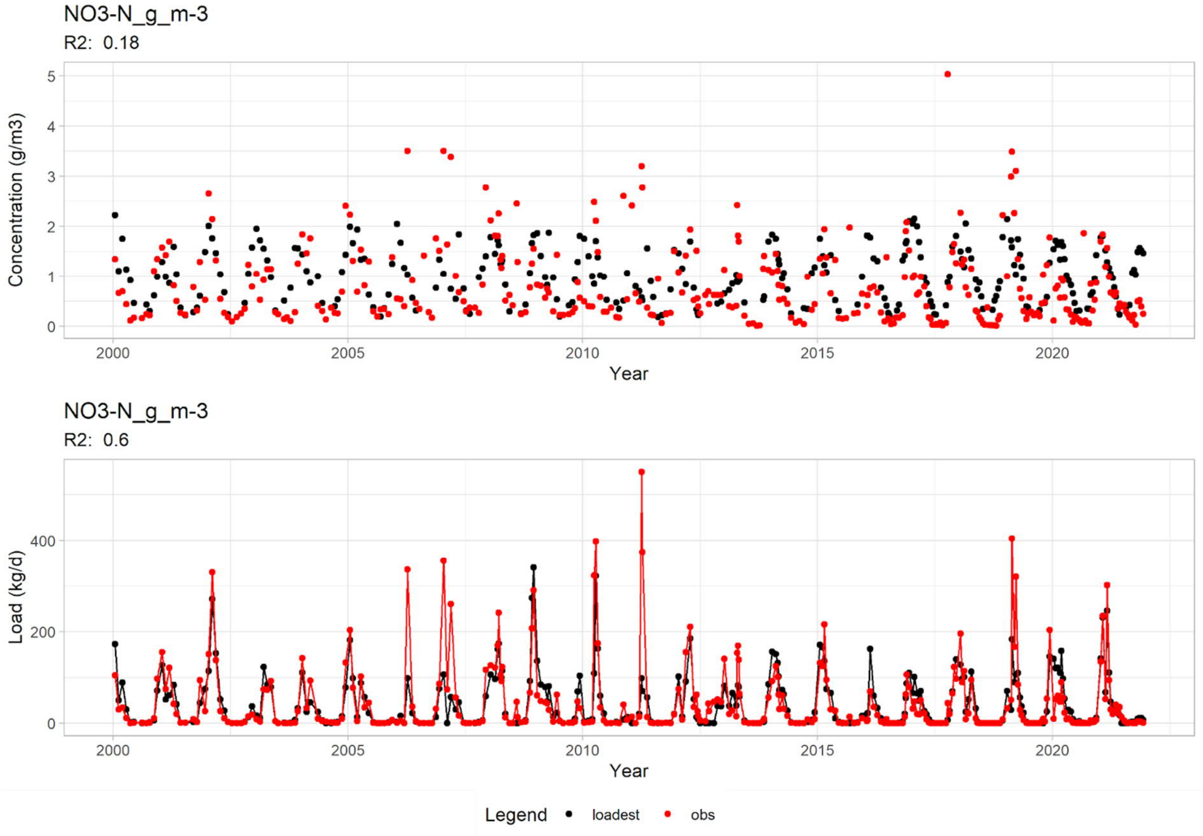
		RMSE			R^2		
	Depth (m)	All	Cal.	Val.	All	Cal.	Val.
NH4	3	0.014	0.015	0.011	0.136	0.121	0.214
	15	0.043	0.035	0.057	0.067	0.071	0.112
	all	0.025	0.022	0.032	0.142	0.144	0.166
NO3	3	0.043	0.041	0.048	0.593	0.640	0.475
	15	0.034	0.031	0.040	0.133	0.165	0.083
	all	0.041	0.039	0.046	0.535	0.588	0.414
O2	3	1.284	1.248	1.339	0.618	0.635	0.593
	15	2.070	2.065	2.080	0.779	0.774	0.792
	all	1.730	1.809	1.604	0.715	0.701	0.744
PO4	3	0.012	0.013	0.011	0.381	0.406	0.289

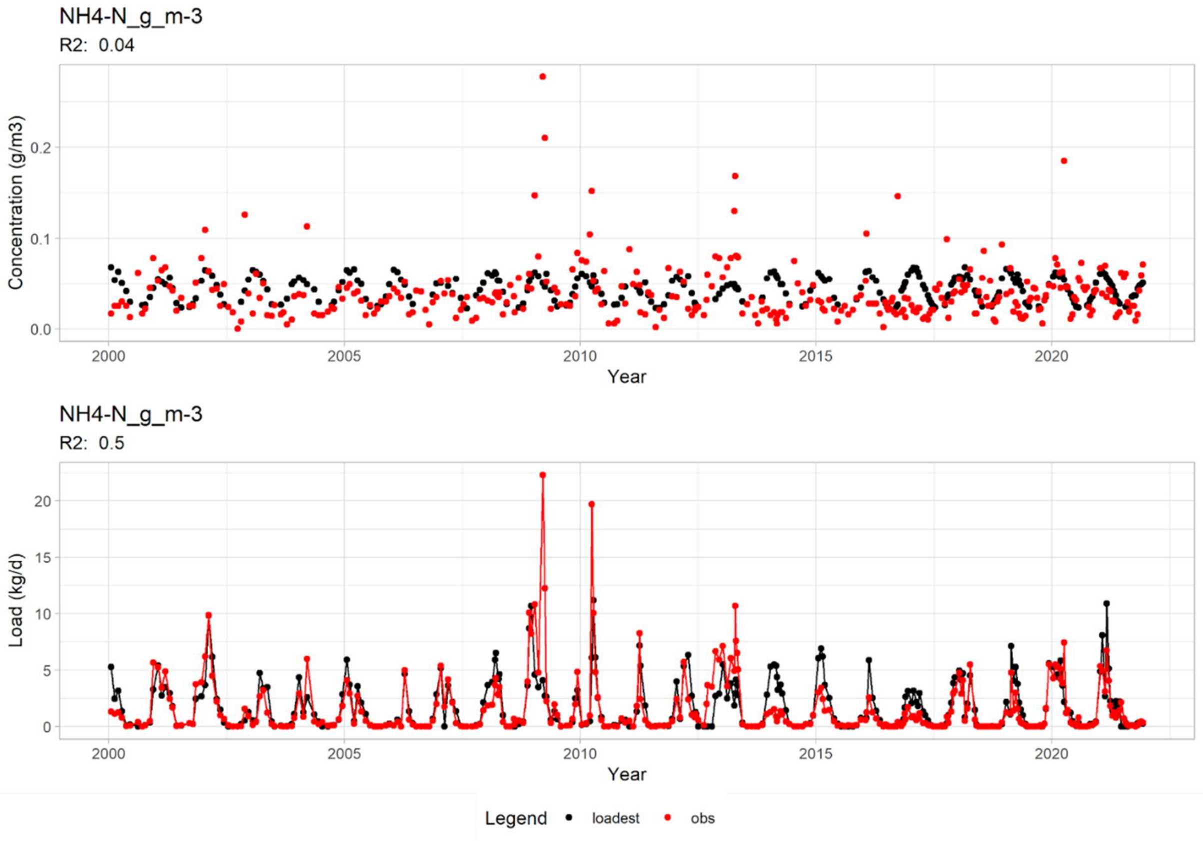
	15	0.037	0.036	0.040	0.119	0.168	0.026
	all	0.022	0.022	0.023	0.213	0.251	0.116
SiO2	3	0.640	0.569	0.792	0.016	0.061	0.037
	15	0.918	0.849	1.057	0.008	0.003	0.091
	all	0.726	0.655	0.877	0.084	0.095	0.224
temp	3	0.768	0.800	0.690	0.988	0.986	0.992
	15	1.136	1.142	1.123	0.946	0.940	0.957
	all	1.001	1.078	0.859	0.969	0.950	0.983
chla	3	5.482	4.892	6.807	0.277	0.351	0.155
TP	3	0.010	0.011	0.008	0.550	0.561	0.539
	15	0.036	0.035	0.039	0.182	0.243	0.061
	all	0.021	0.020	0.022	0.282	0.324	0.178

Supplement B – LOADEST fit for Lake Erken inflow nutrient concentrations
(DOP = Dissolved Organic Phosphorus, DIP = Dissolved Inorganic Phosphorus, DON = Dissolved Organic Nitrogen, DIN = Dissolved Inorganic Nitrogen)



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101017861.





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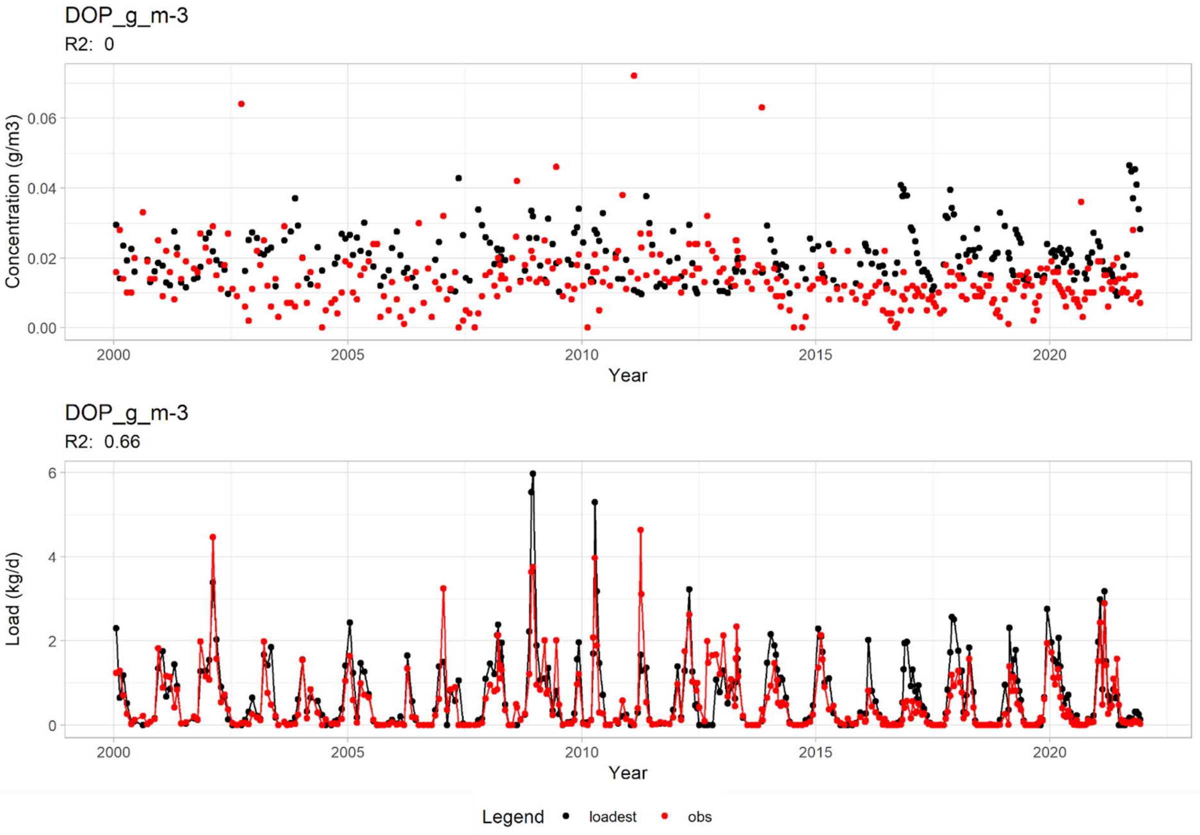
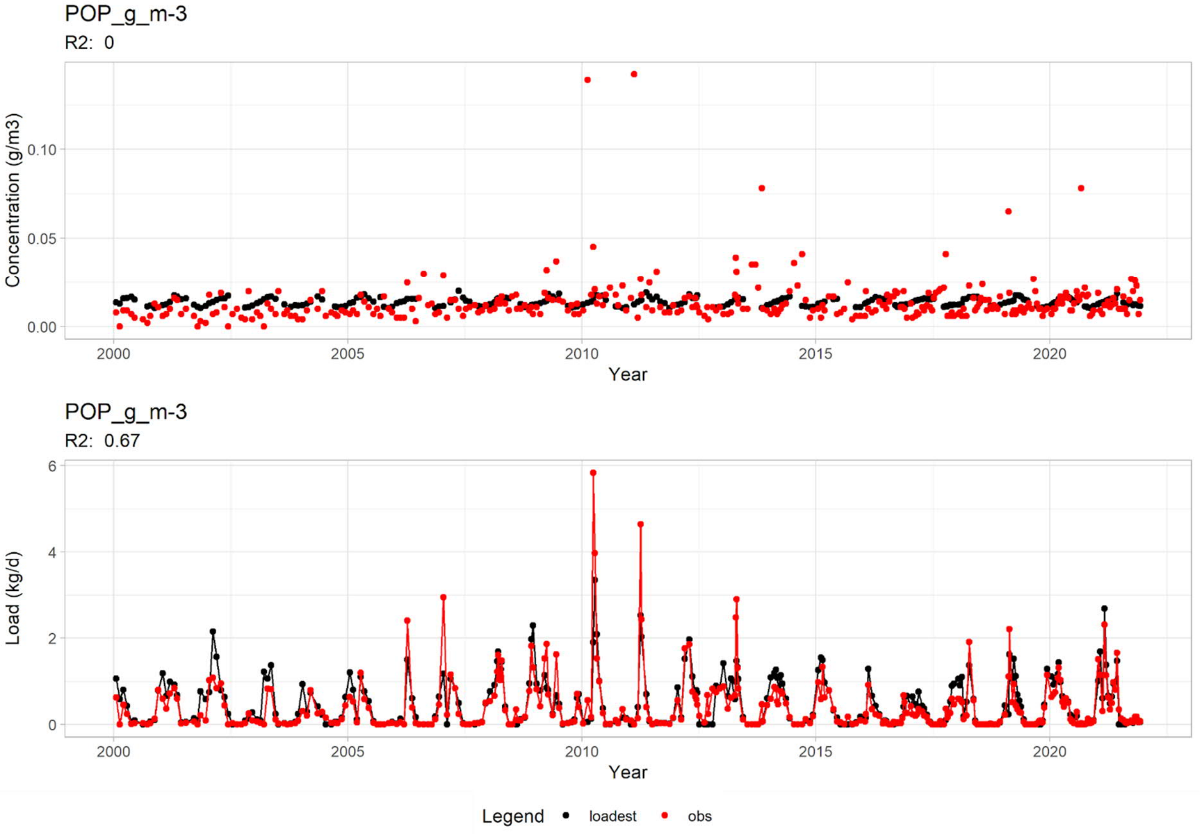
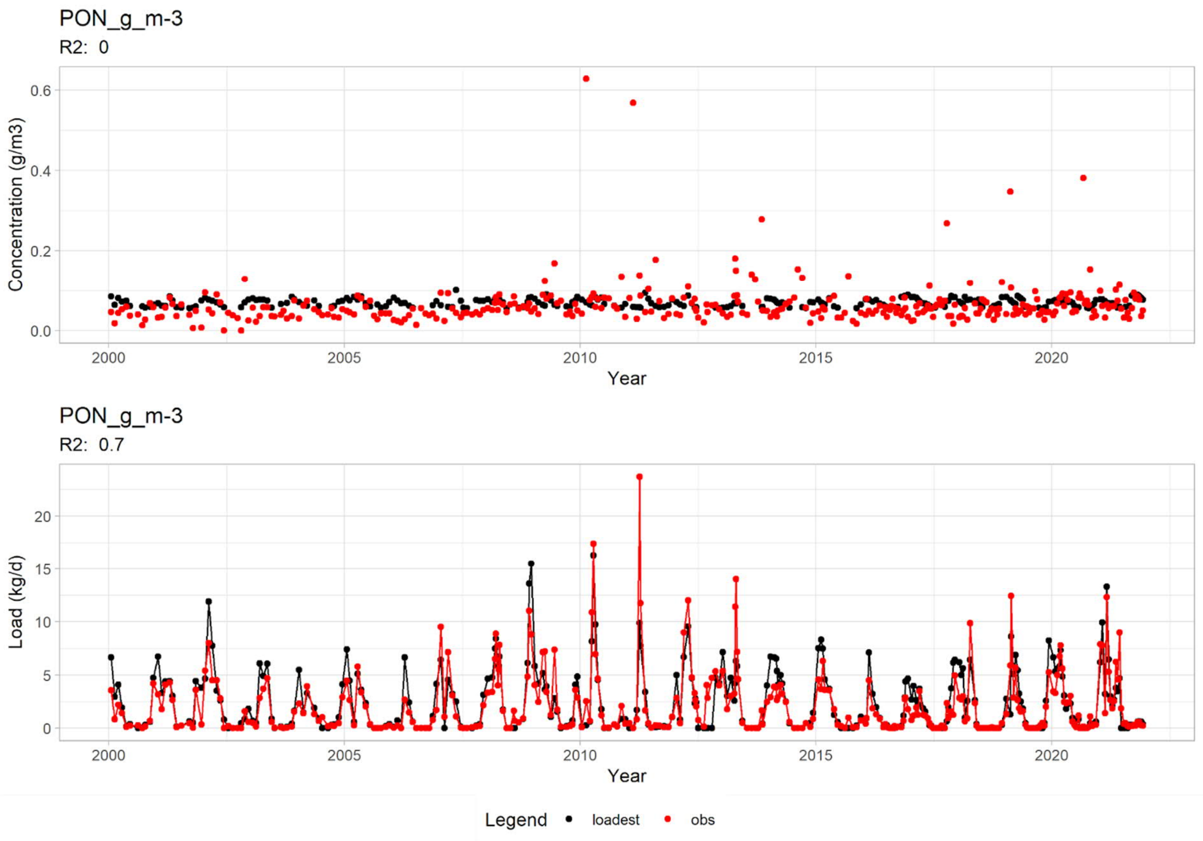
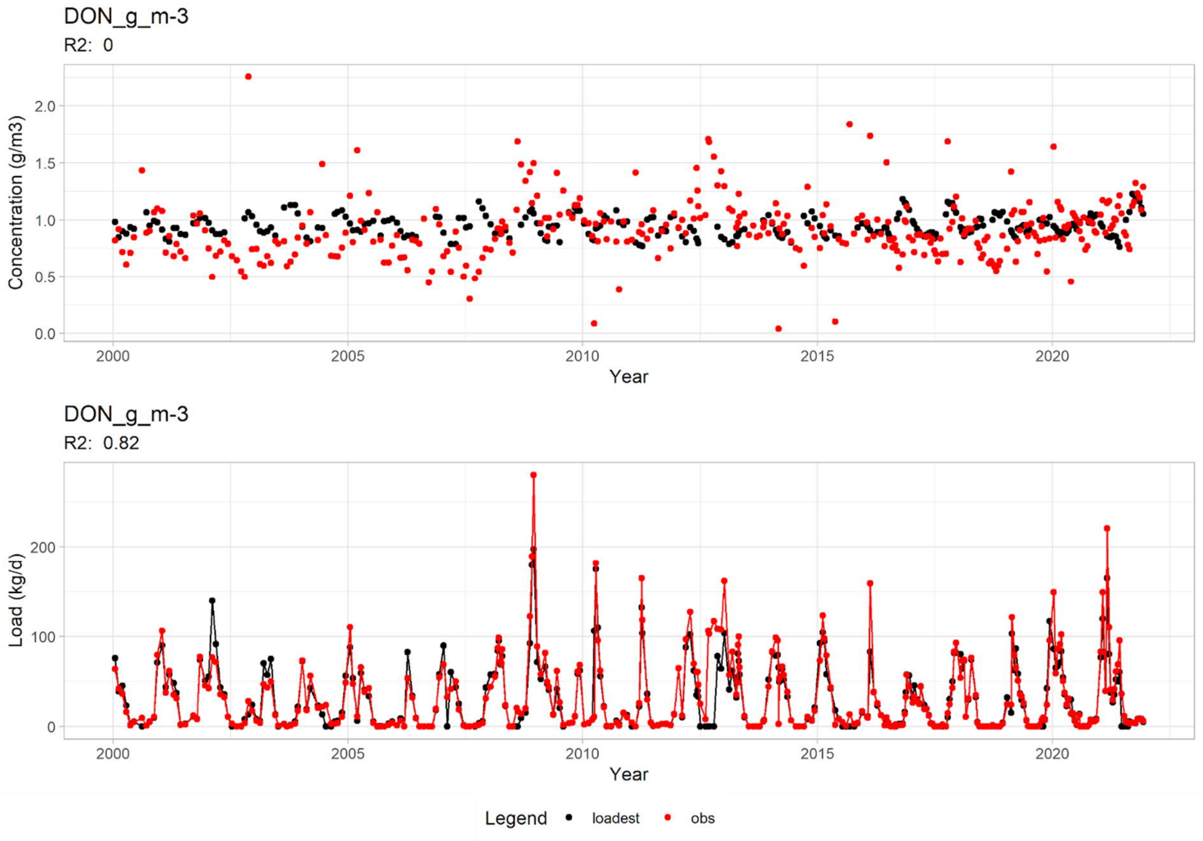
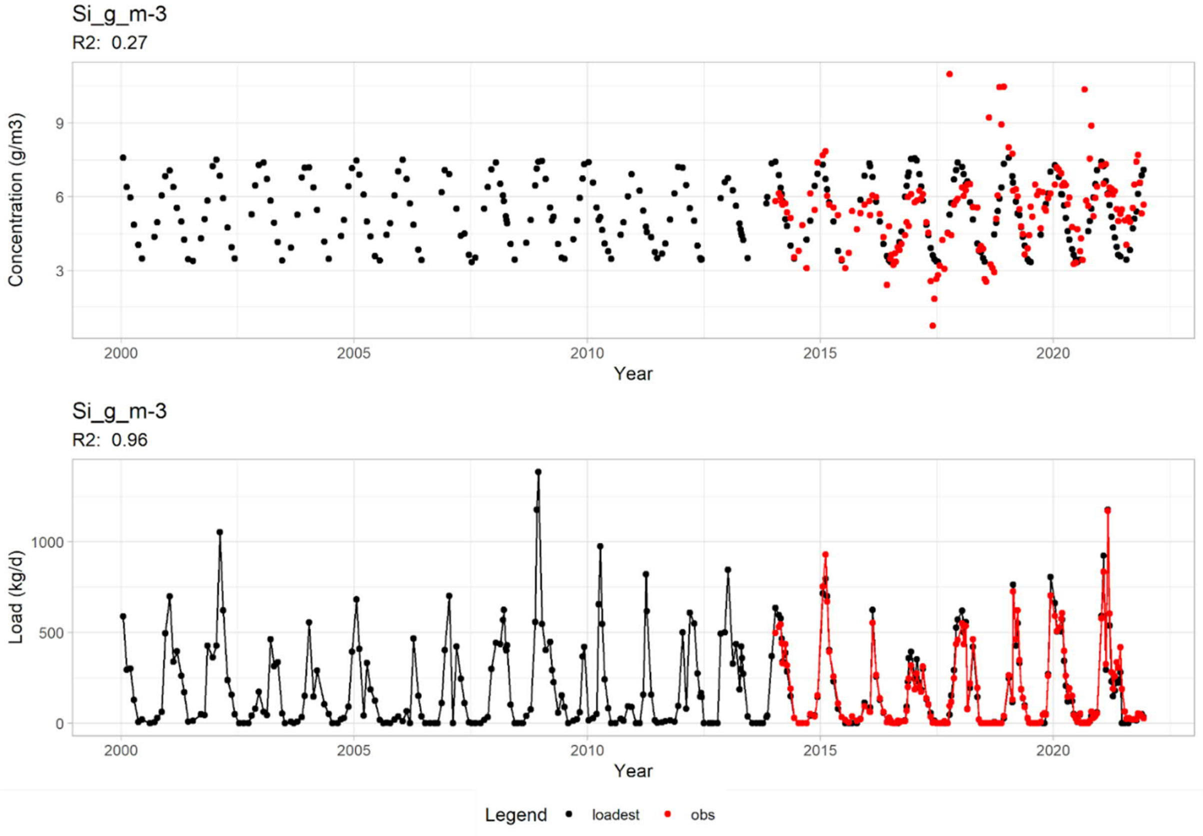

DOP_g_m-3
R2: 0
Concentration (g/m3)
0.00
0.02
0.04
0.06
2000
2005
2010
2015
2020
Year
DOP_g_m-3
R2: 0.66
Load (kg/d)
0
2
4
6
2000
2005
2010
2015
2020
Year
Legend
● loadest
● obs


POP_g_m-3
R2: 0
Concentration (g/m3)
0.00
0.05
0.10
2000
2005
2010
2015
2020
Year
POP_g_m-3
R2: 0.67
Load (kg/d)
0
2
4
6
2000
2005
2010
2015
2020
Year
Legend
● loadest
● obs


PON_g_m-3
R2: 0
Concentration (g/m3)
0.6
0.4
0.2
0.0
2000
2005
2010
2015
2020
Year
PON_g_m-3
R2: 0.7
Load (kg/d)
20
15
10
5
0
2000
2005
2010
2015
2020
Year
Legend ● loadest ● obs


DON_g_m-3
R2: 0
Concentration (g/m3)
2.0
1.5
1.0
0.5
0.0
2000
2005
2010
2015
2020
Year
DON_g_m-3
R2: 0.82
Load (kg/d)
200
100
0
2000
2005
2010
2015
2020
Year
Legend ● loadest ● obs


Si_g_m-3
R2: 0.27
Concentration (g/m3)
9
6
3
2000
2005
2010
2015
2020
Year
Si_g_m-3
R2: 0.96
Load (kg/d)
1000
500
0
2000
2005
2010
2015
2020
Year
Legend
● loadest
● obs

SMARTLAGOON

End of Deliverable 3.2

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