WP 2 – Integrative tools

Optimized impact model chain for seasonal and future climate predictions at WATExR case study site

Date

May 2019

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Table of Contents

Contents

1. Introduction

An overarching goal of the WATExR project is to advance the development of model-based forecasts of lake and reservoir water quality. Both seasonal and future climate simulations are being tested, the latter by participating in the lake sector of the Inter-Sectoral Impact Model Intercomparison Project (ISIMIP). In most cases these forecasts and simulations are complex, using a coupled system of watershed and lake/reservoir models with the input to this modeling chain being the output of complex climate models that operate at seasonal or decadal time scales.

As a result, in order to achieve optimal simulation results there are a number of steps that must be taken in the modeling exercise. These include the initial set up and testing of the model, model calibration, model verification, and then producing the final model simulation and forecast. Such forecasts are usually made in the form of a group of simulations based on multiple model ensemble members and also can be made using multiple climate models. This in turn results in multiple forecasts so that the variability in this output can be used to evaluate the uncertainty in the forecast predictions.

In Deliverable 3.1 we described the model workflows to be used at each case study, and in Deliverable 2.1 we described the protocols and procedures to be used within WATExR to ensure high quality model calibration and evaluation, including some examples of model calibration and hindcast simulations from select case study sites. Here the main objective is to describe the additional work that is needed beyond the initial setup and calibration, to ensure that model predictions are optimal for each case study site given the common limitations related to climate data. The goal of this report is to show examples of how each case study in the WATExR project has validated a modeling workflow that provides a methodology to assess seasonal or future climate predictions. Some of the case study workflows described here are formalized in a QGIS interface, as has been described in Deliverable 3.1.

2. Modeling workflows in WATExR

The following sections show the results from forcing the impact models, using the seasonal forecast data or/and future climate data. The impact model setups, calibration and validation procedures and uncertainty analyses are described in in Deliverables 2.1 and 3.1). The workflows implemented in each case study have a particular objective according to the end-user requirements and impact model configuration, but the uncertainty analysis associated with the climate data is common to all cases studies. The next sections show the results of the workflows applied in each case study.

2.1 Modeling workflow for Swedish site: Lake Erken

The Swedish case study Lake Erken is the first site used to test future climate simulations for the ISIMIP lake sector (https://www.isimip.org/). As part of the WATExR contribution to ISIMIP we developed future climate simulations of Erken's thermal structure, and developed an optimal simulation strategy for use of the GOTM hydrothermal model. This served as an example for the over 60 lakes that are presently being processed in the ISIMIP lake sector with the GOTM model used here and also with four or more additional lake models.

The first phase of ISIMIP simulations were by design simple focusing only on hydrothermal simulations. The reason for this was twofold. First it is the hydrodynamic simulations produced by models such as GOTM that form the foundation of more complex water quality model simulations. It is the variations of water temperature, timing of thermal stratification and changes in mixed layer depth that ultimately regulate all biogeochemical processes occurring in lakes. Secondly, in cases where there are only small seasonal variations in lake water level, simulations that only examine lake thermal structure can reduce the need for watershed input to the lake, and therefore, simplify the lake modeling system by eliminating the need for watershed model predictions. This is important to the ISIMIP as it allows the first phase of Lake Sector simulations to proceed rapidly. The workflow described for Lake Erken is therefore somewhat different from those in the remaining WATExR case studies. Only a single model (GOTM Burchard et al. 2006) is used, and its long-term future climate rather than near term seasonal forecasts that are being simulated. Despite this apparent simplicity there was still significant work involved in developing correct model calibration, and post processing the data from the future climate simulations. The modeling workflow developed here will be embedded into a QGIS interface that will allow any of the many lakes that serve as case studies for the ISIMIP to be simulated. This will provide an educational application that will allow students visiting the Erken laboratory to simulate future changes in Erken's thermal structure, and compare these changes with simulations from other lakes participating in the ISIMIP.

2.1.1 Steps in future climate simulation workflow.

1) Ensure optimal calibration with minimal parametrization. While the initial calibrations of GOTM provided good results as described in WATExR D2.1, further tests on our optimizations run using the ACPy program (https://bolding-bruggeman.com/portfolio/acpy/) were required to ensure that all model parameter were occurring within physically realistic ranges, and that the model was calibrated by adjusting the minimal amount of parameters. Since the hydrodynamic calculations in GOTM are largely based on well-known physical relationships we strived to avoid over-tuning the model, which could provide some small improvements in the simulations of historical conditions, but may lead to less representative simulations of future climate conditions. Initially seven model parameters were adjusted during model calibration. We found we could simplify the calibration of the processes affecting the attenuation of solar radiation in the water column by fixing two parameters to realistic physical values and adjusting only one additional parameters. This resulted in a final calibration strategy that adjusted five rather than seven model parameters. The remaining four parameters all scale the processes and inputs that affect the surface heat flux and distribution of heat in the water column. These were checked and found to have realistic values. ACPy provides some capabilities to visualize the difference between simulated and measured water temperature. We developed additional visualizations (**Figs 2.1.1-2.1.3**) to better understand the performance of GOTM by comparing simulated and measured water temperatures at different depths and in different water layers and the ability of simulations to reproduce important metrics of thermal stratification.

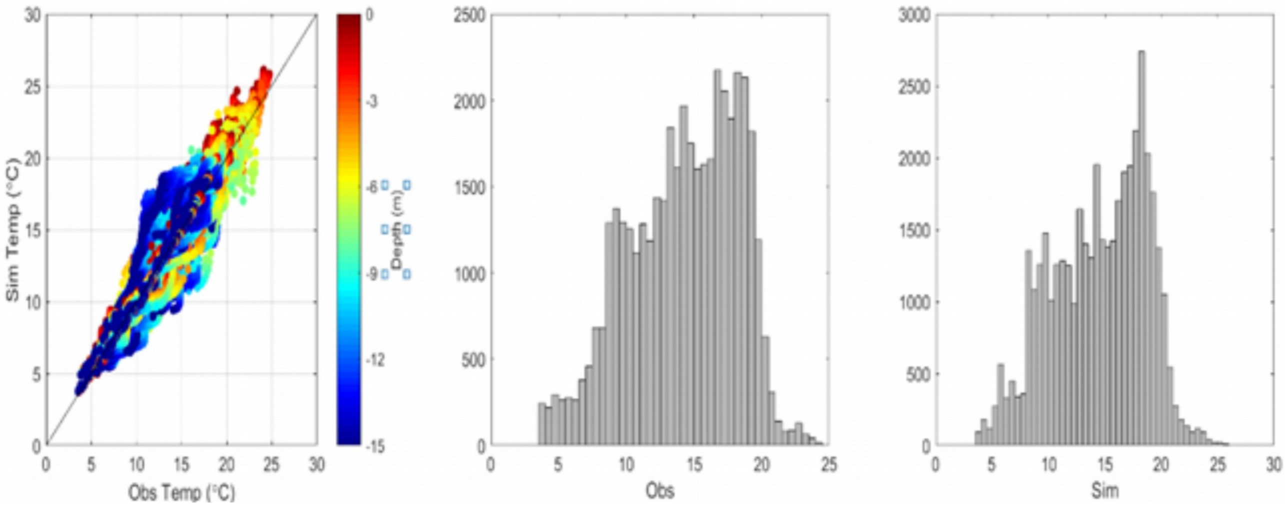

Figure 2.1.1 Advanced visualization used to improve model calibration. Observed vs measured temperature colored to show depth, and the frequency distributions of the observed and simulated temperatures.

Model fit was judged by visual comparison of simulated and measured values and by calculation of common estimates of model fits such as the mean absolute error (MAE), root mean square error (RMSE) and the Nash–Sutcliffe efficiency (NSE) as described in WATExR Deliverable 2.1

Figure 2.1.2 Advanced visualization used to improve model calibration. These graphs show a comparison between metrics of thermal stratification derived from the observed and measured temperature data using the Lake Anlayzer program (Read et al. 2011).

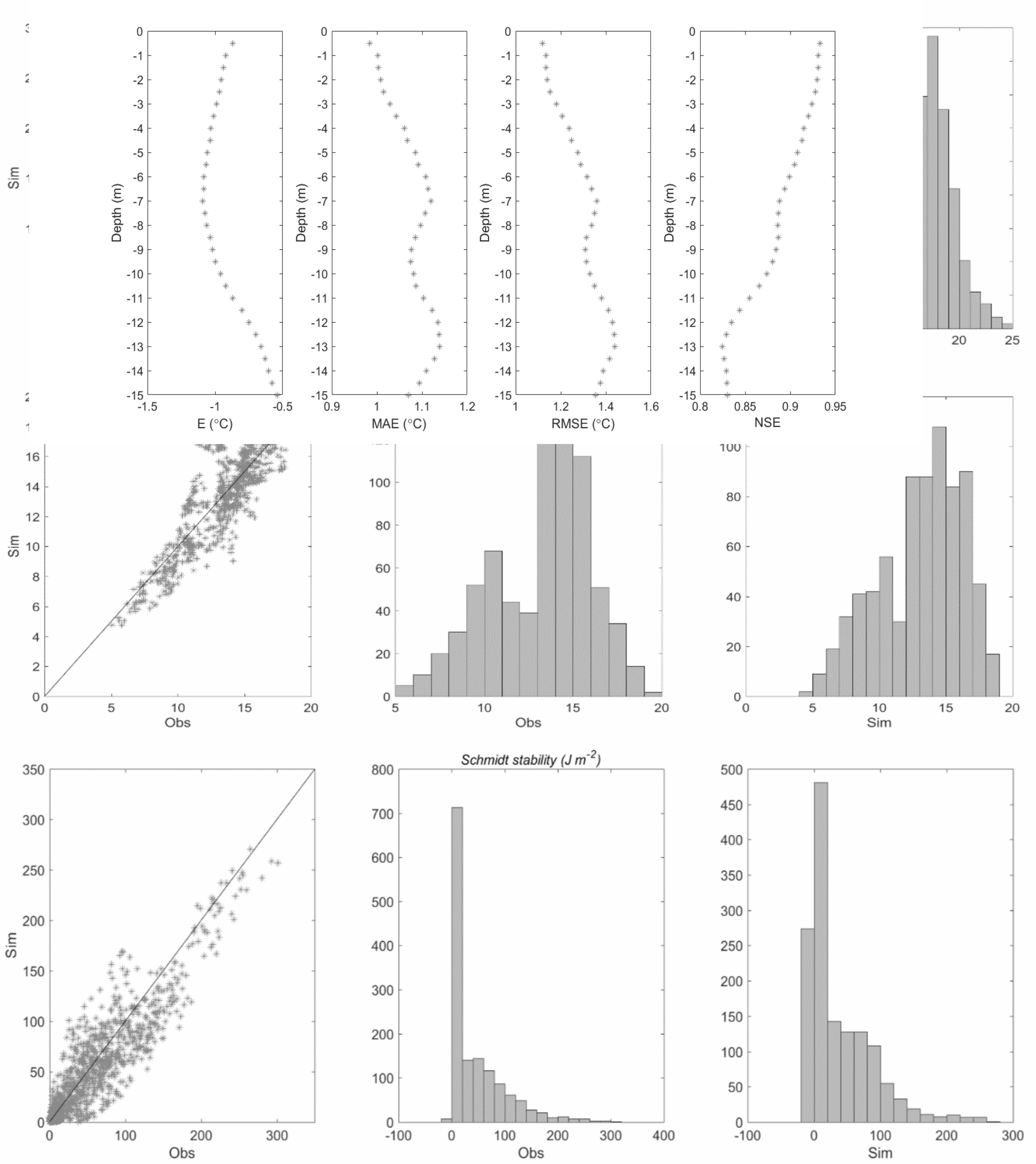
Depth (m)
E (°C)
MAE (°C)
RMSE (°C)
NSE
Sim
Obs
Schmidt stability (J m-2)

Figure 2.1.3 Advanced visualization used to improve model calibration. Measures of model fit or error calculated used simulated and measured water temperature data from 0.5 m vertical intervals

2) Running future climate scenarios. Using the final calibrated model, future climate scenarios are simulated by forcing the model with meteorological variables provided in the future climate scenarios. Specifically for Lake Erken, and for the ISIMIP lake sector simulations in general, it is the ISIMIP experiment 2B simulations(Frieler 2006) that are being used, as described in the ISIMIP 2B protocol (https://www.isimip.org/protocol/#isimip2b) There are four GCM models (**Figure 2.1.4**) obtained from the CMIP5 data archive (https://esgf-node.llnl.gov/projects/cmip5/) For use in the ISIMIP these have been consistently bias corrected based on comparison of GCM output during the historical period with gridded meteorological data from the European Centre for Medium-Range Weather Forecasts (ECMWF), and the Climate Research Unit TS2.1 dataset (Hempel 2013)

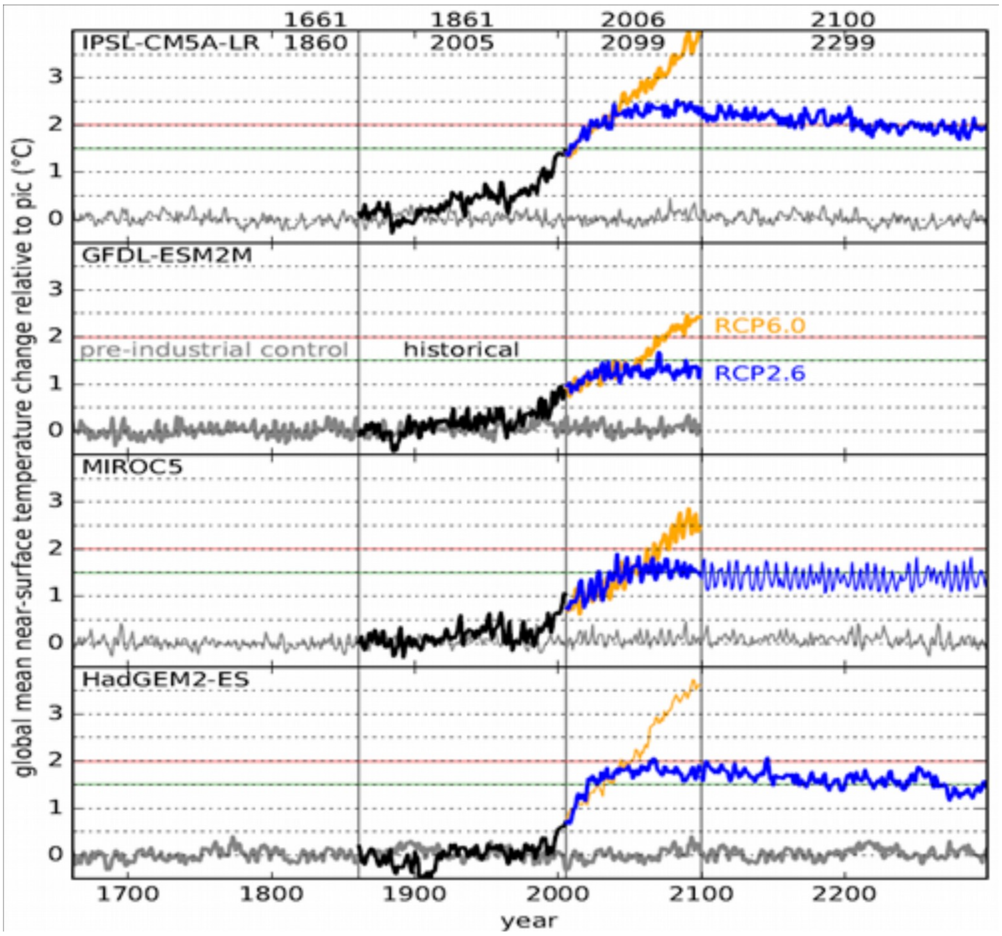

Figure 2.1.4 Illustration of the 16 scenarios that are available for four GCMs in the ISIMIP phase 2b project. Light grey is a long-term pre-industrial control scenario where

atmospheric CO2 is held at pre-industrial levels. Black shows scenarios based on historically measured CO2 concentrations. Blue (RCP 2.6) is an optimistic future climate scenario where reduced carbon emissions leads to an approximately 1.5 degree increase in global surface temperature as specified in the COP 21 Paris agreement. The orange (RCP 6.0) is shows a more moderate less optimistic scenario.

For each bias corrected GCM the ISIMIP provides data sets representative of four different emission scenarios (Fig. 2.1.4) These include the necessary data (air temperature, surface pressure, humidity, wind speed, and solar radiation) needed to force the GOTM model, except for cloud cover, which can be estimated from short wave radiation using the method of Martin&McCutcheon (1999). Over all, there are 1372 years of daily time step simulations that are run for each GCM. Consequently there was a need to develop effective methods for post processing and visualizing these data. A summary showing the average thermal structure of Lake Erken for each of the different scenarios of the ISPL model is shown in **Figure 2.1.5**, but to more precisely quantify the simulated changes in lake thermal structure the daily temperature profiles associated with each combination of GCM and emission scenario were processed with the program Lake Analyzer (Read et al. 2011) to obtain additional metrics of thermal stratification such as the Schmitt stability, thermocline depth and the duration of the stratified period. Outputs based on the simulated temperature profiles and the Lake Analyzer derived metrics are presented in summary figures that evaluate the mean response for a scenario and probabilistic differences between scenarios (**Figure 2.1.6**) There are clear shifts in the distributions of these parameter, which illustrates that under future conditions surface water temperatures will be warmer, the duration of thermal stratification will be longer, and the vertical gradient in temperature will greater leading to more stable stratification.

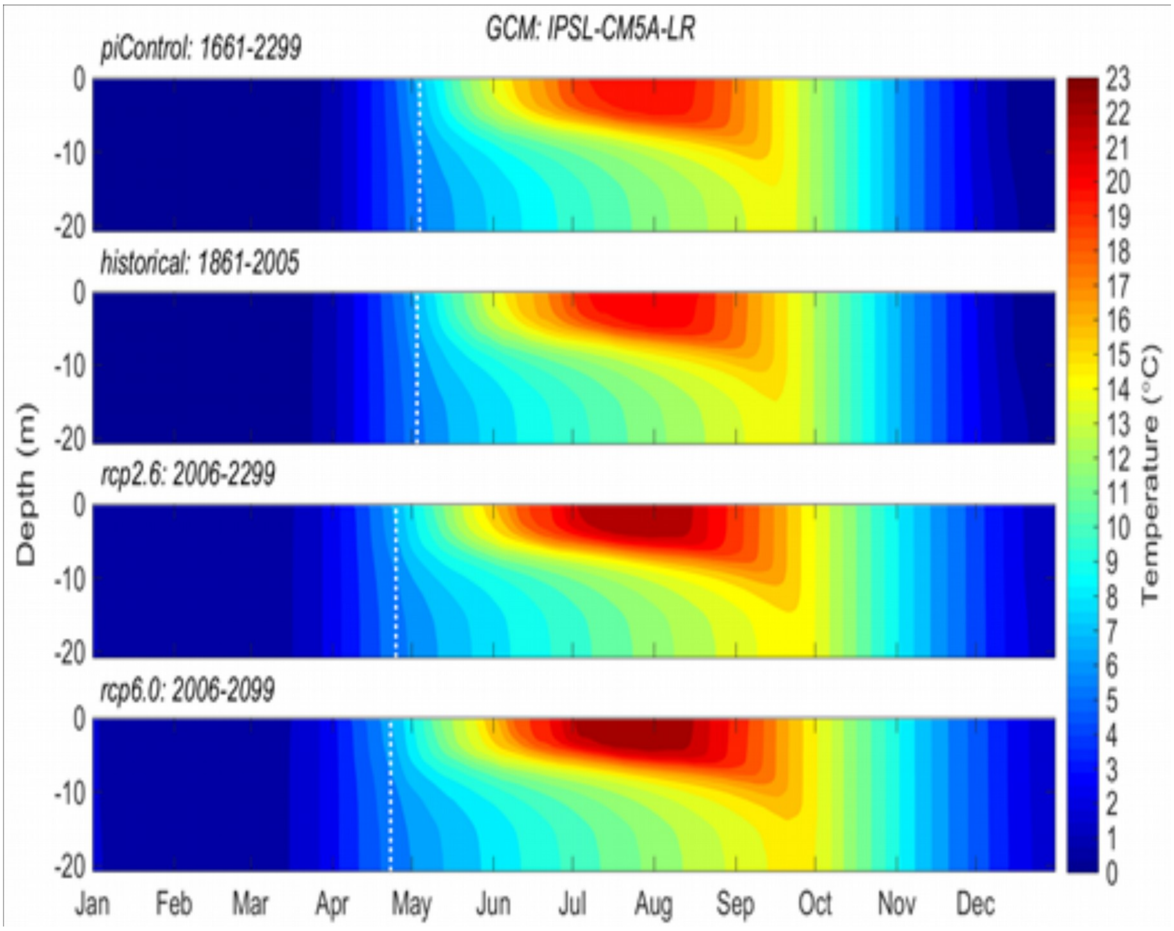

Figure 2.1.5 Illustration of the average changes in Lake Erken thermal structure that would be expected in each of the four emission scenarios for the IPSL GCM. The colored isopleth plots are based on 365 daily temperature profiles that are the average of all years in each scenario. The white dashed line shows the onset of thermal stratification.

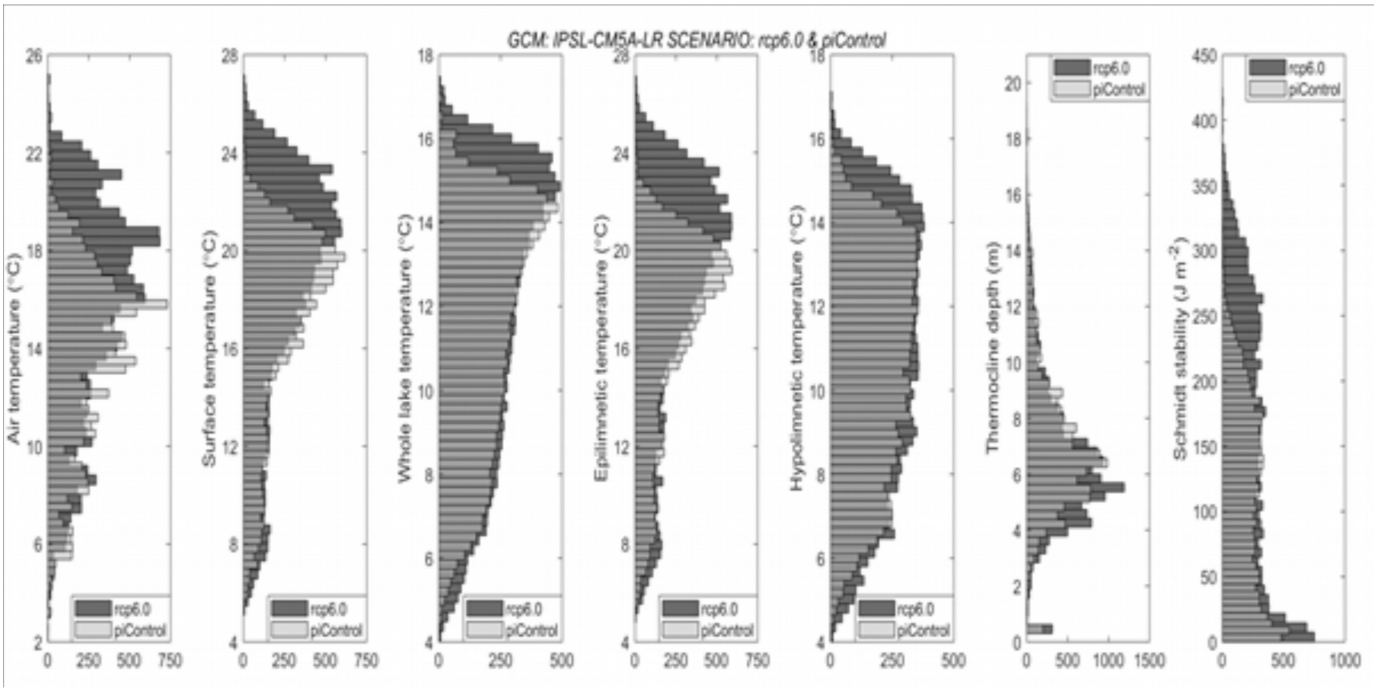

Figure 2.1.6 comparison of the frequency distributions of daily metrics of lake thermal structure for the PI control (grey) and RCP 6.0 (black) emission scenarios of the IPSL GCM simulations. These distributions include all days of the RCP 6.0 scenario and an equal number of days from the PI control scenario. There are clear shifts in the magnitude and distribution of these metrics of lake thermal structure under future climate conditions.

2.2 Modeling workflow for Spanish site: Sau Reservoir and its catchment

The Spanish target system is the Sau Reservoir (capacity of 165 km^3 with a mean inflow of 10 m^3/s), which is a recreational and water supply system for the Barcelona metropolitan area (ca. 3 million people), and the Ter river watershed which has an area of 1680 km^2 as the main source of water for the reservoir. This particular watershed and lake were selected because there is an increasing interest, from the management stakeholders and the communities that depends on the water supply, to provide seasonal predictions of water flows into and water quality of the reservoir.

The Spanish end-user is the ATLL Concessionària de la Generalitat de Catalunya, which is the water supply company for Barcelona and the main user of the water stored in the Sau Reservoir. This end-user is interested in a model based solution, which can readily be used as an aid to decision making and water management. Through developer/enduser interactions, the Spanish partners have agreed on a modeling solution comprising of the mHM (mesoscale Hydrologic Model) for describing the catchment dynamics, including water discharge to Sau Reservoir, and GOTM (General Ocean Turbulence Model) for describing the dynamics within the lake. These two impact models are being forced by S4 forecast system by the European Centre for Medium-Range Weather Forecasts (ECMWF). More details about linking seasonal forecasting data and impact models, model calibration procedures and initialization of the workflow can be found in deliverables 2.2, 2.3 and 3.1.

2.2.1 Results of applying seasonal forecasting on hydrologic model: Ter River

The hydrologic model was run using the seasonal climate forecast system considered here (System 4) provided by the European Centre for Medium-Range Weather Forecasts (ECMWF:) as the forcing meteorological data. The model was previously calibrated and validated using observational data, EWEMBI in this case, more information is presented in Deliverable 2.1. Using this parametrization, reinitialization runnings were implemented to run the hydrological model using System 4: the model was warmed up with 7 previous years using EWEMBI (observations), then a 4 month long simulation was run driven by System 4 forecast data for each initialization (e.g. February for spring), where the last 3 months correspond to the target season, more information can is presented in Deliverable 2.2. This was implemented with the aim of analyzing the discharge response of the Ter River when forced by a seasonal forecast system. Figure 2.2.1a shows the resulting time series of discharge when forced by observational meteorological data (EWEMBI) and seasonal forecast data (System4) for 2003, it shows and underestimation when forced by System4.

This is supported by the cumulative discharge for the same year (2003) showed in Figure 2.2.1b. The Figure 2.2.2 shows the resulting tercile plots from the runnings, some skill is obtained for the Ter River discharge resulting from the hydrological model in Summer for the normal category.

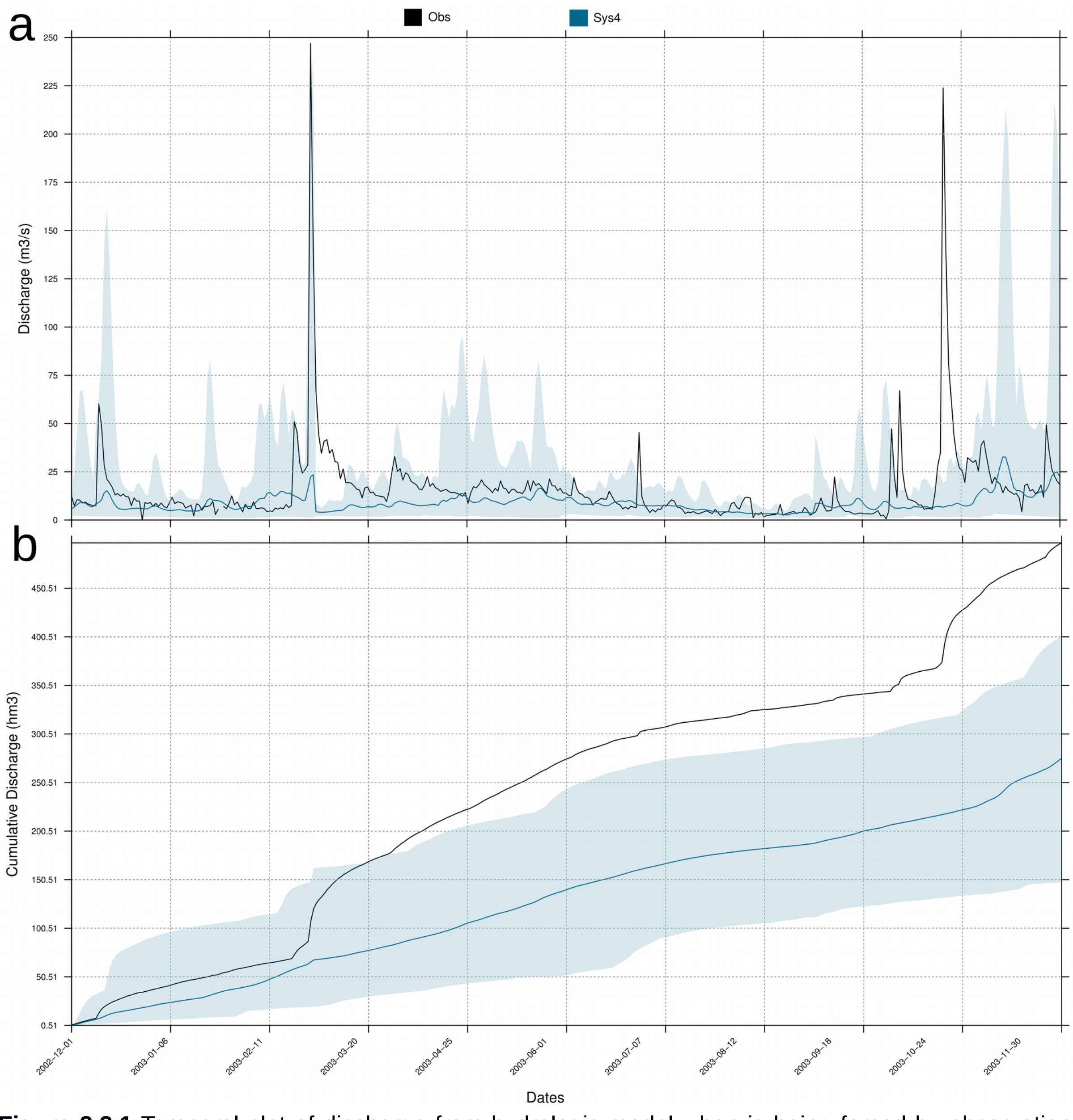

Figure 2.2.1 Temporal plot of discharge from hydrologic model when is being forced by observation (EWEMBI, black line) and system forecast data (System4, blue lines) as meteorological input. The shaded lines represent each of the 15 members from System4 while the solid line represent the average of these members. The dates are reduced (1986-2009) respect the original System4 dates (1980-2009) due to the warm-up period required in the hydrologic model.

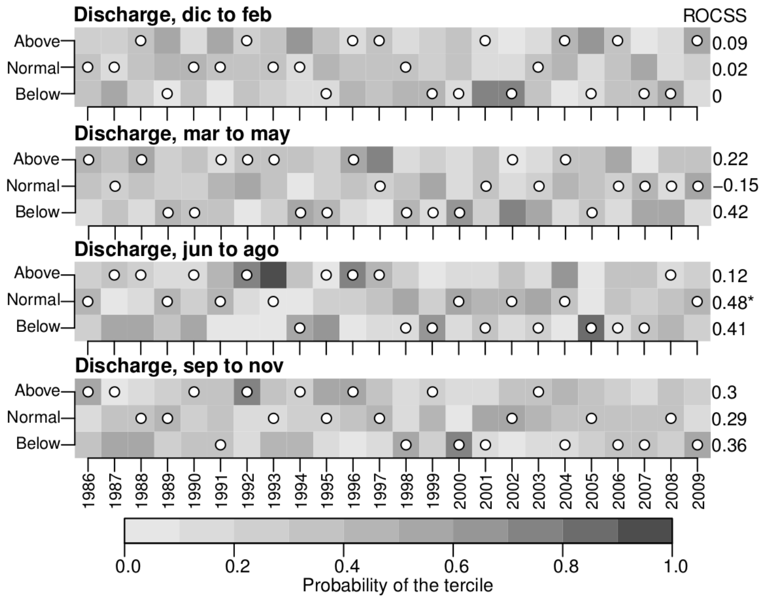

Figure 2.2.2 Tercile plot of discharge for hydrologic model implemented in Ter River. The grayscale shows the probability of each tercile given by the ratio between the number of members of System4 falling in each tercile and the total number of members. White dots show, for each year, the observed tercile when using EWEMBI. The asterisk indicates statistically significant ROCSS values.

2.2.2 Results of applying seasonal forecasting on lake model: Sau Reservoir

The GOTM lake model was run using meteorological inputs from the System4 seasonal forecasts. This was implemented with the aim of analyzing the response of the Sau Reservoir when forced by a seasonal forecast system. There are several key-variables that are of interest to the end-user, such as temperature, organic matter, chlorophyll and oxygen. However, only temperature data are shown here since as this time the model is only calibrated for this variable. Simulations are under development to add the additional key-variables. The resulting time series of water temperature at 1, 30 and 50m depth when forced by observational meteorological data (EWEMBI) and seasonal forecast data (System4) are shown in Figure 2.2.3, in general, the temperature is overestimated near the surface when using System 4, this estimation is improved when going deeper. This is supported by the increasing skill in the terciles when going from 1m to 50m depths as is shown by tercile plots in Figure 2.2.4.

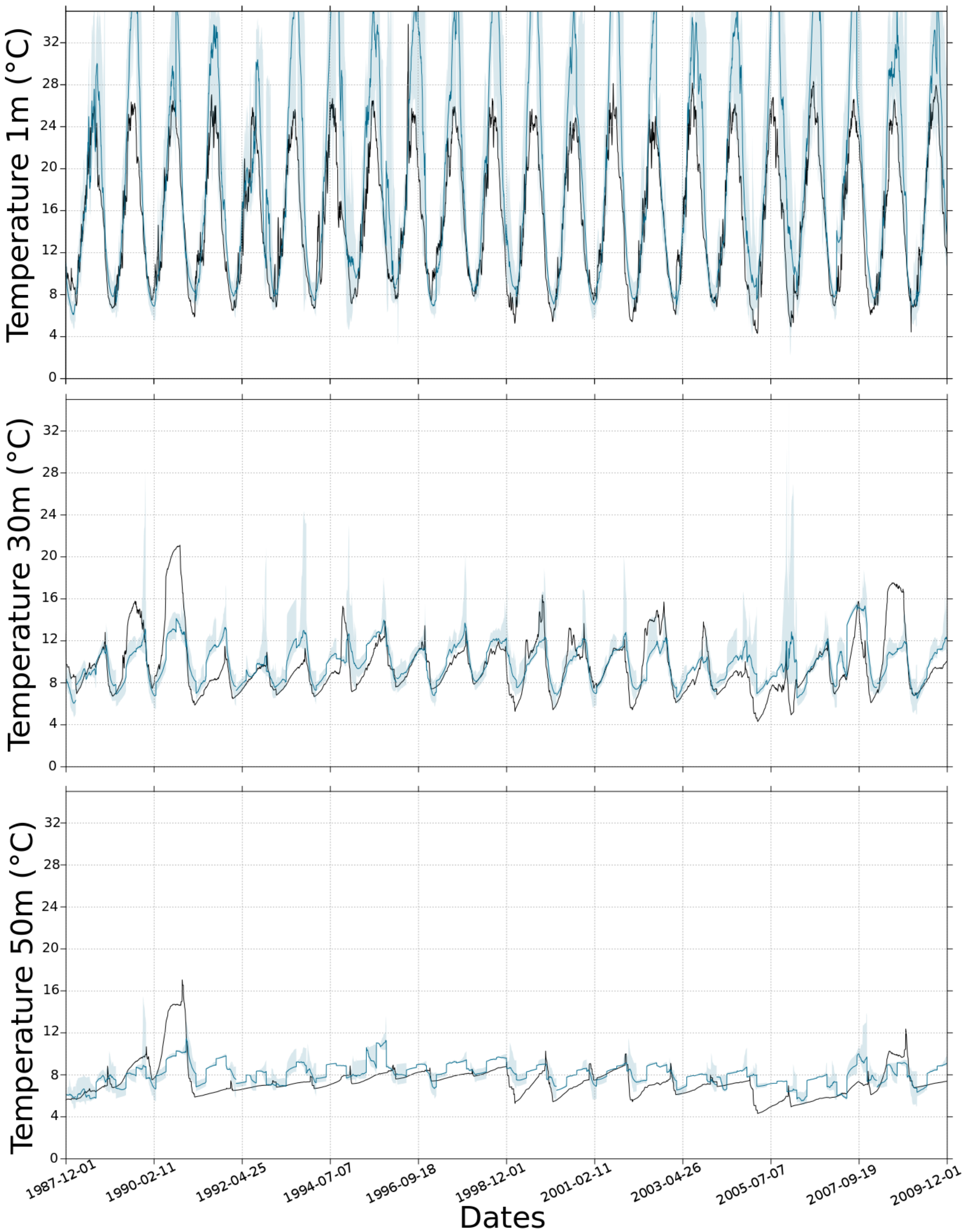
Temperature 1m (°C)
Temperature 30m (°C)
Temperature 50m (°C)
0
4
8
12
16
20
24
28
32
1987-12-01
1990-02-11
1992-04-25
1994-07-07
1996-09-18
1998-12-01
2001-02-11
2003-04-26
2005-07-07
2007-09-19
2009-12-01
Dates

Figure 2.2.3 Temporal plot of temperature at 1, 30 and 50 m depth from the lake model when is being forced by observation (EWEMBI, black line) and system forecast data (System4, blue lines) as meteorological input. The shaded lines represent each of the 15 members from System4 while the solid line represent the average of these members. The dates are reduced (1987-2009) respect the original System4 dates (1980-2009) due to the warm-up period required in the hydrologic and lake models.

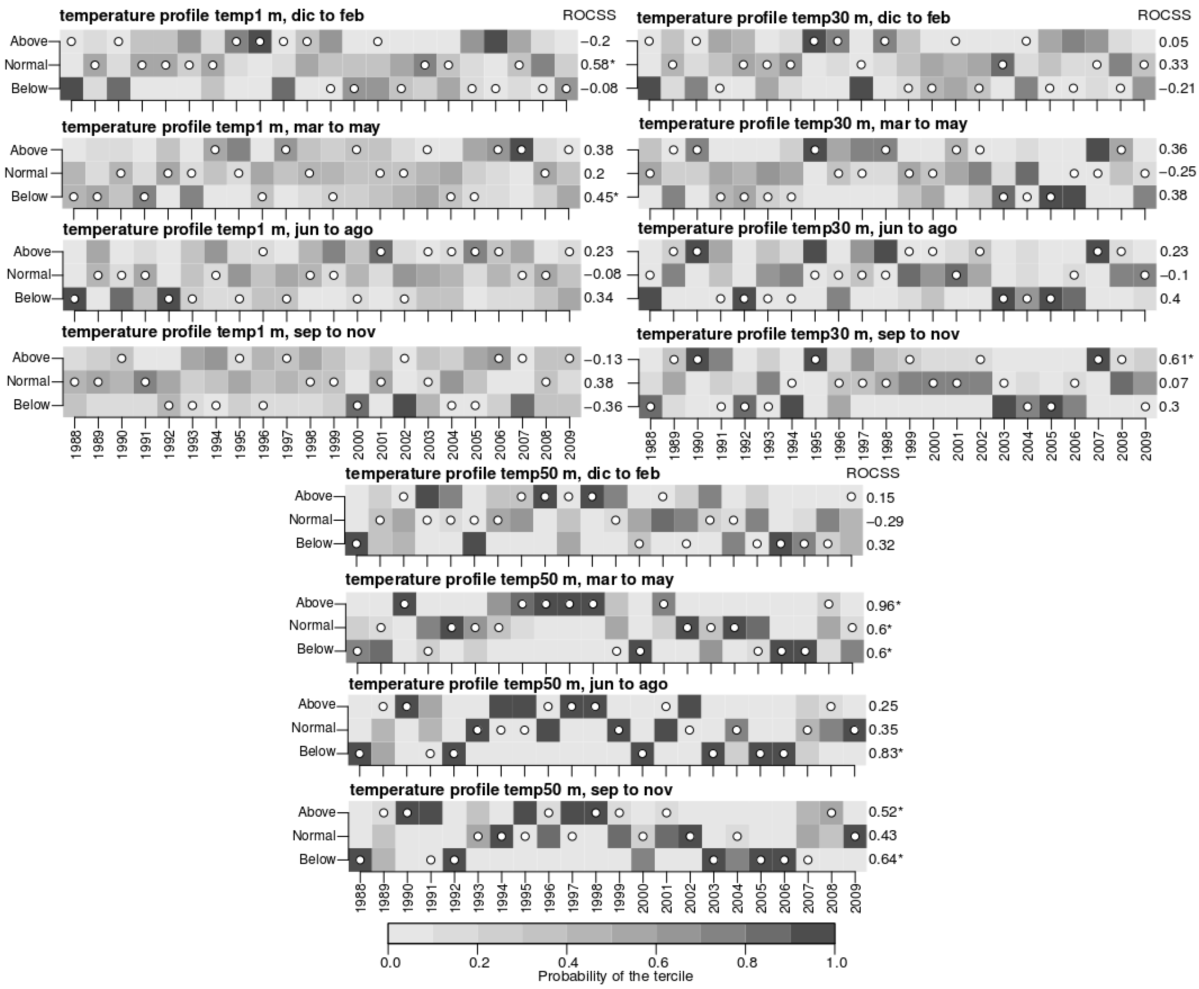

Figure 2.2.4 Tercile plot of temperature at 1, 30 and 50m depth for lake model implemented in Sau Reservoir. The grayscale shows the probability of each tercile given by the ratio between the number of members of System4 falling in each tercile and the total number of members. White dots show, for each year, the observed tercile when using EWEMBI. The asterisk indicates statistically significant ROCSS values.

2.3 Modeling workflow for Danish site: Lake Arreskov and its catchment

The Danish study site represent a typical Danish, shallow, eutrophic lake, namely, Lake Arreskov and its catchment (Nielsen et al. 2014). The lake is situated in the upper parts of the catchment to the Odense Fjord estuary. The Danish end-user is the Danish Ministry for the Environment (MFE), and key challenges, which they would like WATExR solutions to address include compliance with the EU Water Framework Directive (WFD) with focus on phytoplankton and the proportion of blue-green algae, fish and the proportion of piscivorous fish, and the abundance of submerged vegetation.

The MFE has a key interest in an impact model solution, which can readily be adapted to other lakes in Denmark, so that it can potentially be applied much more widely for water management planning (and not only for the study case in WATExR). The chosen modelling workflow in WATExR include the SWAT model (Soil and Water Assessment Tool) for describing the catchment dynamics, including water discharge and nutrient loads to Lake Arreskov, and the WET model (Water Ecosystems Tool) for describing the ecosystem dynamics within the lake. The SWAT model has already been implemented in a detailed, open source, QGIS plugin, which allows new model set ups, execution of the model, and a range of output visualizations (https://swat.tamu.edu). As part of WATExR, WET has now also been implemented in a QGIS plugin, which allow a lake model to read stream output directly from a SWAT model run, and use that as inflow to WET.

The SWAT model was initially set up and calibrated for the Lake Arreskov catchment based on gridded, observed, daily meteorological data provided by the Danish Meteorological Institute (DMI). SWAT simulated streamflow and nutrient transport (Fig. 2.3.1) were calibrated using SWATCUP, based on the SUFI2 auto-calibration routine, following a similar logic as that outlined in Deliverable 2.1.

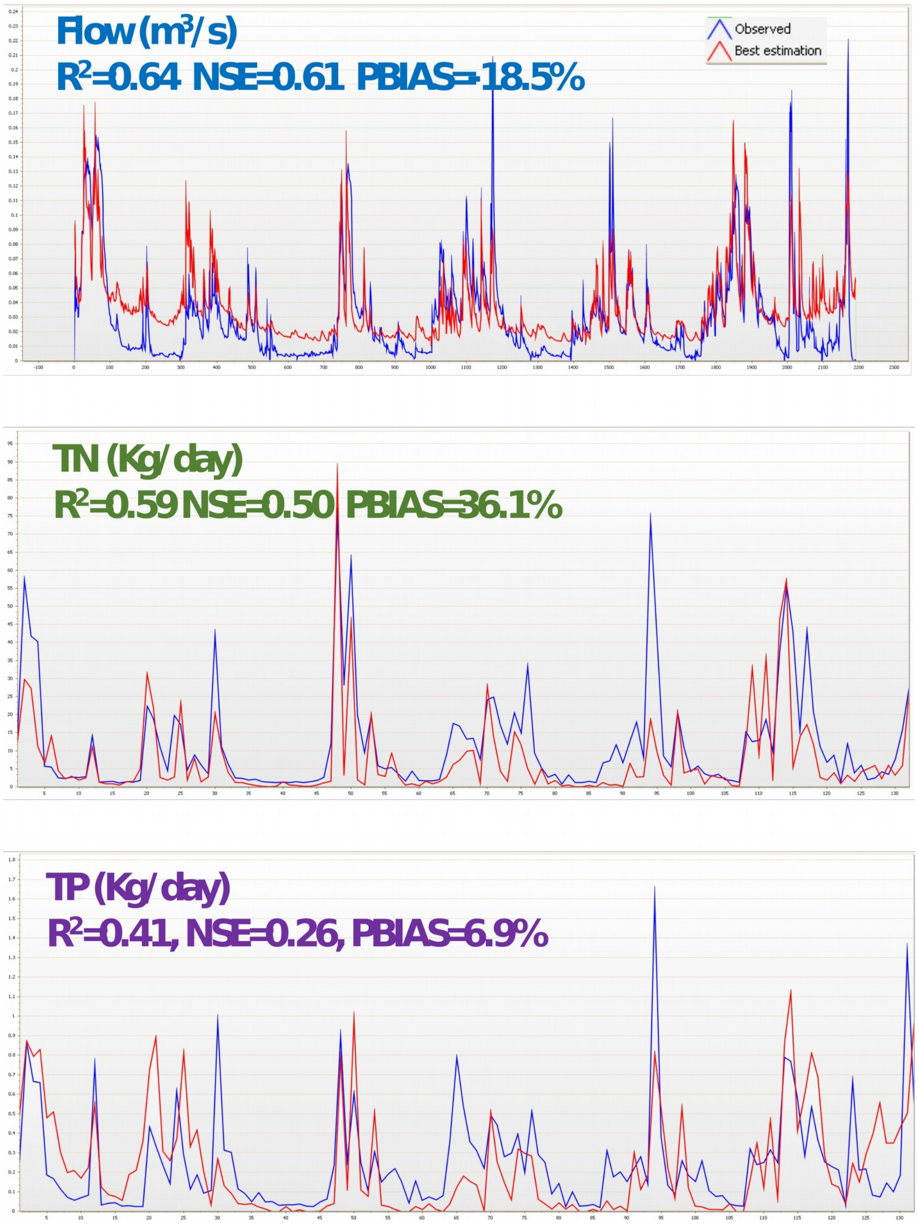

Figure 2.3.1 Example of calibration results for discharge and nutrient transport in the largest inflowing stream to Lake Arreskov.

The WET model has been set up based on the ERA-interim (subdaily) meteorological data provided by the European Center for Medium- and Short-term Weather Forecasts (ECMWF). Simulated dynamics of water temperature, oxygen, nutrients and phytoplankton is calibrated (Fig. 2.3.2) based on the semi-automatic ACPy routine, as outlined in Deliverable 2.1. At the time of writing this Deliverable, additional calibration (following also improvements to the core model code) is ongoing. The Danish team plan to continue improving the model core and model calibration throughout the lifetime of WATExR, thereby constantly also improving the basis for plausible seasonal predictions by the model.

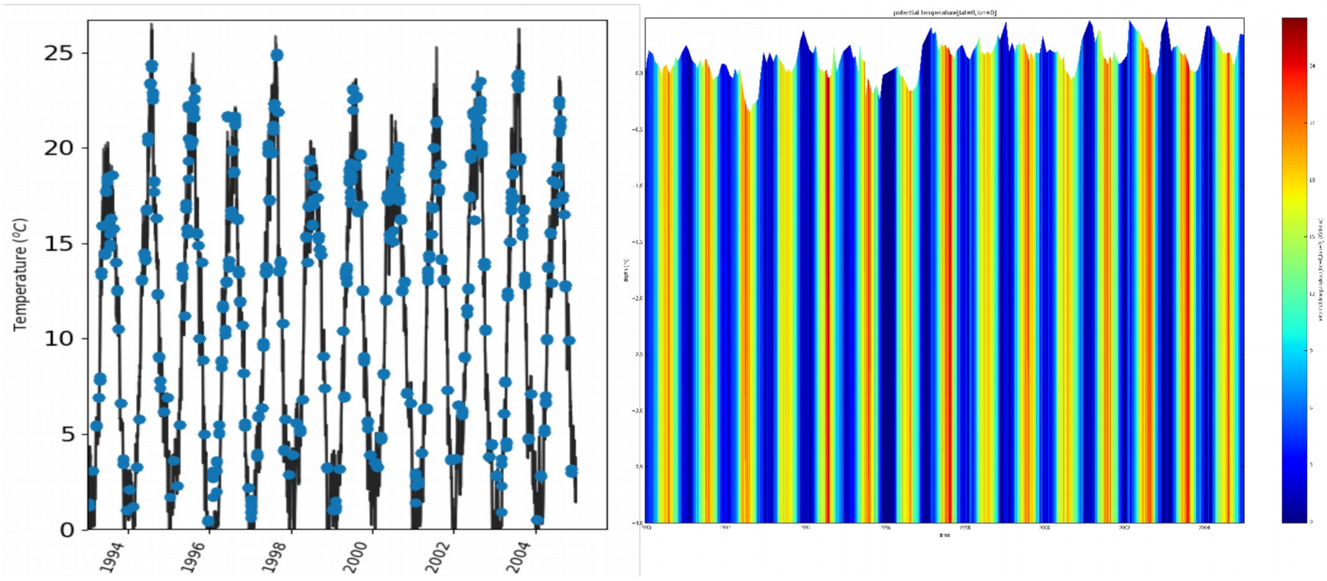

Figure 2.3.2 Example of calibration results for temperature in Lake Arreskov. Simulated (line) and observed (full circles) surface temperature in left panel, and complete temperature profiles (with variable water level), in right panel.

2.3.1 Results of applying seasonal forecasting for lake model

An example of a complete cycle of a seasonal prediction through the SWAT-WET model chain is presented in Deliverable 3.1. Here, the catchment and lake models are first "warmed-up" through a 10-year simulation, followed by a four month 15-member ensemble run for the seasonal prediction (**Figure 2.3.3**).

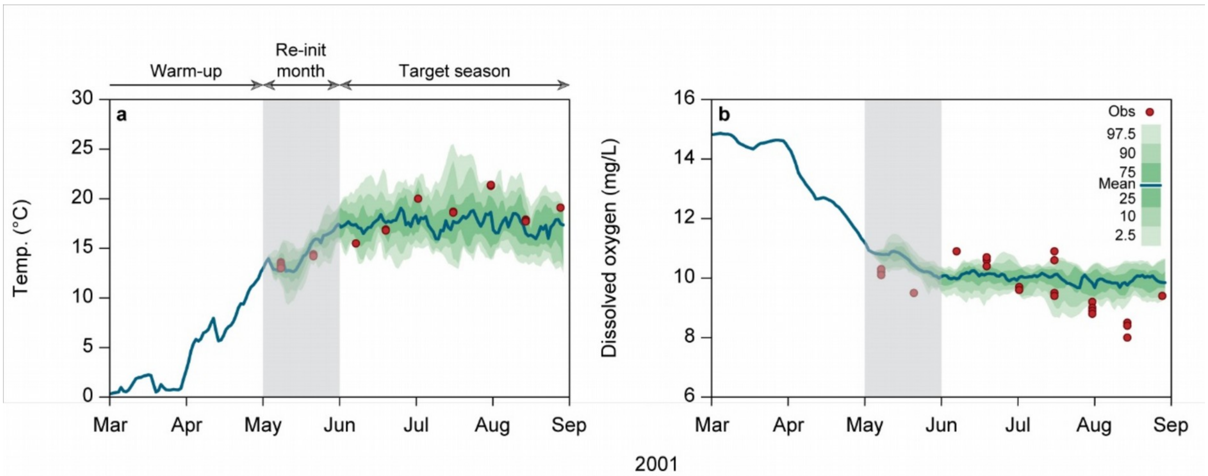

Figure 2.3.3 Example of a seasonal ensemble prediction through the model chain, here represented by lake surface temperature and oxygen (modified from Fig. 4 in Deliverable 3.1). Target period for the seasonal forecast example is Jun-Aug.

2.3.2 Key challenges to be addressed for Lake Arreskov and catchment

As the model cores of SWAT and WET continues to be improved, so may the reliability of their predictions. Ongoing work in relation to WET (in complementary research projects) include improvements to the macrophyte module, more “intelligent” fish dynamics (e.g. vertical movements), improvements to the model’s ability to represent subtropical and tropical systems, and inclusion of an explicit ice-module in the GOTM physical model (used by WET).

In addition to improvements to the conceptual catchment and lake models themselves, more reliable meteorological forcing data will likely also result in more reliable impact model predictions. A key challenge identified for Lake Arreskov, when testing the seasonal predictions, was the inadequate quality of the meteorological data used for the 10-year warmup period. The project team has experimented with both EWEMBI data and ERA-interim data, both of which exhibit considerably less precipitation than the observed data by DMI (around 400-500 mm/yr vs approx. 900 mm/yr in the DMI observations). As a result, we tried recalibrating the lake model based on inflow data derived from SWAT using ERA-interim precipitation, to produce potentially more reliable seasonal predictions (as presented in Deliverable 3.1). For the remainder of the WATExR project, the Danish team will try experimenting with the newer ERA5 reanalysis dataset by ECMWF, which will likely improve the model warmup, and potentially also the following seasonal prediction.

2.4 Modeling workflow for German site: Wupper reservoir and its catchment

The German target system is the Wupper reservoir and its catchment area, the Upper Wupper catchment. The upper Wupper catchment covers an area of 212 km^2 including upstream river flow that is regulated by a series of reservoirs. The reservoir is characterized as slightly eutrophic and dimictic, and its water level fluctuates widely. The reservoir has a maximum volume of 26 million m^3, an average depth of 11 meters and the maximum depth reaches 31 meters. The German stakeholder is the Wupperverband, the water board responsible for the management of water resources for the entire Wupper catchment.

The hydrological model used for simulating the upper Wupper catchment and the reservoir network is TALSIM-NG. This model includes a classical hydrological model coupled to a dynamic reservoir storage model and is therefore able to simulate discharge generation and reservoir management in a coherent framework. In our workflow, TALSIM is generating the inflow discharges into the Wupper Reservoir in response to meteorological drivers and the storage dynamics of the upstream reservoirs.

The lake model that was implemented is GLM (General Lake Model, see Hipsey et al 2018). This is a 1D hydrodynamic model simulating the thermal structures in lakes and reservoirs including the dynamics arising from inflows/outflows, surface energy fluxes, and hydrodynamics using a Lagrangian layer structure. In this Langrangian structure, the thickness and volume of each layer change dynamically during the runtime of the model as driven by inflows and depth-specific withdrawal.

Both TALSIM-NG and GLM were forced by ERA-Interim reanalysis data (https://www.ecmwf.int/en/forecasts/datasets/reanalysis-datasets/era-interim) and hindcast data of the forecasting system System 4 by the European Centre for Medium-Range Weather Forecasts (ECMWF) as meteorological input. The System 4 forecasting system consists of an ensemble with 15 members. The seasonal forecasting workflow focuses on the spring season from March until the end of May and documents the coupling of the two impact models to produce seasonal forecasts. The simulation period set for the hydrological model was 1998-2010 with a two-year warm-up period (1998-2000). The lake model was simulated for the time period 2000-2010 with a one-year warm-up period (2004-2005).

2.4.1. Results of applying seasonal hydrological forecasting: Wupper River

The hydrological model was forced with the ERA-Interim reanalysis data for the model warm-up period which provided the initial conditions for the seasonal forecasting scenarios for the 1st of March of each year. Later the model was forced every year with the 3-month seasonal forecasting scenarios (all 15 ensemble members) for spring. The resulted discharge time series from the model sub-catchments leading to the outlet on the Upper Wupper catchment were summed up and used as input for the lake model (inflow to the main dam). **Error: Reference source not found** compares the simulated discharge derived from the seasonal forecasts to the observed data from the water gauge Hückeswagen, which is located upstream of the main dam of the reservoir. More specifically, it shows the spread of the simulated discharge resulted for the 15 System 4 ensemble members, the ensemble mean and the measured discharge at the reference station.

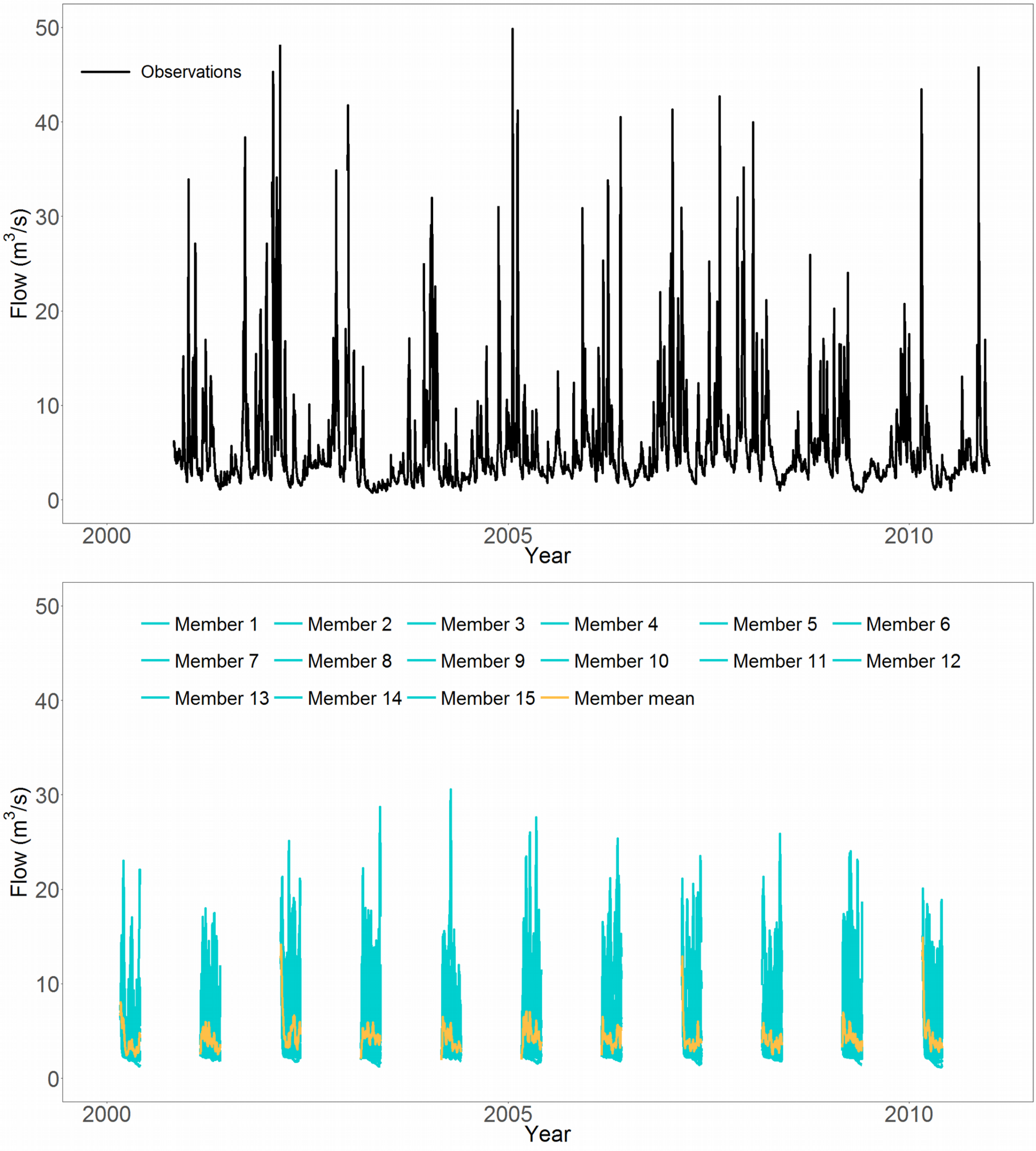

Figure 2.4.1 Simulated discharge (ensemble mean) and observed discharge at the inflow of Wupper reservoir

2.4.2 Results of seasonal forecast using the Wupper Reservoir lake model

Lake simulations will be carried out using GLM in order to fully simulate the hydrodynamics and stratification dynamics in the lake. For this deliverable, however, we concentrate on showing just the surface water temperatures although in all simulations the whole vertical temperature distributions were modelled. As a first step, the reservoir was simulated once for the entire time of 2004-2010, using the ERA-Interim reanalysis data of as meteorological forcing data. Figure **2.4.2** shows a scatter plot of the simulated surface temperature in Wupper reservoir using reanalysis data as meteorological input as well as the observed surface temperature for the days when measurements took place. The results indicate a good agreement between modelled and observed water temperature and give confidence in using the reanalysis data to drive the model for the warm-up period.

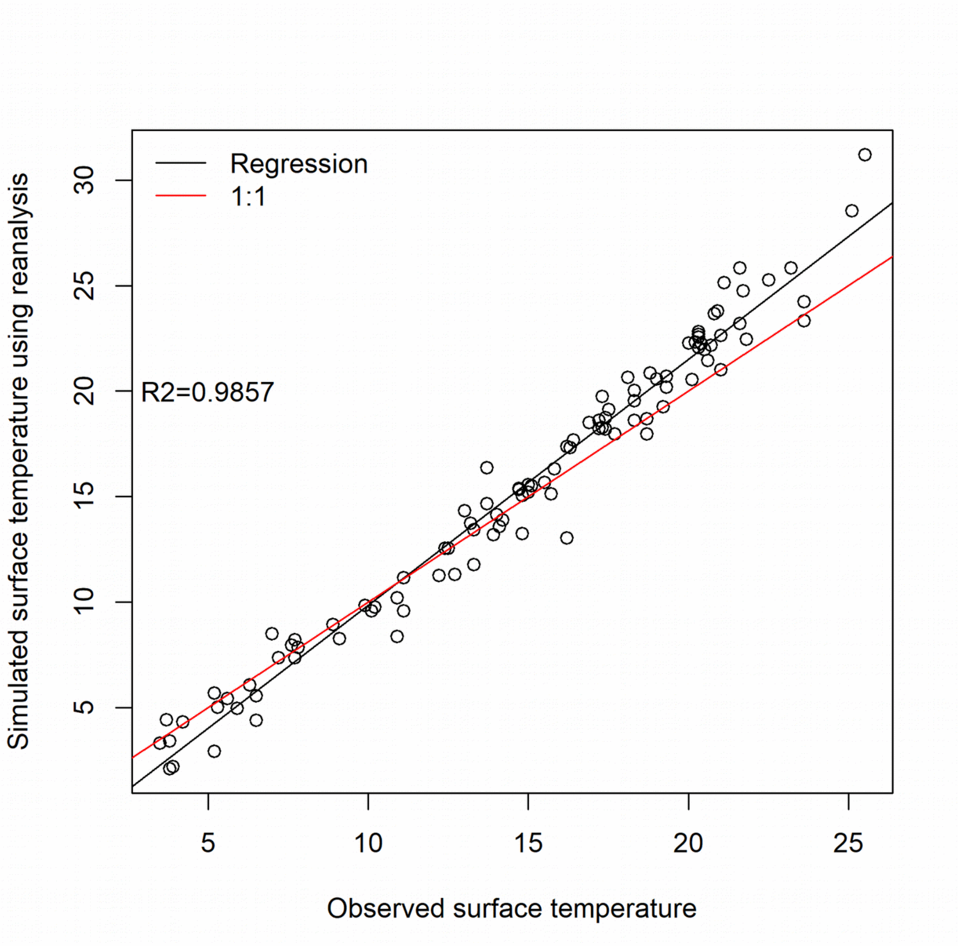

Figure 2.4.2 Scatter plot of surface water temperatures obtained by a simulation using reanalysis data as meteorological input and the observed surface water temperatures.

In a second step, the model was first driven by reanalysis data until the beginning of spring in each year as a spin-up period for the hydrodynamic model. Then the seasonal forecasts were used to provide the meteorological input data to GLM during the three months of the seasonal spring forecasts. During these seasonal forecast simulations, the predicted inflow discharges from TALSIM-NG for each ensemble member were simultaneously used as hydrological inputs to GLM. During other times of the year, the hydrological inputs to GLM was simply taken from the observed inflow dynamics

The GLM simulation requires inflow temperatures although measurements were not available for the entire time series. Therefore, a statistical model was developed to link the inflow temperatures to air temperature in order to create a continuous time series of inflow water temperatures. During spring, i.e. for the seasonal forecast simulations, this statistical model was used to generate inflow temperatures for each of the seasonal forecast ensemble member by using the air temperatures associated with them.

To produce the final spring seasonal forecasts therefore, required multiple levels of model simulation: hydrologic simulations of the reservoir inflow using the TALSIM-NG model; statistical estimation of inflow temperatures based of the seasonal forecast air temperature data; and finally GLM simulated hydrothermal simulations driven by the output of the first two simulation levels and the seasonal forecast meteorological variables. Due to this procedure, the seasonal forecast ensemble and its products were introduced to the model on multiple levels (i.e. as meteorological input and as inflow temperature input). With 7 years and 15 members of the seasonal forecast, simulations were run a total of 105 times to produce the ensemble of the surface temperature for the 15 members. In **Figure 2.4.3** the results are shown for the spring period seasonal forecasts for each year along the simulated surface temperature simulated over the entire year that were forced with the ERA-Interim reanalysis data.

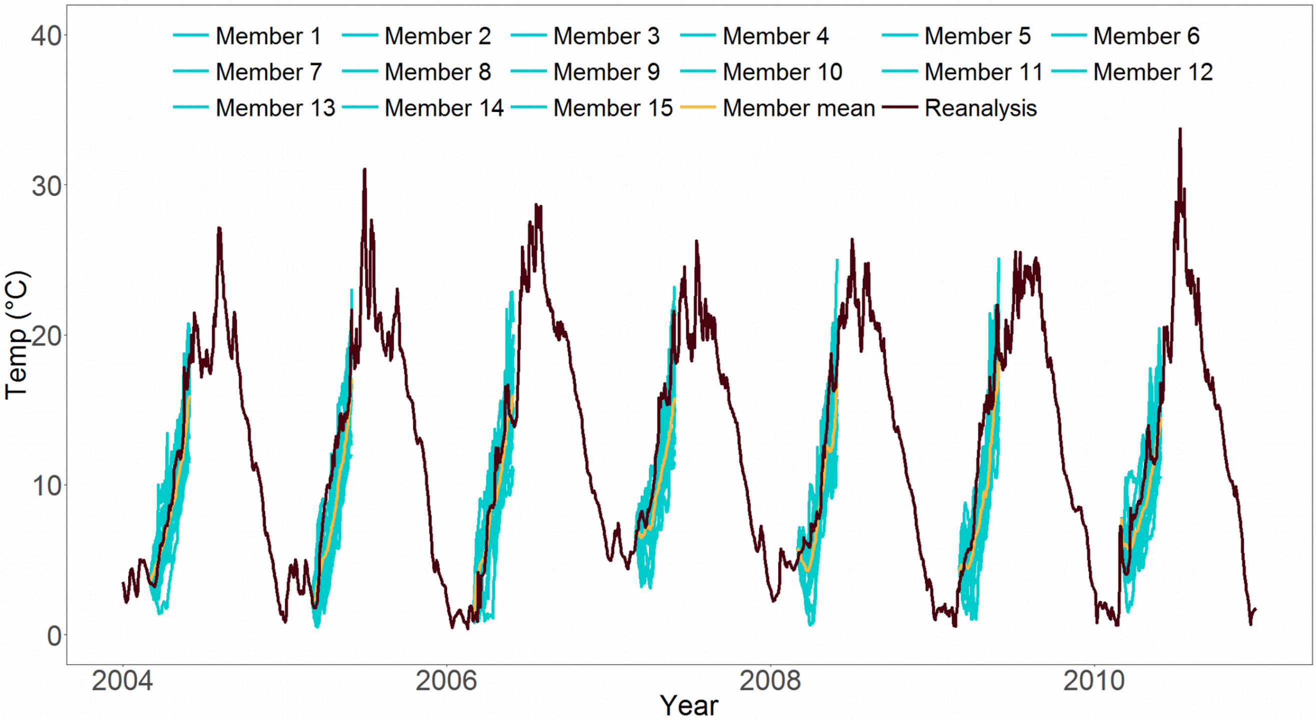

Figure 2.4.3: Simulated surface water temperatures in Wupper Reservoir using seasonal forecast in spring and reanalysis data at other times of the year.

In order to show the spread of the ensemble of the surface water temperatures and inherent variation within the seasonal forecasts we show model results beginning in the summer 2005 with spin-up simulations driven by the ERA-Interim reanalysis data and forecast simulatons driven by ECMWF System 4 seasonal forecasts until the spring 2006 in **Figure 2.4.4**. We also included observed surface water temperatures from Wupper Reservoir in order to show the performance of the seasonal forecasts. In conclusion, the ensemble mean of the seasonal forecasts gives a good approximation of the observed dynamics but the spread among the ensemble members appears to be rather large.

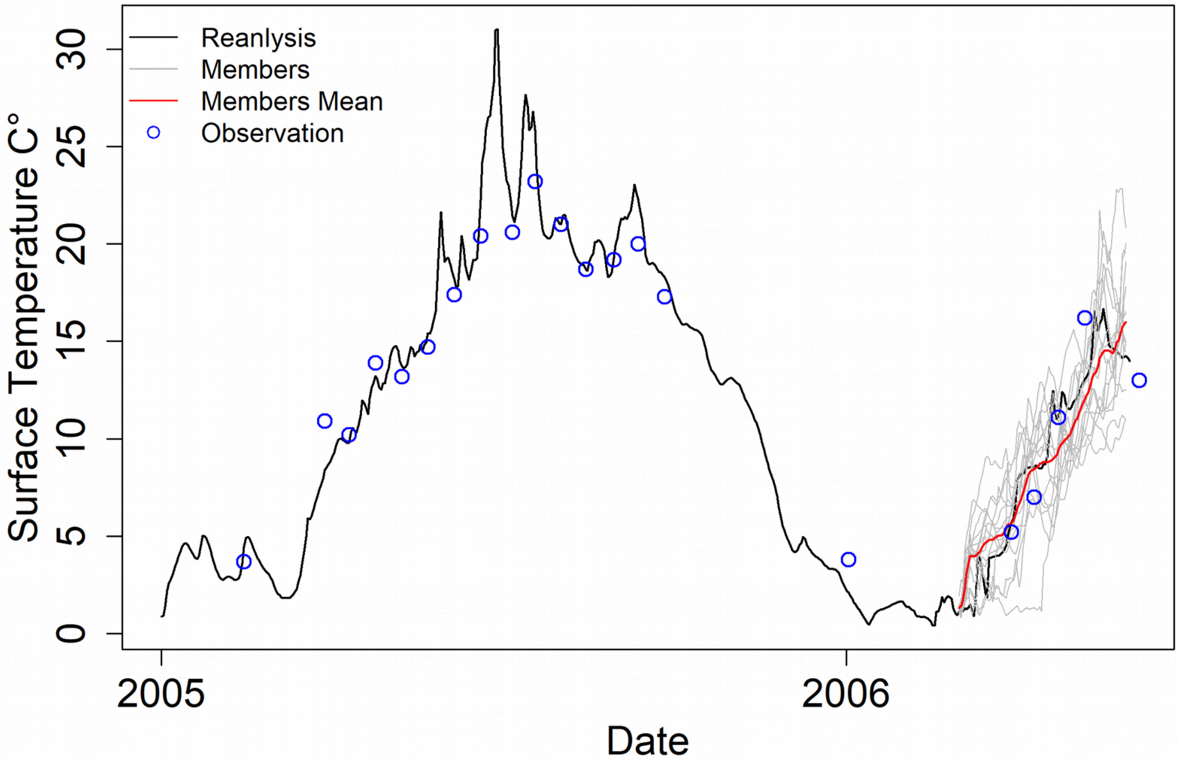

Figure 2.4.3: Simulated and observed surface water temperature in Wupper reservoir for the years 2005 and 2006.

2.5 Modeling workflow for Norwegian site: Lake Vansjø and its catchment

2.5.1 Study site and previous work in the catchment

Lake Vansjø lies in south-eastern Norway, in one of the most agricultural areas of the country. The Norwegian end-user is the Morsa river basin authority, who are responsible for EU Water Framework Directive (WFD) implementation in the catchment and wider area, and are a partnership organisation representing many interested parties in the catchment. The Morsa river basin authority are particularly interested in receiving early warning of seasons where there is a higher than usual risk of failing to meet good ecological status (under the Water Framework Directive), of poor bathing water quality, or of poor drinking water quality. Key variables which need to be forecasted to enable such predictions are in-lake phytoplankton abundances (chl-a, and in particular the abundance of potentially toxic cyanobacteria). Lake water colour is also of interest to the water company, and lake TP concentration may be required to predict WFD status.

Prior to WATExR, a coupled model workflow had been set up for the catchment/lake and used to simulate the target chemical and ecological variables under future scenarios of climate and land use change, e.g. as part of the EU FP7 REFRESH and MARS projects (Couture et al., 2018). This workflow of models consisted of:

> PERSiST (catchment hydrology) → INCA-P (catchment phosphorus) →
> MyLake (lake physics and chemistry) → Bayesian Belief Network
> (cyanobacteria, WFD status)

The first three models are relatively complex process-based/conceptual models, whilst the Bayesian Belief Network (BBN) is a statistical model. This modeling workflow provides a useful starting point for WATExR, but has a number of issues which reduce its applicability in an operational, open source seasonal forecasting tool. Key issues are over-complexity, with too much attention paid to processes which may not be so important when producing seasonal forecasts, and the use of proprietary software (Matlab and Netica). For the WATExR operational seasonal forecasting model, we therefore decided to remove the process-based models and replace them with an extended BBN, adding extra weather and chemistry nodes to the original Vansjø BBN. BBNs are probabilistic graphical models that represent a set of variables and their conditional dependencies. They are particularly suitable for combining various types of data and information, modelling ecological status classes, and incorporating uncertainty into predictions. A BBN therefore has the potential to be a very suitable tool for seasonal water quality forecasting.

2.5.2 Model adaptation for seasonal forecasting

To design the new, expanded BBN, we first needed to define the variables to include in the BBN, based on a statistical analysis of all variables which appear to be most strongly linked to the target variables. To do this, we first created a large number of potential explanatory variables, based on measurements of both the water shed and lake biogeochemistry. This included variables such as discharge, precipitation, air temperature, lake chlorophyll and lake total phosphorus concentrations. We derived variables such as lags, sums and averages over the previous 1-3 months, winter sums or averages, averages from the previous summer, precipitation intensity, snow melt inputs, potential evapotranspiration, etc. For each of the target variables, we then used feature selection algorithms (regression tree analysis and recursive feature selection) to pick key features. This work is not yet complete, but a summary of key variables identified so far is provided in Table 2.5.1.

Table 2.5.1. Preliminary results of feature selection for the western basin (Vanemfjorden) of Lake Vansjø, to help in BBN design.

Target variable	Key features
Chl-a	Lake chl-a (previous month) Temperature (current month and previous month) Discharge (previous month) Chl-a (previous summer) Lake TP concentration
Cyanobacteria	Lake chl-a (current month) Lake colour (current month) Lake chl-a (previous summer) Cyanobacteria (previous summer) Chl-a (previous summer)
TP	Lake TP conc (previous month) Lake TP conc in upstream lake Lake TP conc (previous summer)

As a result of this analysis, a preliminary BBN structure has been constructed as shown in Fig. 2.4.1. The next stage is to populate the conditional probability tables which make up each node in the network using a combination of observed data and statistical techniques.

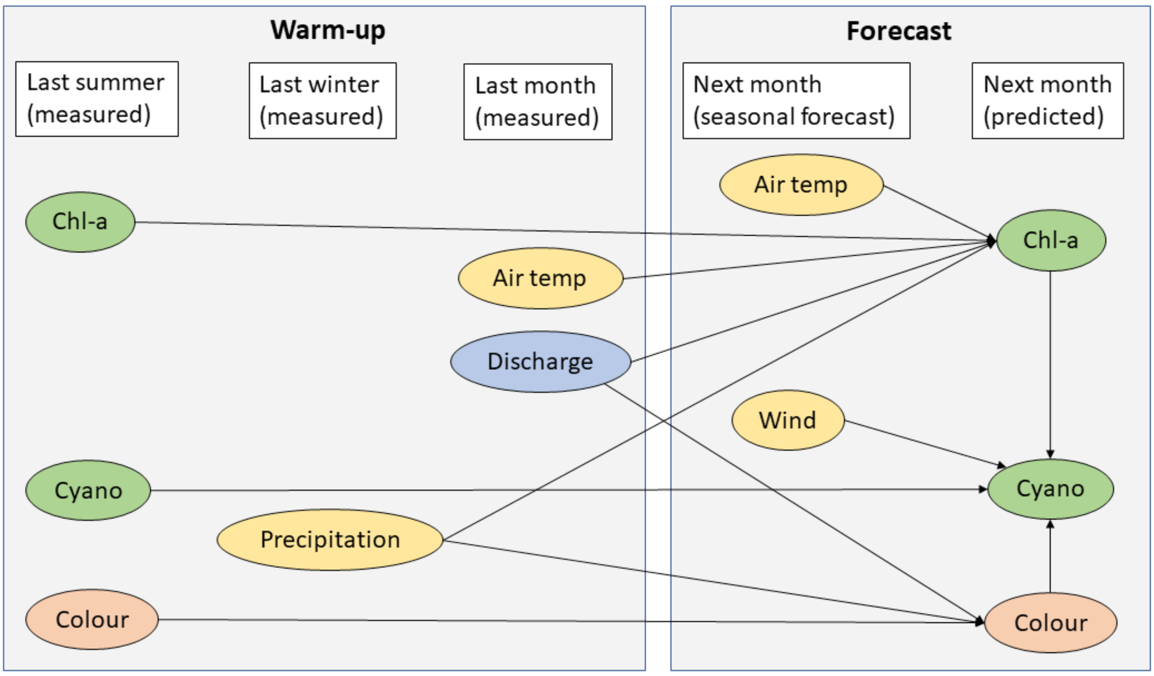

Figure. 2.5.1. Conceptual design of the Bayesian Belief Network which will form the core part of the seasonal forecasting workflow at the Norwegian site.

2.5.3 Model workflow

The workflow for seasonal water quality and ecology forecasting in the Lake Vansjø catchment will include:

1. Data preparation:
    a. Download meteorological data:
        i. Long-term meteorological observations (from met.no), and gridded reanalysis data (ERA-Interim for the hindcast experiment, ERA5 for the operational forecasting tool)
        ii. Seasonal forecasting data (System4/System5 to start with)
        iii. Bias correct reanalysis and seasonal forecast data using observed data
    b. Download other supporting water chemistry and ecology data
    c. Process data to produce chemical/biologically-relevant features (e.g. calculate winter precipitation sum, temperature and precipitation monthly/seasonal means and sums, and lagged versions, water chemistry and ecology in the previous summer, etc.)
2. BBN model: Model defined as described in Section 2.4.3, and updated as new observed data becomes available
3. Seasonal forecast: Simulate water chemistry and ecology by driving the BBN using features derived from the seasonal forecast projections

This model workflow is expected to work in operational forecasting mode. In addition, it will be used for a hindcast period, driving the model for every season and year in the period using:

- Observed data: to assess the skill of the BBN
- Hindcast seasonal forecast data: to assess the skill of the whole forecasting system, incorporating uncertainty in both the BBN and the seasonal weather forecast

2.5.4 Model comparison exercise

In the Norwegian case study site we will also explore model-related uncertainty in seasonal predictions. While the BBN will be the main model used in our operational forecast, we are also developing other models to produce seasonal forecasts, and we will compare results from the different modeling systems for the hindcast period. Additional models to be considered include:

1. A process-based modelling chain: SimplyP (catchment hydrology and phosphorus) – MyLake – BBN. This is similar to the pre-existing modelling chain, but replaces

PERSiST and INCA-P with SimplyP, a much simpler model which performs as well during calibration and validation (Table 2.5.2 and Fig. 2.5.2).

2. A pure data-based model. So far we have produced forecasts using Facebook's Prophet procedure with mixed results, but other machine learning algorithms will be explored.

Table 2.5.2. Model performance statistics for SimplyP during calibration and validation, and comparison to INCA-P.

Variable	**Calibration period** 11 yrs, 1979 to 1990	**Validation period** 24 yrs, 1990 to 2014	**Whole period*** 32 yrs, 1982 to 2014	
			SimplyP	**INCA-P**
Discharge	0.61	0.66	0.66	0.66
Suspended sediment	0.1	0.19	0.14	0.34
Total phosphorus	0.14	0.17	0.17	-2.1

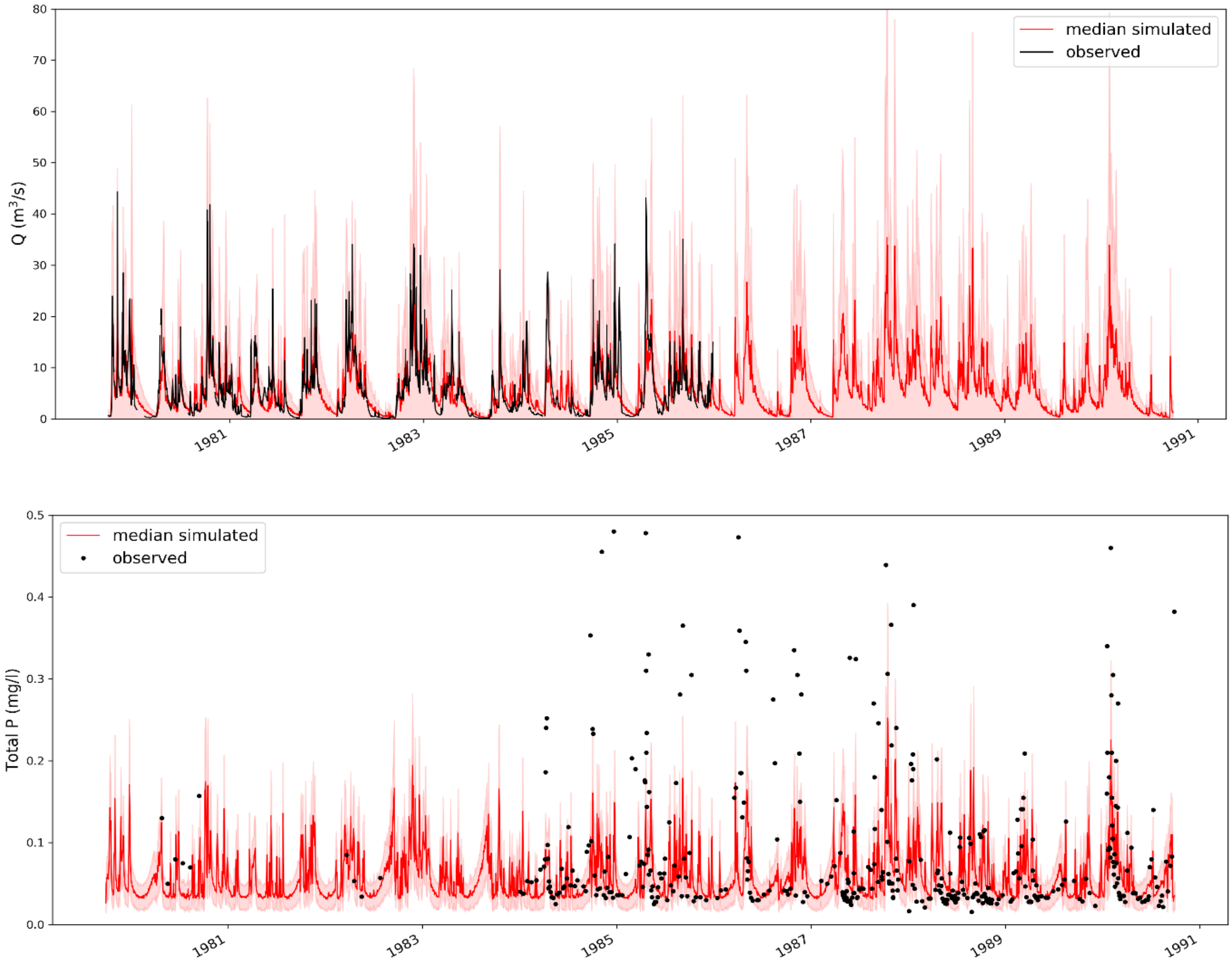

Figure. 2.5.2. Simulated discharge (upper) and total phosphorus concentrations (lower) in the Hobølelva river at Kure for the calibration period. Light pink band marks the uncertainty.

2.6 Modeling workflow for Irish site: Burrishoole catchment

2.6.1 Case study background

The Burrishoole catchment (~100km^2) drains into inner Clew Bay on the Atlantic west coast of Ireland. Fish traps between the marine and freshater habitats in this catchment enable a full census of the downstream and upstream movements of three diadromous fish species, Atlantic salmon (*Salmo salar*), European eel (*Anguilla anguilla*) and anadromous brown trout (*Salmo trutta*). This census has been carried out every day since 1970. Each of the three species exhibits a seasonal movement pattern, which is commonly termed “the run”; juvenile salmon and trout move downstream in spring, and maturing eels move downstream in autumn. The timing of downstream migration of diadromous fishes is related to local meteorology at a seasonal scale owing to each species’ necessity to undergo physiological and morphological preparation for marine survival. For example, juvenile Atlantic salmon undergo smoltification, whereby the time taken to smoltify is correlated with accumulated thermal units (degree days) in early spring (Zydlewski et al., 2005). Inter-annual variation in salmonid smolt run and eel run timings are of interest to the Marine Institute for practical purposes in terms of fish trap operation and research procedures such as tagging, which requires careful organization and an optimum number of staff to minimize stress to fish. Furthermore, the timing of migration is of interest to those managing hydroelectric infrastructure, owing to their obligation to ensure unimpeded passaged and avoid injuries and mortalities to migrating fishes.

2.6.2 End user requirements and research objectives

The case study stakeholder, the Marine Institute, Ireland, would like to understand the extent to which the seasonal migrations of diadromous fishes are predictable using seasonal meteorological forecasts. To this end, a three-step modelling procedure was required:

(i) Identify an appropriate method to quantify the migration phenology of Atlantic salmon (*Salmo salar*), European eel (*Anguilla anguilla*) and anadromous brown trout (*Salmo trutta*) from a daily count census.

(ii) Develop a model that predicts daily migration of diadromous fishes using daily census data and knowledge of each species' ecology in relation to local meteorology and other environmental factors.

(iii) Use seasonal forecast ensemble data to simulate daily migration counts of diadromous fishes, and, in so doing, illustrate the extent to which seasonal forecasting of fish migration phenology is practicable.

2.6.3 Workflow example for European eel

Quantifying fish migration phenology

The first objective of the workflow (and introductory panel of the QGIS plugin) is to provide the end user with definitions of anomalous migration phenology. In so doing, the end user will be able to interpret forecasts.

To estimate overall anomalies in fish migration phenology, we stratified each migration run into terciles, whereby the middle proportion (between the 33.3rd and 66.6th percentiles) of migrants are (on average) counted between two dates that delineate the "middle tercile". As such, 33.3% of migrating fish are counted by the end of the first tercile and 66.6% are counted by the start of the third tercile.

To quantify the average middle tercile, we first extracted the ordinal dates during which 33.3% and 66.6% of each run in the 1970 to 2017 time series had migrated and calculated their respective means. For each biological year, we then calculated the summed percentage of counts occuring before, after and within the average middle tercile and their means and 95% (Wald-type) confidence intervals. We then defined anomalous phenology for those years during which the percentage of counts occurring within each tercile fell outside the 95% confidence intervals of the averaged tercile percentages (**Figure 2.6.1**).

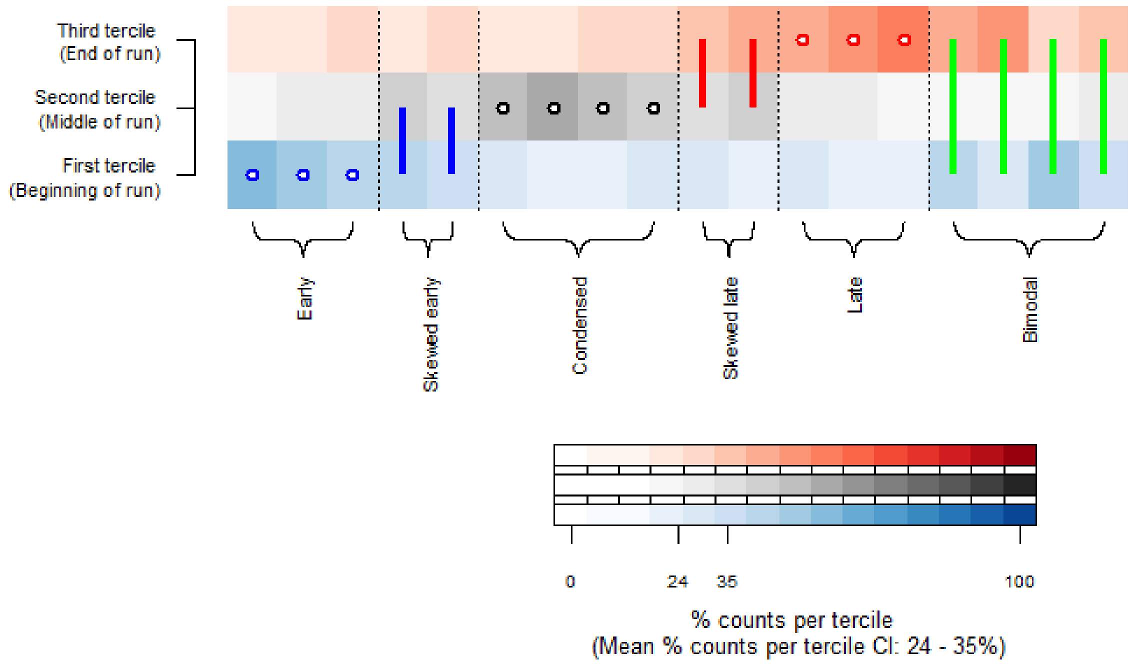

Figure 2.6.1. Schematic illustration of definitions of migration phenology anomalies. Each anomaly definition is represented in the schematic by between two and four examples. Note that the sum of count percentages per definition example adds up to 100%. For illustrative purposes, the 95% CIs for each tercile are identical (25 - 34%).

To provide the end user with a historical context, we provide an illustration of the complete daily census in terms of interannual variation in phenology (**Figure 2.6.2**).

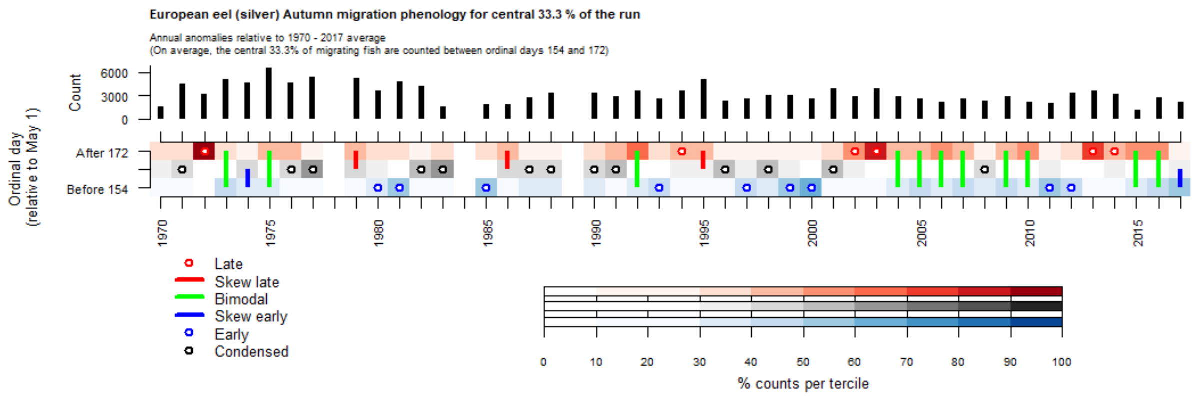

Figure 2.6.2. European eel migration phenology anomalies 1970 – 2017.

Development of a daily fish count model (using reanalysis meteorological data)

Modelling Europen eel migration timing is complex, owing to a variety of environmental factors acting at a range of temporal scales. During a migration run, the number of eels that migrate per day is associated with current environmental conditions such as moon illumination, rainfall and water temperature (i.e., the immediate "tolerability" of conditions for movement; (Sandlund et al., 2017)). Migration rates are also associated with seasonally quantifiable factors such as growing degree days (or declines in water temperature), which faciliate (or indeed trigger) physiological changes that prepare migrating cohorts for marine endurance. Daily counts of migrating eels are therefore primarily associated with environmental variation at two temporal scales. However, interannual variation in total numbers of freshwater "yellow" catchment resident eels that have the potential to achive physical size to ”silver” into silver eels and migrate adds a third (less easily quantifiable) factor into the mix.

We used a generalised linear mixed effects modelling approach to model daily counts for each "eel year" in the census. The GLMM approach allowed us to take into account variation at a range of temporal scales and was flexible enough to account for violations of statistical assumptions, such as overdispersion (Brooks et al., 2017). Eel years were defined in relation to water temperature thresholds related to growth (which is associated with pre-migration silvering (Daverat et al., 2012)) - in the interests of generalisability, this threshold may be manually altered by the end user in accordance with local knowledge.

We used reanalysis ERA interim meteorological data to calibrate our model, as these data are used for initialisations in seasonal forecast System 4; NOTE - we maintained flexibility in our modelling scripts to allow the end user to incorporate alternative data (e.g., ERA 5 and System 5) for re-calibration of the fish count model as and when new meteorological reanalysis and seasonal forecasts data become available.

Statistical validation

We validated our model(s) (statistically) by visually inspecting residual plots and autocorrelation function plots as per the DHARMa R package (Hartig, 2019) (see

Figure 2.6.3 for an example model diagnostic plot related to a special case of residual overdispersion: zero-inflation).

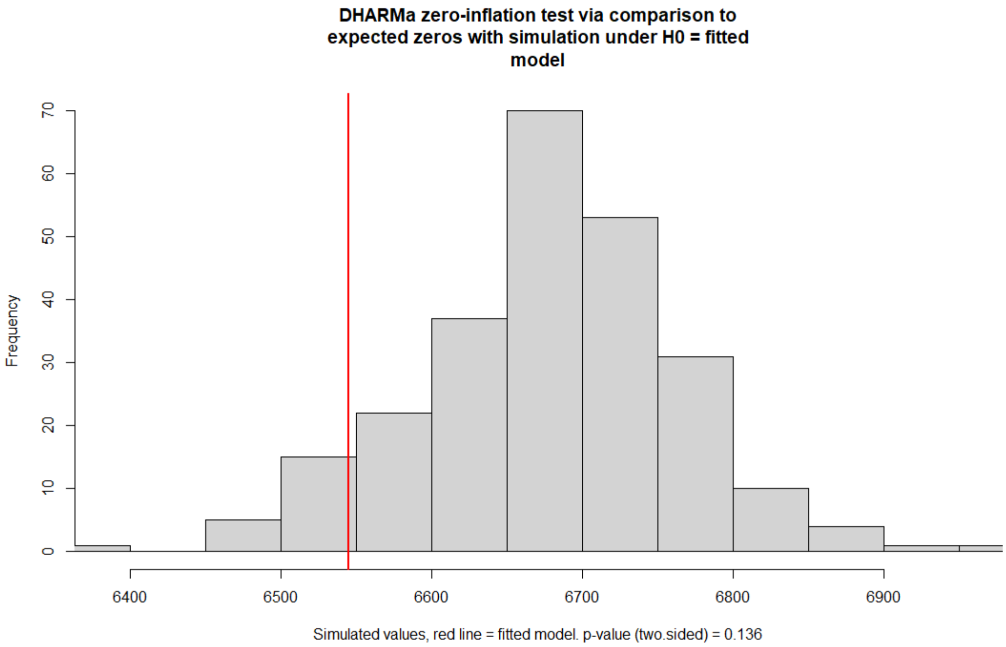

Figure 2.6.3. Example model diagnostic plot illustrating non-significant difference in number of zeros predicted by the model and number of zeros observed in the resampled model training dataset.

Model prediction efficacy

Following model statistical validation, we explored model prediction efficacy – the ability of our specified models to accurately predict daily migration counts for ”forward” held-out data. In so doing, we aimed to explore prediction efficacy under ”operational conditions”. We plotted observed vs predicted counts along a time axis along with 95% bootstrapped (percentile) confidence intervals to illustrate stochastic uncertainty (**Figure 2.6.4**).

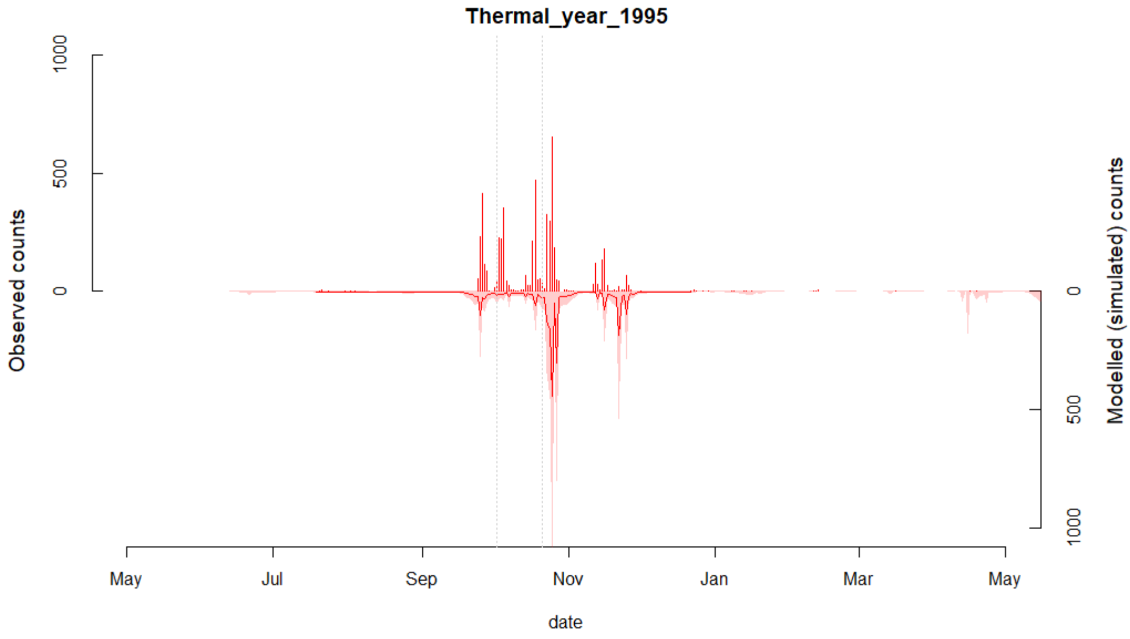

Figure 2.6.4. Example plot illustrating prediction efficacy of a GLMM to predict downstream silver eel migation counts during the ”forward” held-out 1995 run (i.e., the model was trained on data for 1981 to 1994). Tercile boudaries are illustrated by vertical grey dashed lines. The shaded area in the lower half of the plot illustrates the 95% bootstrapped percentile prediction intervals for the model prediction (median; 50th percentile). NOTE (i) - Uncertainty in predicted counts owing to model parameter estimate uncertainties is not illustrated here, but could be implemented, for example, by resampling parameter estimates from a multivariate normal distribution. NOTE (ii) – The matching colour (red) of observed and simulated counts indicateds that the phenology anomalies observed and predicted were both a ”late” run.

Using a statistical model and seasonal forecast enemble data to forecast migration counts

The primary limitation to the usefulness of a seasonal forecast system for eel migration at Burrishoole relates to the accuracy of seasonal meteorological (climate) forecasts in the West of Ireland. As a demonstrative project, each WATExR case study serves to demonstrate the application of state-of-the-art seasonal climate forecasts in relation to: (i) an appropriate workflow, and (ii) clear communication of forecast uncertainties. To this end, the final step in the workflow of the eel migration forecast system is to use seasonal forecast ensemble data to simulate counts from the daily count model to produce a probabilistic forecast.

Figure 2.6.5 illustrates modelled water temperature based on 15 ensemble members, whereby these data were used to simulate eel counts from our trained model for the held out 2008 eel run. Moreover, **Figure 2.6.5** illustrates the phenology anomolay prediced by each ensemble member (along with other predictors) by colour (red = late, blue = early, green = bimodal). A probablistic forecast based upon the data illustrated in **Figure 2.6.5** and our defined anomalies would have low predictive confidence, as no single anomaly dominates (5 of 15 blue (early), 5 of 15 red (late), 4 of 15 green (bimodal), 1 of 15 grey (condensed).

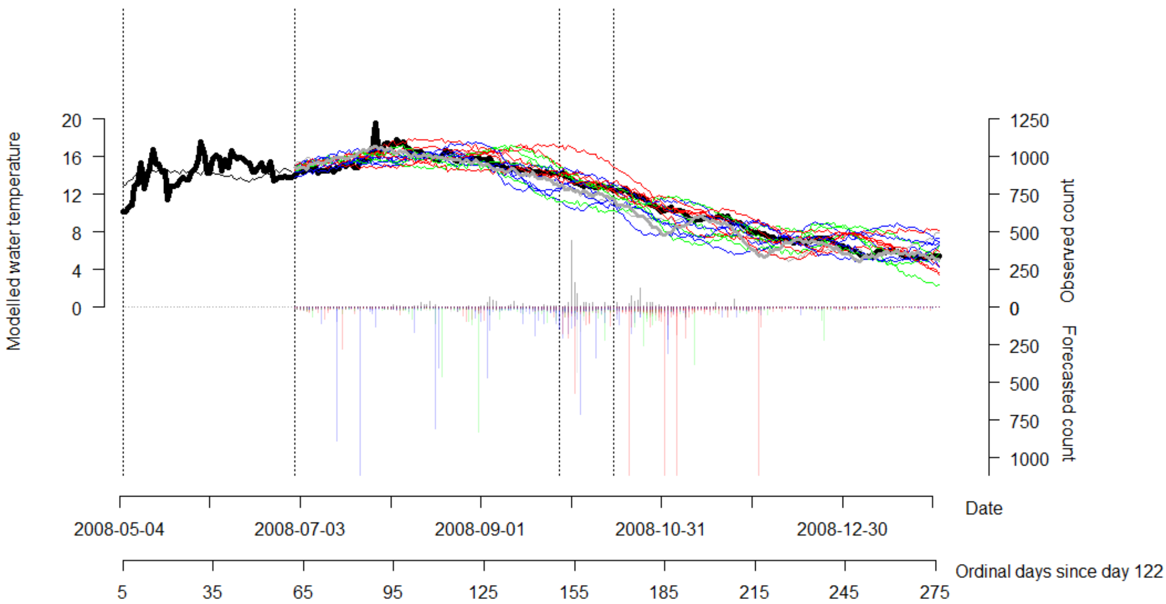

Figure 2.6.5. Illustration of seasonal forecast ensemble data applied to an air to water temperature model and daily fish count model. The broadest black line illustrates the observed (measured) water temperature; the broad grey line illustrates modelled water temperatured from reanalysis data (i.e., it is not a seasonal forecast ensemble member).

An important step in validation of our forecast (not included in this section) is to evaluate forecast skill (i.e., the trust stakeholders should have in any given seasonal forecast). Seasonal forecast skill in the Burrishoole catchment for a variety of meteorological variables and seasons is assessed in Deliverable 2.2. The current qualitative assemssment of forecast skill for the eel migration at Burrishoole (i.e., in absence of a calculated ROC skill score for phenology anomalies) is low owing to the strong association between rainfall (a seasonal forecast variable with low skill in all seasons at Burrishoole) and fish movement. Nevertheless, with developements in daily count modelling ongoing (including for other diadromous fishes; i.e., salmon and trout) and alternative definitions of migration phenology anomalies (described in section **2.6.4**), optimism in seasonal forecasting of diadromous fish migrations is not necessarily misplaced.

2.6.4 Outstanding issues

Air to water temperature prediction

We used a simple air to water temperature model (Mohseni et al., 1998) to estimate water temperature at the Burrishoole catchment. There are a range of models available (including lake models used for other WATExR case studies) that we may choose to substitute into the workflow.

Alternative methods for quantifying phenology (reducing the number of defined anomalies)

A lack of confidence in seasonal forecasts remains as a result of our definition of 6 anomaly types. While we will likely redefine our anomalies to increase the confidence in forecasts, the current set of definitions remain a biologically useful description as they descibe when the majority of eels are moving. One future approach that would solve the issue of low confidence would be to define the date on which a certain percentage of migrating fishes have been observed (e.g., the 50th percentile or ”mid point” of the run. Defining anomalies as late or early in relation to the mid point would reduce the biological value of the forecast, particularly as counts (of eels) are strongly heterogenous (clustered) with time. Such an alternative approach might be more approporate for juvenile salmonids, but, ultimately, a compromise must be agreed between the developers and the stakeholders to produce a meaningful forecast.

2.7 Modeling workflow for Australian site: Mt. Bold Reservoir and its catchment

2.7.1 Study site and previous work

The Australian target system is Mt. Bold reservoir and its two inflows, Echunga Creek and the Onkaparing river. Mt. Bold Reservoir is a moderately eutrophic reservoir located in the Lofty Ranges outside Adelaide in South Australia (35.12 S 138.70 E). The reservoir has a maximum depth of 41.4m which fluctuates seasonally. It has two inflows; the Onkaparinga River and the Echunga Creek. The Onkaparinga River also receives water which is pumped from the Murray River. This water is added to ensure the reservoir water level does not drop too low as this reservoir supplies drinking water to the inhabitants of Adelaide.

The hydrological model used for simulating both inflows into Mt. Bold reservoir is GR4J. The GR4J is a four-parameter lumped rainfall-runoff which accounts for PET, evaporation and percolation and allows for simulation of the lag between rainfall and discharge (Edijatno et al. 1999; Perrin et al. 2003). In our workflow, we will be using GR4J to simulate the inflows into Mt. Bold Reservoir. Within the reservoir, the 1-dimensional hydrodynamic model GOTM will be used to simulate the thermal structure of the lake (Burchard et al., 2006).
GR4J and GOTM were forced using data from ERA-Interim reanalysis data and hindcast data of the forecasting system System4 as meteorological input. GR4J is calibrated using EWEMBI data and observed streamflow data and GOTM for the lake is calibrated

2.7.2 Preliminary Results

Data from ERA-interim reanalysis data was used to spin up both the hydrological and lake hydrodynamic model. Then 4-months from the System 4 forecast was used to forecast, the first month of this forecast is used as a re-initialization month and the following three months are used as the target period. The 95% confidence intervals are calculated from the spread of the forecast from the 15 members used in the forecast.
The main target variables that are demonstrated here are streamflow and surface temperature and summer being the season of most interest due to the risk of drought, which could cause low water level, and elevated phosphorus levels in the reservoir.

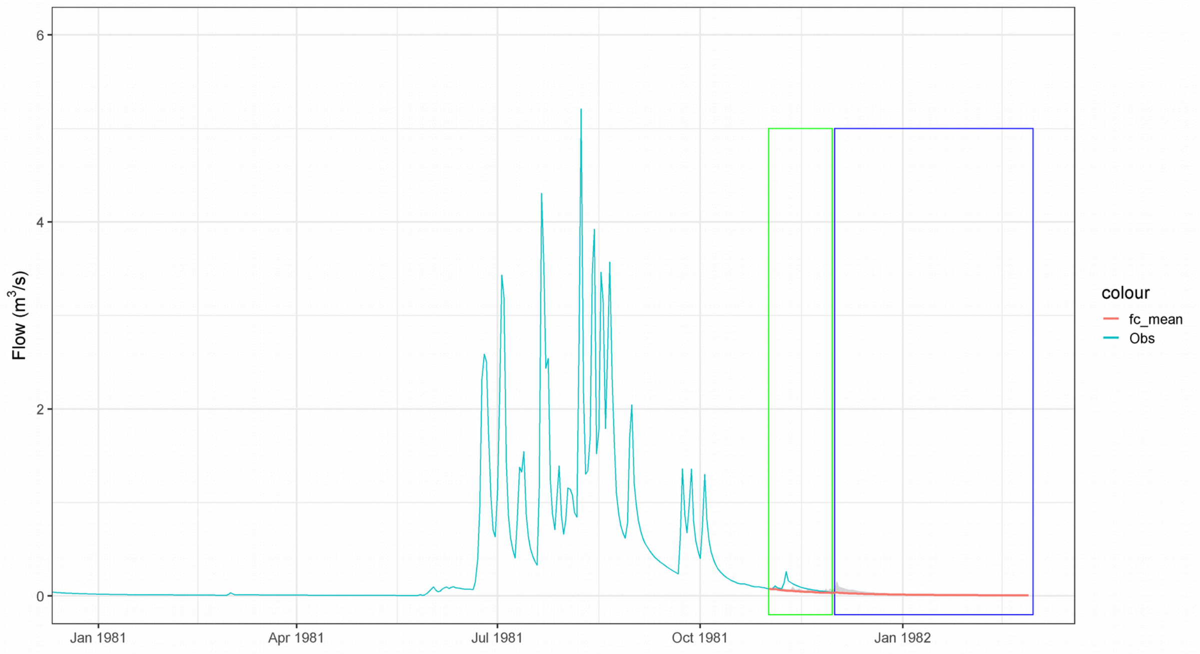

Figure 2.7.1 Observed discharge for the Onkaparinga river (cyan) with the re-initialization period (green box) and the seasonal period (blue box) with the 95% confidence intervals for the forecast (shaded grey area) and the forecast mean (red line). The forecast period was summer (December, January and February).

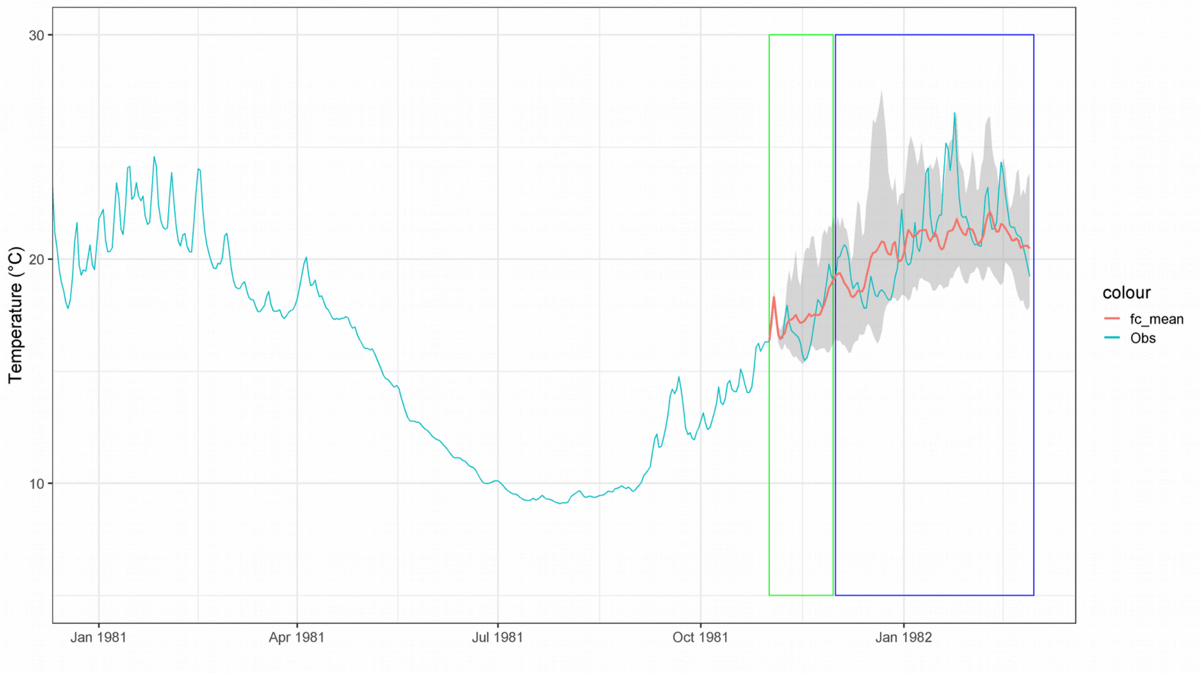

Figure 2.7.2 Observed surface water temperature for Mt. Bold (cyan) with the re-initialization period (green box) and the seasonal period (blue box) with the 95% confidence intervals for the forecast (shaded grey area) and the forecast mean (red line). The forecast period was summer (December, January and February).

The future goal will be to incorporate the SELMA biogeochemical model to simulate phosphorus concentrations at the bottom of the reservoir as this is where the outtake for the reservoir is. A hindcasting experiment will be carried out to develop a trust score for these forecasts.

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