Supplementary material: Forecasting water temperature in lakes and reservoirs using seasonal climate prediction

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1. Catchment-lake systems

Table 1: Main characteristics of lakes and reservoirs studied

Case study	*Country*	*Altitude (m)*	*Surface area (ha)*	*Volume (hm^3)*	*Water retention time (years)*	*Max. depth (m)*	*Mixing regime*
Sau	Spain	425	575	165	0.20	60	monomictic
Mt. Bold	Australia	244	254	46.4	0.2 - 0.6 years	44.5	monomictic
Vansjø	Norway	26	3600	252	1.1 years	19	dimictic
Wupper	Germany	250	211	26	0.20 years	31	dimictic

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1.1. Sau Reservoir (Spain)

Sau reservoir is part of a chain of reservoirs that form the water supply system to the Barcelona metropolitan area, while it is also used for recreation. The reservoir has a capacity of 165 hm^3 and a mean inflow of 14 m^3/s. Sau reservoir is part of the Ter River catchment, which has an area of 1680 m^2 and is the main source of water for this reservoir. This particular catchment/lake system was selected due to its relevant role on water supply and the availability of long-term monitoring data. There is a growing interest to have improved tools to inform the water quality management decisions taken by stakeholders at Sau reservoir, owing to recurring water quality impairment episodes related to anoxia development and algal blooms (Marcé and Joan, 2010).

1.2. Mt. Bold Reservoir (Australia)

Mount Bold (Mt. Bold) reservoir is the largest reservoir in South Australia. It has a capacity of 0.046 hm^3 and was completed in 1938. At full water level (41.5 m) the reservoir has a surface area of 2.5 km^2. It receives water from the Onkaparinga catchment (325 km^2) and the Echunga Creek Catchment (32 km^2). In addition to these inflows, the Onkaparinga river is supplemented with water from the Murray River *via* a pipeline. This pipeline crucially provides water during the summer and autumn seasons where there is little to no precipitation. Mt. Bold reservoir provides water to the Happy Valley reservoir further downstream which is a drinking water reservoir for Adelaide and the surrounding Mount Lofty Ranges. Mt. Bold reservoir was selected as a case study because the seasonal variations in water level are critically important for managing the quantities of water that are released downstream. Moreover, pumping water from the Murray is a large economic expense so having prior knowledge with regards to how the hydrology of the catchment is going to respond can inform decisions on whether or not to pump the water into the Onkaparinga. In addition, there have been historical issues with regards to high levels of re-suspension of phosphorus from the sediments which have contributed to the historic occurrence of algal blooms in Happy Valley reservoir.

1.3. Lake Vansjø (Norway)

Lake Vansjø (36 km^2; 252.2 hm^3), located in southeastern Norway, provides drinking water to three municipalities ($\sim$ 60000 inhabitants) and is a major recreational and fishing area in the region. Its catchment (690 km^2) comprises mainly forest (78%), agricultural area (15%), and open water (7%; (Skarbøvik et al., 2019). The lake is composed of several sub-basins, of which the two largest are Storefjorden (eastern basin, sub-catchment of 244 km^2, surface area of 23.8 km^2), and Vanemfjorden (western basin, sub-catchment of 58 km^2, surface area: 12.0 km^2). The water flows through the deeper Storefjorden basin (max depth: 41 m, mean depth: 8.7 m, and residence time: 0.85 $year$) through a channel to the shallower Vanemfjorden basin (max depth: 19.0 m, mean depth 3.8 m, and residence time: 0.21 $year$). The physicochemical and ecological status of Vanemfjorden is typically moderate (Haande et al., 2011), and remediation measures implemented in the past few years in the catchment have only partially improved this status (Skarbøvik and Skjelbred, 2019). Several blooms of cyanobacteria have been recorded in the 2000's causing beach closures (Moe et al., 2016). Lake Vansjø, which has been monitored since 1980, is thus a case study of high interest for stakeholders to implement sustainable measures to improve its ecological status and understand possible risks of deterioration.

1.4. Wupper Reservoir (Germany)

The Wupper Reservoir is located in the West of Germany near Cologne (51.2N, 7.3E) at an altitude of 251 m.a.s.l. The reservoir dams the river Wupper and receives water from an upstream catchment of about 215 km^2. At full storage (maximum depth 31m), the reservoir has a maximum surface of 2.12km^2 and a maximum volume of 26 hm^3. The dimictic reservoir has a canyon-like shape, a mean depth about of 11m, a residence time of 0.2 years, and a stratification period between May and September (Scharf, 2008b). The main purposes are flood control, environmental flows, and recreation. Accordingly, water level fluctuations are large with the highest levels in spring and lowest in autumn (Scharf, 2008a). Management of Wupper reservoir would benefit from prior information at seasonal scales with respect to the identification of optimum storage dynamics, balancing the needs of flood protection (i.e., maintenance of excess storage capacity to absorb large inflow events) and environmental flows (i.e., maintenance of sufficient stored water for supplementing outlets during summer). Furthermore, reservoir operators want to use seasonal forecasts to help avoid strong water level drawdowns associated with the occurrence of cyanobacterial blooms during hot summers and low water levels.

2. Climate data

2.1. Reanalysis (ERA5-ECMWF)

The latest reanalysis (Hersbach et al., 2020) produced by the ECMWF (https://www.ecmwf.int/) within the Copernicus Climate Change Service (C3S, https://climate.copernicus.eu/) is ERA5. It covers the entire globe at 0.25° horizontal and hourly temporal resolution. The reanalysis was used for three main purposes. Firstly, the reanalysis was used to provide climate pseudo-observations for retrospective blueperformance (skill) evaluation of seasonal climate forecasts explicitly. Secondly, the reanalysis was used to implement the bias correction of the seasonal forecasting system. Thirdly, the reanalysis was used to derive multi-decade temporal coverage (pseudo-)observations for catchment hydrology (i.e., discharge) and lake/reservoir thermal metrics (i.e., water column temperatures at multiple depths) for the hindcast period against which probabilistic seasonal forecasts of hydrologic and lake-reservoir could be evaluated for retrospective skill. In this third case, hydrologic models were forced with ERA5 precipitation and mean, minimum and maximum daily temperatures, and lake models were forced with ERA5 mean temperature, wind speed (u and v components), air pressure, relative humidity, cloud cover, solar radiation, and precipitation. Both hydrologic and lake models were calibrated against local observations while being forced by the reanalysis ERA5, these resulting hydrologic and lake/reservoir simulations were highly consistent with real observations. Reanalysis data for the period from 1988 to 2016 were considered in this study.

2.2. Seasonal forecast (SEAS5)

A seasonal forecasting system provides an ensemble of coupled ocean-atmosphere model runs (known as members), whereby each member represents a prediction of the medium-term (weeks to months) evolution of the climate system (i.e., a co-varying multi-variable system) with global coverage. This ensemble of members must be used together with a reanalysis with historical observations (ERA5 in this study), it is imposed by the complexity, uncertainties, and non-linear interactions in the Earth climate system.

The latest seasonal forecasting system provided by the ECMWF is SEAS5. This forecasting system provides (i) real-time seasonal forecasts and (ii) retrospective seasonal forecasts for past years (hindcasts). In this study, only retrospective seasonal forecasts (hindcasts) were used, since is is an inevitable step to validate and it is a forecast itself. Due to the intrinsic probabilistic nature of seasonal forecasts, it is essential to provide measures of the quality (reliability, accuracy, etc) of the seasonal forecast system, and hindcast is used for this forecast verification. A hindcast with 25 members was considered for the period 1993-2016 running. For each month (e.g. February) the seasonal forecast is able to cover up to the next 7 months (e.g. February to August).

2.2.1. Bias correction

Prior to hydrologic and lake model forcing and retrospective forecast blueperformance (skill) evaluation, seasonal climate forecast members must be pre-processed to minimise systematic bias implicit in the raw gridded outputs of global climate models (relative to climate (pseudo-)observations; ERA5 reanalysis in this case). Following the approach defined in the framework of the COST Action VALUE (2012 - 2015) project (Maraun et al., 2015), an experiment of inter-comparison of state-of-the-art calibration/downscaling methods (Gutiérrez et al., 2018), the Quantile mapping technique was selected to correct the global climate model data used. We used the empirical approach (EQM) due to its ability to deal with multivariate problems (Wilcke et al., 2013). EQM adjusts 99 percentiles and linearly interpolates inside this range every two consecutive percentiles; outside this range, a constant extrapolation (using the correction obtained for the 1st or 99th percentile) is applied (Déqué, 2007). In the case of precipitation, we applied the wet-day frequency adaptation proposed by Themeßl et al. (2012). The resulting bias-corrected data were used for hydrologic and lake models meteorological forcing, noting that we implemented bias-correction using leave-one-(year)-out cross-validation. Therefore, for each year, seasonal climate forecast member predictions were adjusted with the bias correction parameters derived from training with all other years; after which all bias-corrected data were appended to obtain a corrected (i.e., locally calibrated) time series of seasonal climate forecasts for the full period for each case study. Finally, to use the bias-corrected data as meteorological forcing for hydrologic and lake models, we used bilinear interpolation (*akima* method), whereby we specified lake/reservoir coordinates from which seasonal climate forecast data from surrounding pixels were interpolated.

Following seasonal climate forecast bias-correction, time-series for appended ERA5-SEAS5 meteorological hydrologic and lake model forcing variables revealed smooth transitions from climate (pseudo-)observations during the warm-up period (ERA5) to the seasonal climate forecast ensemble predictions during initialisation and target season (SEAS5); we found no evidence of discontinuities or "jumps".

3. Hydrologic modeling

3.1. Mesoscale Hydrologic Model (mHM)

The mesoscale Hydrologic Model (mHM v5.9: http://www.ufz.de/mhm) was used to implement the hydrologic simulations in the Ter River catchment in the Sau Reservoir case study. This is an open source and spatially distributed model with grid pixel as the main hydrologic unit and a multiscale parameter regionalization approach. It has the capacity to represent the main physical processes for the temporal and spatial scales of this study (e.g, soil moisture dynamics, infiltration and surface runoff, subsurface processes, canopy interception, and snowmelt processes). Apart from being driven by meteorological variables (precipitation, temperature and potential evaporation), it also depends on land cover, leaf area index (LAI), soil, and hydrogeologic maps.

The model has three levels of resolution to represent the surface characteristics (i.e, soil, land cover, terrain), the hydrologic processes and geological formations, and the variability of the meteorological forcing. Accordingly, the model was set up using the resolutions 100, 1000 and 10000 meters, respectively. These resolutions were selected according to (i) the area of our catchment and terrain resolution, (ii) the resolution of the meteorological forcing used and (iii) the suggestions from the user manual of the model. Additionally, the Jarvis equation (Jarvis, 1989) to represent soil moisture processes and the Muskingum approach (McCarthy, 1939) to represent the routing conditions were selected.

The hydrologic model was auto-calibrated using a Shuffled Complex Evolution optimization algorithm and NSE (Nash–Sutcliffe model efficiency coefficient) as objective function $(1.0 - 0.5 * (NSE + log(NSE)))$, to calibrate high and low flows. The observed data to implement the calibration was provided by the water treatment plant company in charge of the reservoir (Ens d'Abastament Ter-Llobregat (ATL)). More details of calibration and validation results are found in the Table 1 of the main paper in the "Hydrologic and lake temperature modeling" section, where the NSE and Kling-Gupta efficiency (KGE) metrics are calculated.

3.2. GR4J & GR6J

To model the inflows for the Wupper Reservoir and the Mt Bold Reservoir (Onkaparinga and Echunga Creek), the *Génie Rural* (GR) models were used within the R package "*airGR*" (Coron et al., 2017). These are a range of lumped conceptual rainfall-runoff models that can be applied at varying timescales from annual to hourly (Perrin et al., 2013). These models have been demonstrated to accurately simulate hydrologic flow regimes across a variety of different catchments such as mountainous terrain (Coron et al., 2017), near-natural catchments with high precipitation (Broderick et al., 2016) and across climatic shifts (Brulebois et al., 2018).

The GR4J and GR6J models are parsimonous model which are forced by precipitation and potential evapotranspiration (PET). Catchment size is the other required variable that is used in the computation of discharge. There are four parameters that can be calibrated within GR4J: production store capacity, intercatchment exchange coefficient, routing store capacity and unit hydrograph time constant. While GR6J (Pushpalatha et al., 2011) includes the same four parameters it comes along with two extra parameters: intercatchment exchange threshold and coefficient for emptying exponential store.

To calibrate the model, first a manual screening process was performed using a predefined grid to identify a 'good parameter set'. This is then used as the initial conditions for starting a steepest descent local search algorithm. Similarly to mHM, NSE was the objective function used within the calibration algorithm. However, for the German case study, the GR6J was calibrated using KGE as an objective function in order to ensure better representation of base flows since the reservoir was otherwise prone to drying out. More details of calibration and validation results are found in Table 1 of the main paper in the "Hydrologic and lake temperature modeling" section.

3.3. SimplyQ

SimplyQ, used to model the inflows to Lake Vansjø (Norway), is the hydrologic module of the catchment model for phosphorus SimplyP and described in detail by Jackson-Blake et al. (2017). Briefly, SimplyQ is forced by precipitation and air temperature, and computes snow accumulation and melt, evapotranspiration, terrestrial (soil, quick-surface and groundwater flows) and in-stream hydrologic processes. Six parameters were manually calibrated: degree-day evapotranspiration, degree-day factor for snow melt, proportion of precipitation that contributes to quick flow, baseflow index, groundwater time constant and soil water time constant. As for the other models, NSE was the objective function used during calibration, more details of calibration and validation results are found in Table 1 of the main paper in the “Hydrologic and lake temperature modeling” section.

4. Lake temperature modeling

4.1. General Ocean Turbulence Model (GOTM)

The General Ocean Turbulence Model (GOTM: http://gotm.net) was used for simulating the thermal dynamics of Sau Reservoir (Spain) and Lake Vansjø (Norway). GOTM is an open source ocean model adapted to lakes, which assumes a one-dimensional water column model for studying hydrodynamic and biogeochemical processes in marine and limnic waters. It models the state-of-the-art of the main physical processes in lakes: vertical turbulent fluxes of momentum, heat, and dissolved and particulate matter. To execute, it must be forced by meteorological data (precipitation, winds, pressure, air temperature, relative humidity, cloud fraction and solar radiation) and associated river inflow data (river discharge and water temperature). Additionally, for the Spanish case study, the water level fluctuations in the lake depend also on the historical outflow controlled by the water supply company, which was supplied as an observed forcing.

The model was calibrated against observed water temperature profiles using the ParSAC autocalibration tool (https://bolding-bruggeman.com/portfolio/parsac/) and the Maximum Likelihood optimization method. The parameters considered during calibration were the scale factor for short-wave solar radiation, scale factor for surface heat fluxes, scale factor for wind, minimum turbulent kinetic energy (TKE), and the light extinction coefficient. For Lake Vansjø, two additional parameters were calibrated for the ice dynamics: the ice albedo and the minimum threshold ice thickness.

The same parameters from the calibration were then used to run all time period for the water temperature data period using ERA5. The outflows are managed everyday according to the real-time changes in the water quality column in SAU reservoir and it reproduces a natural flow in the Vansjo lake. In Sau reservoir then, any difference between ERA5 inflows from mHM model (hydrologic) could lead to a dry out in the GOTM model (lake).

According to the most common statistical parameters (Nash-Sutcliffe Efficiency (NSE) and Root-Mean-Square Error (RMSE)) to evaluated calibration and validation in lake modeling (see Table 1 of the main paper in the "Hydrologic and lake temperature modeling" section), the fit between modelled and observed temperatures is better when closer to surface. However, it has to be noticed that when going deeper the amount of observations decreased affecting the statistical parameters to evaluate the fitting.

4.2. General Lake Model (GLM)

The General Lake Model (GLM) is a 1-D lake model that calculates the water balance and models thermal stratification within lake water bodies (Hipsey et al., 2019). It can be coupled to ecological and biogeochemical models through the Framework for Aquatic Biogeochemical Models (FABM) and also has an own Aquatic Ecosystems Dynamics library (AED) (Hipsey et al., 2013). It includes the impact of inflows, outflows, internal mixing, heat fluxes and ice formation. Within the model, a flexible Lagrangian layer structure is incorporated, which allows the layer thickness to change in response to inflows, outflows, internal mixing and heat and mass fluxes. It has been used to model lake hydrodynamics at regional scales (Read et al., 2014), reservoir operation (Feldbauer et al., 2020), lake management strategies (Ladwig et al., 2018), and has undergone rigorous stress testing across 32 lakes globally distributed (Bruce et al., 2018).

The model was calibrated slightly differently at Wupper Reservoir and Mt. Bold. In both cases, modelled temperatures were compared to observed temperatures but also considerable effort was made to ensure that the water balance and thus the water level simulated within the model reasonably replicated observed changes. Accurately capturing the water balance is critically important owing to the sensitivity of the heat budget to the volume of water.

For Mt. Bold Reservoir, assumptions were made in regards to the withdrawal and the Murray Bridge pipeline delivering water to the Onkaparinga. Using historically observed data, an average annual cycle was calculated for both and then replicated throughout the entire timeseries. While this assumption does not allow for inter-annual variation, it allowed for simulation of water level fluctuation each year that represented the seasonal cycle apparent within Mt. Bold. For calibration, residuals were visualized and it was identified that mixing of heat to lower depths was the largest. Using an automatic calibration for two parameters, scaling factor on the wind and scaling factor on the incoming long-wave radiation a RMSE of 1.17 degrees for the calibration period was achieved.

For Wupper Reservoir, a statistical model was developed to calculate the reservoir's outflow based on the inflow using the historical observations for each discharge simulation of the catchment model. Such an approach allows mimicking the outflow decision and approximately resembling the observed water-level to avoid the cases of dry-outs or exceedingly low volumes of water due to inflow underestimation. Moreover, this method could also help in future operational forecastings, aiming to represent a realistic water balance while respecting the reservoir's operational rules during the system run-time. The calibration function of the R package "glmtools" was used to set the values of the wind factor, light extinction coefficient, and long-wave radiation. Since the reservoir has a short residence time and is substantially affected by the inflow dynamics, the inflow parameters (i.e. streams drag coefficient, slope, and width angle) were also calibrated.

5. Calibration of hydrologic and lake models

All hydrologic models were calibrated and validated using the Nash–Sutcliffe efficiency coefficient (NSE) as objective function. More details of calibration and validation results are found in Table 2, where the NSE and Kling-Gupta efficiency (KGE) metrics are presented. In addition, more details about each particular hydrologic model may be found in the supplementary material.

blueThe lake models for each case was calibratedto ensure modeled temperatures were consistent with observations; however, considerable effort was also made to ensure that the water balance, and thus simulated water levels, reasonably reflected observed changes. Accurately capturing the water balance is critically important owing to the sensitivity of the heat budget to the volume of water.

According to the most common statistical goodness-of-fit parameters to evaluate calibration and validation in lake modeling, NSE and Root-Mean-Square Error (RMSE) (see Table 3 for our models), the goodness-of-fit between modeled and observed water temperatures declines with depth. How-

Table 2: Summary of the configuration of the hydrologic model for each catchment-lake system

Country	*River*	*Model*	*Warm-up*	*Calibration*			*Validation*		
				Time	*NSE**	*KGE**	*Time*	*NSE**	*KGE**
Spain	Ter	mHM	5 years	1997-2007	0.60	0.66	2008-2018	0.54	0.63
Australia	Echunga Creek	GR4J	5 years	2003-2007	0.64	0.70	2008-2013	0.80	0.75
Australia	Onkaparinga	GR4J	5 years	1999-2002	0.80	0.84	2003-2006	0.65	0.54
Norway	Vansjø	SimplyQ	5 years	2005-2010	0.51	0.56	2011-2015	0.57	0.57
Germany	Wupper	GR6J	1 year	1991-2011	0.71	0.85	2012-2016	0.63	0.81

*Calculated from daily values of discharge

ever, we acknowledge that data is increasingly sparse at increasing depths, which affects the calculation of goodness-of-fit statistics. Moreover, the influence of bathymetry on goodness-of-fit statistics at deeper depths should also not be neglected, particularly for the 1D models used in this study. Specific details of each lake model calibration may be found in the supplementary materials.

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Table 3: Summary of the configuration of the lake temperature model for each case study

Country	*Lake*	*Model*	*Warm-up*	*Calibration*			*Validation*		
				Time	*NSE**	*RMSE**	*Time*	*NSE**	*RMSE**
Spain	Sau	GOTM	1 year	1997-2007	0.93	1.63	2008-2018	0.94	1.45
Australia	Mt. Bold	GLM	1 year	2014-2016	0.91	1.17	2016-2018	0.78	1.50
Norway	Vansjø	GOTM	1 year	2005-2010	0.92	1.12	2011-2015	0.93	1.10
Germany	Wupper	GLM	1 year	1993-2010	0.93	1.31	2011-2016	0.91	1.53

*Calculated from daily values of surface water temperature

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