

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

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1 You can find all the codes, inputs and plots related to this manuscript at  
2 <https://git.io/J3tDN> and [https://nivanorge.github.io/seasonal\\_forecasting\\_watexr/](https://nivanorge.github.io/seasonal_forecasting_watexr/)

## 3 **1. Catchment-lake systems**

### 4 *1.1. Sau Reservoir (Spain)*

5 Sau reservoir is part of a chain of reservoirs that form the water supply  
6 system to the Barcelona metropolitan area, while it is also used for recreation.  
7 The reservoir has a capacity of  $165 \text{ hm}^3$  and a mean inflow of  $14 \text{ m}^3/\text{s}$ . Sau  
8 reservoir is part of the Ter River catchment, which has an area of  $1680 \text{ m}^2$   
9 and is the main source of water for this reservoir. This particular catch-  
10 ment/lake system was selected due to its relevant role on water supply and  
11 the availability of long-term monitoring data. There is a growing interest

12 to have improved tools to inform the water quality management decisions  
13 taken by stakeholders at Sau reservoir, owing to recurring water quality im-  
14 pairment episodes related to anoxia development and algal blooms (Marcé  
15 and Joan, 2010).

### 16 1.2. Mt. Bold Reservoir (Australia)

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

### 36 1.3. Lake Vansjø (Norway)

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

### 56 1.4. Wupper Reservoir (Germany)

57 The Wupper Reservoir is located in the West of Germany near Cologne  
58 ( $51.2\text{N}$ ,  $7.3\text{E}$ ) at an altitude of  $251 \text{ m.a.s.l.}$  The reservoir dams the river  
59 Wupper and receives water from an upstream catchment of about  $215 \text{ km}^2$ .  
60 At full storage (maximum depth  $31\text{m}$ ), the reservoir has a maximum surface

61 of  $2.12\text{km}^2$  and a maximum volume of  $26\text{ hm}^3$ . The dimictic reservoir has a  
 62 canyon-like shape, a mean depth about of 11m, a residence time of 0.2 years,  
 63 and a stratification period between May and September (Scharf, 2008b).  
 64 The main purposes are flood control, environmental flows, and recreation.  
 65 Accordingly, water level fluctuations are large with the highest levels in spring  
 66 and lowest in autumn (Scharf, 2008a). Management of Wupper reservoir  
 67 would benefit from prior information at seasonal scales with respect to the  
 68 identification of optimum storage dynamics, balancing the needs of flood  
 69 protection (i.e., maintenance of excess storage capacity to absorb large inflow  
 70 events) and environmental flows (i.e., maintenance of sufficient stored water  
 71 for supplementing outlets during summer). Furthermore, reservoir operators  
 72 want to use seasonal forecasts to help avoid strong water level drawdowns  
 73 associated with the occurrence of cyanobacterial blooms during hot summers  
 74 and low water levels.

## 75 **2. Climate data**

### 76 *2.1. Reanalysis (ERA5-ECMWF)*

77 The latest reanalysis (Hersbach et al., 2020) produced by the ECMWF  
 78 (<https://www.ecmwf.int/>) within the Copernicus Climate Change Service  
 79 (C3S, <https://climate.copernicus.eu/>) is ERA5. It covers the entire globe at  
 80  $0.25^\circ$  horizontal and hourly temporal resolution. The reanalysis was used  
 81 for three main purposes. Firstly, the reanalysis was used to provide climate  
 82 pseudo-observations for retrospective blueperformance (skill) evaluation of  
 83 seasonal climate forecasts explicitly. Secondly, the reanalysis was used to  
 84 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 it is an inevitable

110 step to validate and it is a forecast itself. Due to the intrinsic probabilistic  
111 nature of seasonal forecasts, it is essential to provide measures of the quality  
112 (reliability, accuracy, etc) of the seasonal forecast system, and hindcast is  
113 used for this forecast verification. A hindcast with 25 members was consid-  
114 ered for the period 1993-2016 running. For each month (e.g. February) the  
115 seasonal forecast is able to cover up to the next 7 months (e.g. February to  
116 August).

#### 117 *2.2.1. Bias correction*

118 Prior to hydrologic and lake model forcing and retrospective forecast  
119 blueperformance (skill) evaluation, seasonal climate forecast members must  
120 be pre-processed to minimise systematic bias implicit in the raw gridded  
121 outputs of global climate models (relative to climate (pseudo-)observations;  
122 ERA5 reanalysis in this case). Following the approach defined in the frame-  
123 work of the COST Action VALUE (2012 - 2015) project (Maraun et al., 2015),  
124 an experiment of inter-comparison of state-of-the-art calibration/downscaling  
125 methods (Gutiérrez et al., 2018), the Quantile mapping technique was se-  
126 lected to correct the global climate model data used. We used the empirical  
127 approach (EQM) due to its ability to deal with multivariate problems (Wilcke  
128 et al., 2013). EQM adjusts 99 percentiles and linearly interpolates inside this  
129 range every two consecutive percentiles; outside this range, a constant ex-  
130 trapolation (using the correction obtained for the 1st or 99th percentile) is  
131 applied (Déqué, 2007). In the case of precipitation, we applied the wet-day  
132 frequency adaptation proposed by Themeßl et al. (2012). The resulting bias-  
133 corrected data were used for hydrologic and lake models meteorological forc-  
134 ing, 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

159 processes, canopy interception, and snowmelt processes). Apart from being  
160 driven by meteorological variables (precipitation, temperature and potential  
161 evaporation), it also depends on land cover, leaf area index (LAI), soil, and  
162 hydrogeologic maps.

163 The model has three levels of resolution to represent the surface character-  
164 istics (i.e, soil, land cover, terrain), the hydrologic processes and geological  
165 formations, and the variability of the meteorological forcing. Accordingly,  
166 the model was set up using the resolutions 100, 1000 and 10000 meters, re-  
167 spectively. These resolutions were selected according to (i) the area of our  
168 catchment and terrain resolution, (ii) the resolution of the meteorological  
169 forcing used and (iii) the suggestions from the user manual of the model.  
170 Additionally, the Jarvis equation (Jarvis, 1989) to represent soil moisture  
171 processes and the Muskingum approach (McCarthy, 1939) to represent the  
172 routing conditions were selected.

173 The hydrologic model was auto-calibrated using a Shuffled Complex Evo-  
174 lution optimization algorithm and NSE (Nash–Sutcliffe model efficiency co-  
175 efficient) as objective function ( $1.0 - 0.5 * (NSE + \log(NSE))$ ), to calibrate  
176 high and low flows. The observed data to implement the calibration was pro-  
177 vided by the water treatment plant company in charge of the reservoir (Ens  
178 d’Abastament Ter-Llobregat (ATL)). More details of calibration and valida-  
179 tion results are found in the Table 1 of the main paper in the “Hydrologic  
180 and lake temperature modeling” section, where the NSE and Kling-Gupta  
181 efficiency (KGE) metrics are calculated.



### 182 3.2. GR4J & GR6J

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

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

201 To calibrate the model, first a manual screening process was performed  
202 using a predefined grid to identify a ’good parameter set’. This is then  
203 used as the initial conditions for starting a steepest descent local search  
204 algorithm. Similarly to mHM, NSE was the objective function used within  
205 the calibration algorithm. However, for the German case study, the GR6J  
206 was calibrated using KGE as an objective function in order to ensure better

207 representation of base flows since the reservoir was otherwise prone to drying  
208 out. More details of calibration and validation results are found in Table 1 of  
209 the main paper in the “Hydrologic and lake temperature modeling” section.

### 210 3.3. *SimplyQ*

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

## 223 4. Lake temperature modeling

### 224 4.1. *General Ocean Turbulence Model (GOTM)*

225 The General Ocean Turbulence Model (GOTM: <http://gotm.net>) was  
226 used for simulating the thermal dynamics of Sau Reservoir (Spain) and Lake  
227 Vansjø (Norway). GOTM is an open source ocean model adapted to lakes,  
228 which assumes a one-dimensional water column model for studying hydrody-  
229 namic and biogeochemical processes in marine and limnic waters. It models

230 the state-of-the-art of the main physical processes in lakes: vertical tur-  
231 bulent fluxes of momentum, heat, and dissolved and particulate matter. To  
232 execute, it must be forced by meteorological data (precipitation, winds, pres-  
233 sure, air temperature, relative humidity, cloud fraction and solar radiation)  
234 and associated river inflow data (river discharge and water temperature).  
235 Additionally, for the Spanish case study, the water level fluctuations in the  
236 lake depend also on the historical outflow controlled by the water supply  
237 company, which was supplied as an observed forcing.

238 The model was calibrated against observed water temperature profiles us-  
239 ing the ParSAC autocalibration tool (<https://bolding-bruggeman.com/portfolio/parsac/>)  
240 and the Maximum Likelihood optimization method. The parameters consid-  
241 ered during calibration were the scale factor for short-wave solar radiation,  
242 scale factor for surface heat fluxes, scale factor for wind, minimum turbu-  
243 lent kinetic energy (TKE), and the light extinction coefficient. For Lake  
244 Vansjø, two additional parameters were calibrated for the ice dynamics: the  
245 ice albedo and the minimum threshold ice thickness.

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

252 According to the most common statistical parameters (Nash-Sutcliffe Effi-  
253 ciency (NSE) and Root-Mean-Square Error (RMSE)) to evaluated calibration  
254 and validation in lake modeling (see Table 1 of the main paper in the “Hy-

255 drologic and lake temperature modeling” section), the fit between modelled  
256 and observed temperatures is better when closer to surface. However, it has  
257 to be noticed that when going deeper the amount of observations decreased  
258 affecting the statistical parameters to evaluate the fitting.

#### 259 4.2. General Lake Model (GLM)

260 The General Lake Model (GLM) is a 1-D lake model that calculates the  
261 water balance and models thermal stratification within lake water bodies  
262 (Hipsey et al., 2019). It can be coupled to ecological and biogeochemical  
263 models through the Framework for Aquatic Biogeochemical Models (FABM)  
264 and also has an own Aquatic Ecosystems Dynamics library (AED) (Hipsey  
265 et al., 2013). It includes the impact of inflows, outflows, internal mixing,  
266 heat fluxes and ice formation. Within the model, a flexible Lagrangian layer  
267 structure is incorporated, which allows the layer thickness to change in re-  
268 sponse to inflows, outflows, internal mixing and heat and mass fluxes. It  
269 has been used to model lake hydrodynamics at regional scales (Read et al.,  
270 2014), reservoir operation (Feldbauer et al., 2020), lake management strate-  
271 gies (Ladwig et al., 2018), and has undergone rigorous stress testing across  
272 32 lakes globally distributed (Bruce et al., 2018).

273 The model was calibrated slightly differently at Wupper Reservoir and  
274 Mt. Bold. In both cases, modelled temperatures were compared to observed  
275 temperatures but also considerable effort was made to ensure that the wa-  
276 ter balance and thus the water level simulated within the model reasonably  
277 replicated observed changes. Accurately capturing the water balance is crit-  
278 ically important owing to the sensitivity of the heat budget to the volume of  
279 water.

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

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

## 304 5. Calibration of hydrologic and lake models

305 All hydrologic models were calibrated and validated using the Nash–Sutcliffe  
 306 efficiency coefficient (NSE) as objective function. More details of calibration  
 307 and validation results are found in Table 1, where the NSE and Kling-Gupta  
 308 efficiency (KGE) metrics are presented. In addition, more details about each  
 309 particular hydrologic model may be found in the supplementary material.

Table 1: Summary of the configuration of the hydrologic model for each catchment-lake system

<i>Country</i>	<i>River</i>	<i>Model</i>	<i>Warm-up</i>	<i>Calibration</i>			<i>Validation</i>		
				<i>Time</i>	<i>NSE*</i>	<i>KGE*</i>	<i>Time</i>	<i>NSE*</i>	<i>KGE*</i>
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

310 blueThe lake models for each case was calibrated to ensure modeled tem-  
 311 peratures were consistent with observations; however, considerable effort was  
 312 also made to ensure that the water balance, and thus simulated water lev-  
 313 els, reasonably reflected observed changes. Accurately capturing the water  
 314 balance is critically important owing to the sensitivity of the heat budget to  
 315 the volume of water.

316 According to the most common statistical goodness-of-fit parameters to  
 317 evaluate calibration and validation in lake modeling, NSE and Root-Mean-

318 Square Error (RMSE) (see Table 2 for our models), the goodness-of-fit be-  
319 tween modeled and observed water temperatures declines with depth. How-  
320 ever, we acknowledge that data is increasingly sparse at increasing depths,  
321 which affects the calculation of goodness-of-fit statistics. Moreover, the influ-  
322 ence of bathymetry on goodness-of-fit statistics at deeper depths should also  
323 not be neglected, particularly for the 1D models used in this study. Specific  
324 details of each lake model calibration may be found in the supplementary  
325 materials.

Table 2: Summary of the configuration of the lake temperature model for each case study

<i>Country</i>	<i>Lake</i>	<i>Model</i>	<i>Warm-up</i>	<i>Calibration</i>			<i>Validation</i>		
				<i>Time</i>	<i>NSE*</i>	<i>RMSE*</i>	<i>Time</i>	<i>NSE*</i>	<i>RMSE*</i>
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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