

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

<i>Case study</i>	<i>Country</i>	<i>Altitude (m)</i>	<i>Surface area (ha)</i>	<i>Volume (hm³)</i>	<i>Water retention time (years)</i>	<i>Max. depth (m)</i>	<i>Mixing regime</i>
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

2 1.1. *Sau Reservoir (Spain)*

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

14 1.2. *Mt. Bold Reservoir (Australia)*

15 Mount Bold (Mt. Bold) reservoir is the largest reservoir in South Aus-
16 tralia. It has a capacity of 0.046 hm^3 and was completed in 1938. At full
17 water level (41.5 m) the reservoir has a surface area of 2.5 km^2 . It receives
18 water from the Onkaparinga catchment (325 km^2) and the Echunga Creek
19 Catchment (32 km^2). In addition to these inflows, the Onkaparinga river is
20 supplemented with water from the Murray River *via* a pipeline. This pipeline
21 crucially provides water during the summer and autumn seasons where there
22 is little to no precipitation. Mt. Bold reservoir provides water to the Happy
23 Valley reservoir further downstream which is a drinking water reservoir for
24 Adelaide and the surrounding Mount Lofty Ranges. Mt. Bold reservoir was
25 selected as a case study because the seasonal variations in water level are
26 critically important for managing the quantities of water that are released

27 downstream. Moreover, pumping water from the Murray is a large economic
28 expense so having prior knowledge with regards to how the hydrology of the
29 catchment is going to respond can inform decisions on whether or not to
30 pump the water into the Onkaparinga. In addition, there have been histori-
31 cal issues with regards to high levels of re-suspension of phosphorus from the
32 sediments which have contributed to the historic occurrence of algal blooms
33 in Happy Valley reservoir.

34 1.3. Lake Vansjø (Norway)

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

52 for stakeholders to implement sustainable measures to improve its ecological
53 status and understand possible risks of deterioration.

54 1.4. Wupper Reservoir (Germany)

55 The Wupper Reservoir is located in the West of Germany near Cologne
56 (51.2N, 7.3E) at an altitude of 251 m.a.s.l. The reservoir dams the river
57 Wupper and receives water from an upstream catchment of about 215 km^2 .
58 At full storage (maximum depth 31m), the reservoir has a maximum surface
59 of 2.12 km^2 and a maximum volume of 26 hm^3 . The dimictic reservoir has a
60 canyon-like shape, a mean depth about of 11m, a residence time of 0.2 years,
61 and a stratification period between May and September (Scharf, 2008b).
62 The main purposes are flood control, environmental flows, and recreation.
63 Accordingly, water level fluctuations are large with the highest levels in spring
64 and lowest in autumn (Scharf, 2008a). Management of Wupper reservoir
65 would benefit from prior information at seasonal scales with respect to the
66 identification of optimum storage dynamics, balancing the needs of flood
67 protection (i.e., maintenance of excess storage capacity to absorb large inflow
68 events) and environmental flows (i.e., maintenance of sufficient stored water
69 for supplementing outlets during summer). Furthermore, reservoir operators
70 want to use seasonal forecasts to help avoid strong water level drawdowns
71 associated with the occurrence of cyanobacterial blooms during hot summers
72 and low water levels.

73 2. Climate data

74 2.1. Reanalysis (ERA5-ECMWF)

75 The latest reanalysis (Hersbach et al., 2020) produced by the ECMWF
76 (<https://www.ecmwf.int/>) within the Copernicus Climate Change Service
77 (C3S, <https://climate.copernicus.eu/>) is ERA5. It covers the entire globe at
78 0.25° horizontal and hourly temporal resolution. The reanalysis was used
79 for three main purposes. Firstly, the reanalysis was used to provide climate
80 pseudo-observations for retrospective blueperformance (skill) evaluation of
81 seasonal climate forecasts explicitly. Secondly, the reanalysis was used to
82 implement the bias correction of the seasonal forecasting system. Thirdly,
83 the reanalysis was used to derive multi-decade temporal coverage (pseudo-
84)observations for catchment hydrology (i.e., discharge) and lake/reservoir
85 thermal metrics (i.e., water column temperatures at multiple depths) for the
86 hindcast period against which probabilistic seasonal forecasts of hydrologic
87 and lake-reservoir could be evaluated for retrospective skill. In this third case,
88 hydrologic models were forced with ERA5 precipitation and mean, minimum
89 and maximum daily temperatures, and lake models were forced with ERA5
90 mean temperature, wind speed (u and v components), air pressure, relative
91 humidity, cloud cover, solar radiation, and precipitation. Both hydrologic
92 and lake models were calibrated against local observations while being forced
93 by the reanalysis ERA5, these resulting hydrologic and lake/reservoir simu-
94 lations were highly consistent with real observations. Reanalysis data for the
95 period from 1988 to 2016 were considered in this study.

96 2.2. Seasonal forecast (SEAS5)

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

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

115 2.2.1. Bias correction

116 Prior to hydrologic and lake model forcing and retrospective forecast
117 blueperformance (skill) evaluation, seasonal climate forecast members must
118 be pre-processed to minimise systematic bias implicit in the raw gridded
119 outputs of global climate models (relative to climate (pseudo-)observations;
120 ERA5 reanalysis in this case). Following the approach defined in the frame-

121 work of the COST Action VALUE (2012 - 2015) project (Maraun et al., 2015),
 122 an experiment of inter-comparison of state-of-the-art calibration/downscaling
 123 methods (Gutiérrez et al., 2018), the Quantile mapping technique was se-
 124 lected to correct the global climate model data used. We used the empirical
 125 approach (EQM) due to its ability to deal with multivariate problems (Wilcke
 126 et al., 2013). EQM adjusts 99 percentiles and linearly interpolates inside this
 127 range every two consecutive percentiles; outside this range, a constant ex-
 128 trapolation (using the correction obtained for the 1st or 99th percentile) is
 129 applied (Déqué, 2007). In the case of precipitation, we applied the wet-day
 130 frequency adaptation proposed by Themeßl et al. (2012). The resulting bias-
 131 corrected data were used for hydrologic and lake models meteorological forc-
 132 ing, noting that we implemented bias-correction using leave-one-(year)-out
 133 cross-validation. Therefore, for each year, seasonal climate forecast member
 134 predictions were adjusted with the bias correction parameters derived from
 135 training with all other years; after which all bias-corrected data were ap-
 136 pended to obtain a corrected (i.e., locally calibrated) time series of seasonal
 137 climate forecasts for the full period for each case study. Finally, to use the
 138 bias-corrected data as meteorological forcing for hydrologic and lake mod-
 139 els, we used bilinear interpolation (*akima* method), whereby we specified
 140 lake/reservoir coordinates from which seasonal climate forecast data from
 141 surrounding pixels were interpolated.

142 Following seasonal climate forecast bias-correction, time-series for ap-
 143 pended ERA5-SEAS5 meteorological hydrologic and lake model forcing vari-
 144 ables revealed smooth transitions from climate (pseudo-)observations during
 145 the warm-up period (ERA5) to the seasonal climate forecast ensemble predic-

146 tions during initialisation and target season (SEAS5); we found no evidence
147 of discontinuities or "jumps".

148 **3. Hydrologic modeling**

149 *3.1. Mesoscale Hydrologic Model (mHM)*

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

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

170 routing conditions were selected.

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

180 3.2. GR4J & GR6J

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

190 The GR4J and GR6J models are parsimonous model which are forced
191 by precipitation and potential evapotranspiration (PET). Catchment size is
192 the other required variable that is used in the computation of discharge.
193 There are four parameters that can be calibrated within GR4J: production
194 store capacity, intercatchment exchange coefficient, routing store capacity

195 and unit hydrograph time constant. While GR6J (Pushpalatha et al., 2011)
196 includes the same four parameters it comes along with two extra parameters:
197 intercatchment exchange threshold and coefficient for emptying exponential
198 store.

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

208 3.3. *SimplyQ*

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

220 in the “Hydrologic and lake temperature modeling” section.

221 **4. Lake temperature modeling**

222 *4.1. General Ocean Turbulence Model (GOTM)*

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

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

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

250 According to the most common statistical parameters (Nash-Sutcliffe Effi-
251 ciency (NSE) and Root-Mean-Square Error (RMSE)) to evaluated calibration
252 and validation in lake modeling (see Table 1 of the main paper in the “Hy-
253 drologic and lake temperature modeling” section), the fit between modelled
254 and observed temperatures is better when closer to surface. However, it has
255 to be noticed that when going deeper the amount of observations decreased
256 affecting the statistical parameters to evaluate the fitting.

257 4.2. General Lake Model (GLM)

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

gies (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

294 due to inflow underestimation. Moreover, this method could also help in
295 future operational forecastings, aiming to represent a realistic water balance
296 while respecting the reservoir’s operational rules during the system run-time.
297 The calibration function of the R package "glmtools" was used to set the
298 values of the wind factor, light extinction coefficient, and long-wave radiation.
299 Since the reservoir has a short residence time and is substantially affected
300 by the inflow dynamics, the inflow parameters (i.e. streams drag coefficient,
301 slope, and width angle) were also calibrated.

302 **5. Calibration of hydrologic and lake models**

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

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

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

Table 2: 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

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

324 Acknowledgments

325 This is a contribution of the WATExR project (watexr.eu/), which is
326 part of ERA4CS, an ERA-NET initiated by JPI Climate, and funded by
327 MINECO-AEI (ES), FORMAS (SE), BMBF (DE), EPA (IE), RCN (NO),
328 and IFD (DK), with co-funding by the European Union (Grant 690462).
329 MINECO-AEI funded this research through projects PCIN-2017-062 and
330 PCIN-2017-092.

Table 3: 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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