Scoping a flexible framework for producing river water temperature projections

Chief Scientist's Group research report

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Professor Doug Wilson
Chief Scientist

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Executive summary

Climate change and particularly warming is expected to change freshwater ecosystems and water quality. Understanding how and where changes may take place and the likely magnitude of these can help to project water quality and target management activity. River systems are highly sensitive to water temperature so it is important to have insight about future patterns. These will not necessarily be a reflection of patterns in air temperature change for which information is readily available.

There are no national-scale approaches to water temperature modelling of contemporary or future dynamics of change in England, although examples exist elsewhere (e.g. Scotland). This limits our understanding of future risks and our ability to target management options to improve resilience to the impacts of climate change. This report provides recommendations for the development of a water temperature modelling framework that can provide projections under current and future climate taking full account of available empirical information.

To develop a flexible framework for river water temperature modelling across England, the following questions were addressed:

1. What methods are available for modelling water temperature, and what are their benefits and limitations?
2. What are the data and modelling requirements, benefits and limitations of using these approaches to produce projections of river water temperature for England under climate change?
3. What is the most suitable methodology for developing these projections given current data availability?

A comprehensive literature review identified four broad groups of modelling approaches for river water temperature: statistical, process-based, machine learning and hybrid. Statistical (regression based) water temperature models are the most established and widely used approach for modelling contemporary water temperature and making projections. Spatial river network models are the current “state of the art” and can facilitate predictions of mean/maximum water temperature but require frequent field measurements (e.g. hourly) for calibration, a topologically correct digital river network and advanced statistical and programming expertise. Process-based models can be potentially more accurate than statistical models for making predictions at unmonitored sites as they represent the physical processes that control warming and cooling of river water. However, they are not well represented in the literature at larger spatial scales (e.g. greater than small sub-catchments) as data requirements for calibration becomes prohibitive. A number of emerging research approaches were identified that may be suitable for large scale modelling in the future. These new approaches are largely associated with machine learning / artificial intelligence approaches.

Two decision trees were developed to facilitate: (1) the identification of the most suitable approach for generating water temperature projections for England given the data constraints, (2) the most suitable approach for a given use case. The first decision tree considers the type of model approach a user wishes to pursue (e.g. statistical vs process-based). The tree structure highlights how different models are interlinked and, in the case of regression-based models, how they can be considered building blocks of increasing complexity towards a model that predicts daily water temperature for the entire river network. The second set of decision trees focuses on the practical considerations that a user may face when attempting to select a suitable model for generating water temperature projections. This second decision tree emphasizes the data requirements, computational requirements and length of time series associated with specific water temperature models. Hence, these decision trees represent a practical tool for choosing a suitable water temperature model for a range of use cases.

Given the data limitations (lack of sub-daily data) and the need for an interpretable and flexible model a statistical approach was required. A multi-site, mixed effect regression model was identified as the most feasible approach for producing temperature projections. This is recommended for application where there is adequate temporal resolution of the water temperature data available for model calibration and validation. A mixed effect regression model has potential to predict to unmonitored locations but should not be used to predict outside the environmental range of the calibration dataset. Furthermore, it represents a building block towards a water temperature model for the entire river network. Detailed instructions are provided in the appendix of this report covering all required steps, including: site/selection, data pre-processing, covariate extraction, exploratory analysis, model selection, model validation for contemporary water temperature and developing future projections.

Finally, recommendations are provided for future data collection to facilitate the development of a water temperature model for the entire river network, including a method to optimise future site selection and avoid data redundancy.

Introduction

Overview

Climate change is expected to cause a deterioration in water quality and river aquatic ecosystems in nutrient rich environments (Whitehead et al. 2009). To maintain or improve water quality and ensure management responses are resilient to future pressures, it is important to identify priority areas for management intervention. Previous modelling exercises to assess how water quality and eutrophication risk are likely to change in the future have highlighted the sensitivity of projections to water temperature (Environment Agency, 2019). Consequently, an accurate representation of future water temperature patterns across England's rivers is required to improve predictions of water quality (Whitehead et al. 2009) and develop effective mitigation strategies for problems where these arise.

River flow regimes shape the river habitats that support biological communities. We have a growing understanding of the role extreme events (droughts and floods) play in shaping these communities (Aspin et al. 2019). Water temperature is also a key control on the structure and function of river ecosystems (Woodward et al. 2010). Understanding likely changes in thermal regime is thus important to guide targeted mitigation strategies (Knouft et al. 2021). For example, tree planting to enhance riparian shading can reduce thermal maxima in some places, but given the long lead time careful targeting is required (Garner et al. 2017). However, there is currently a lack of future water temperature projections to quantify and map water temperature change. However, models to identify where rivers are hottest, most sensitive to climate change and most effectively protected by trees are now available for Scotland (Jackson et al. 2018) and are being used to target riparian tree planting to protect cold water dependent species such as Atlantic salmon and brown trout.

There are a range of potential methods for modelling water temperature that have historically had limitations, making them unsuited to prediction to unmonitored locations or projection into the future (Gallice et al. 2015). Recent advances in the fields of statistics and computer science have yielded new approaches that overcome some of the major issues, in particular those associated with spatial covariance in river networks (Isaak et al. 2014). Given this, there is scope to develop a 'national Future River Water Temperature dataset' that could be used alongside projections of river flows and groundwater levels, such as Future Flows (Prudhomme et al., 2012, 2013) and the ongoing Met Office / CEH eFLaG project which will provide updated estimates of future river flows.

There are many options for modelling water temperature at small scales or for particular sites (Benyahya et al. 2007a), however, decision makers require information at national scales to support strategic planning and inform policy making.

Approaches to estimating future river water temperature range from relatively simple linear and logistic regression (Benyahya et al. 2007a) to complex physically based models using heat exchange principles (Dugdale et al. 2017). The use of regression based approaches that model relationships between air and water temperature, and in some cases how other factors can alter the relationship, have been favoured in the literature (Benyahya et al. 2007a, Letcher et al. 2016, Ouellet et al. 2020). Alternative approaches such as process-based models are useful but often require a large amount of data and are not practical to apply at large scales (see the review in Dugdale et al. 2017). Spatial statistical river network models are well suited to make predictions across large spatial scales and have been shown to provide accurate predictions of contemporary water temperature (Isaak et al. 2017, Jackson et al. 2018). However, data requirements, required model output (e.g. static monthly metrics vs daily metrics), computational demand and availability of software packages to facilitate model development may represent a barrier to implementation. Furthermore, the potential utility of emerging approaches (e.g. machine learning and artificial intelligence) remains largely unknown in the context of large scale water temperature modelling.

Project aim and objectives

There is a clear need for an updated, practitioner focused review of river water temperature modelling. Such a review can then provide the basis for development of a robust framework for river water temperature projection. This report provides a roadmap for this by presenting: (1) an overview of the methods available for modelling contemporary water temperature and for making projections of water temperature under likely future scenarios; (2) decision trees to guide users towards selection of suitable modelling approaches given constraints in data availability, analytical requirements, spatial scale and computational demand; and, (3) a step-by-step, flexible framework (constrained by current data availability) for producing projections of future river water temperature at a range of spatial and temporal scales.

Methodology

Three key steps were undertaken to identify a suitable framework for water temperature modelling that could facilitate future projections and offer a flexibility to accommodate varied use cases. First, a review of the contemporary literature was undertaken to enable identification of the methods available for water temperature modelling. Second, following discussion with Environment Agency specialists, key properties of the models were tabulated to help identify feasible approaches based on reporting priorities and potential limitations (e.g. model time step, data availability, computational demand, etc). Third, decision trees were developed to enable users to identify the best approach for modelling water temperature for a given use case (e.g. across a range of spatial and temporal resolutions). Finally, following further discussion with Environment Agency specialists the most suitable modelling approach was identified (based on current data availability and likely future resource allocation) and a flexible framework for implementation outlined.

Identification of relevant literature

To assess the availability of stream water temperature modelling approaches a systematic review was undertaken following the approach outlined by Pickering and Byrne (2014). The goal was to identify trends in the use of different modelling approaches and emerging methods rather than undertake statistical analysis of evidence, as is common in the meta-analyses of the medical sciences. Utilizing Web of Science automated the process as recent research has highlighted this as the most suitable search engine for systematic review (Gusenbauer & Haddaway 2020). The search results were augmented by manual searches of the literature. The aim was to include papers and studies that explicitly developed or used water temperature models and the search criteria were defined as follows:

TS=("river water temperature" AND model) OR TS =("stream water temperature" A ND model*) ORTS =("stream temperature" AND model*) OR TS =("river temperature " AND model*) OR TS = ("river temperature" AND prediction*) OR TS = ("stream tem perature" AND prediction*) OR TS = ("river water temperature" AND prediction*)*

Here TS = subject area and the * denotes a wildcard that retrieves variants of the word, for example plurals and different spellings. This initial search returned 998 publications. The search criteria were further refined to return only literature published over the last 30 years and then a screening of title and abstract was conducted. This yielded 338 publications (including 5 identified from manual searches) that were used to form the basis of this review

Data availability and spatio-temporal reporting requirements

The Environment Agency has monitored water temperature at ~30,000 sites across England and Wales. Most of the associated 42 million data records are spot measurements that were typically measured twice a month, between 08:00 and 16:00 h. Sub-daily measurements (hourly -15-min resolution) are available for 351 sites but further data quality checks are required to assess the suitability of this data for modelling purposes. The average site record length is 14 years, but this is skewed to sites monitored at weekly – monthly intervals (Orr et al. 2015). It is important to note that no guidance was provided to operatives regarding time of day that sampling should be undertaken; hence this coupled with irregular sampling could introduce systematic bias into the water temperature dataset (Toone et al., 2011).

To understand the impact of climate change on river systems at different times and places the Environment Agency has a range of spatio-temporal reporting requirements. Of particular relevance here are the need for: (1) *Reach scale projections* of changes in water temperature across the river network in England that can indicate absolute and relative change values at different time scales (i.e. daily, monthly, seasonal, annual, 30 year averages). (2) *Station/site specific projections* that can also indicate absolute and relative change at varied time scales. Reach scale projection can provide an understanding of risks and vulnerabilities in different locations, drive water quality models and produce a range of other outputs (for example a network map of future water temperatures). While station specific projections focus on a set of monitoring stations (c.f. Future Flows) and can enable site specific and national understanding of temperature change and risk. The key use of river water temperature projections would be to drive existing water quality models, develop new ecosystem models and produce visualisations of changes in river water temperature.

Given that additional monitoring or data collection is unlikely, any framework for developing future projections will be constrained by data availability (i.e. a lack of sub-daily data for model building). In addition, given the range of potential use cases flexibility of the framework is an important property. In particular it should be adaptable in response to the particular reporting requirements and data availability, with flexibility regarding the spatial and temporal resolution of input data and the modelling outputs. Another important requirement is the ability to predict to sites that are currently unmonitored (i.e. sites with no water temperature records).

Identification of suitable modelling approaches

Papers were examined and retained if modelling approaches were described that could generate reach scale water temperature predications across the entire river network or for specific monitoring stations/sites. Information on these water temperature modelling approaches was then extracted to facilitate the development of summary tables. Four key model groups were apparent: (1) statistical, (2) process-based, (3) machine learning/ artificial intelligence and (4) hybrid approaches. A separate summary table was constructed for each group of models to act as a quick reference guide to models that have potential for river water temperature projection over large scales. For each model summary information was produced on: spatial resolution, potential to predict at unmonitored sites, the input data requirement, calibration requirements, computational requirements, software availability, advantages, constraints and model response metric (See Table 1). Key references were also identified that either provided a technical overview of the modelling approach or showcased a highly relevant application of that specific model.

Development of decision trees

Decision trees were developed for two purposes, namely to:

1. understand available models and how they are related - highlighting in particular how statistical methods can be considered as building blocks allowing development of progressively more complex models.
2. identify suitable modelling approaches based on data availability and other practical considerations (i.e. those applicable to each use case).

Development of flexible framework for water temperature modelling

A detailed step by step approach was developed for making water temperature projections across large spatial scales but with flexibility to increase spatial resolution. The development of this framework was guided by potential use cases and data availability within the Environment Agency. These can be broadly defined as applications that require data that is spatially distributed across the river network (e.g. water quality models such as SAGIS-SIMCAT) or those that require projections for specific points or stations within the river network (e.g. to assess impact of abstractions or develop a *future-flows* analogue). However, the potential to develop a framework that could provide distributed projections is constrained by the availability of input data for model fitting and validation (i.e. availability of a calibration dataset to cover the environmental ranges of the rivers where predictions are required). Hence, the framework outlined in this report represents the best possible approach for the Environment Agency given their objectives and constraints. In particular, the selection was governed by the need for flexibility around the required model timestep, the spatial configuration of projections (i.e. site vs entire network), model interpretability (i.e. not a black-box) and additional variables available for model development.

Table 1. The key attributes of the water temperature models identified by the literature review. The rationale for selecting these attributes is also highlighted.

Model property	Reason for inclusion
Model detailed description	To provide a reference point for the user
Model approach	Identify if the model can produce predictions that vary across time and space
Spatial resolution	To understand the most appropriate spatial scale for using the model approach (e.g. site vs network)
Prediction for unmonitored sites	To identify if the model has potential to predict for sites with no water temperature records
Time step of input	To help the user identify the temporal resolution of data required to use the model (also guidance on the most suitable time step provided)
Input data	To help the user identify the specific data required to use the model (e.g. air temperature, discharge and land cover)
Calibration requirements	To help the user identify the specific calibration requirements
Response metric	To provide the user with information on the output from the model (e.g. daily mean, weekly mean etc). Guidance also provided on the most suitable output metric.
Computational requirements	The expertise and computational requirements required to calibrate and use the model.
Software available	The available software available for running the model (R packages are identified where possible)
Open source	Provide info on whether the code is open source (useful if the model needs to be adapted in the future)
Advantages	An assessment of the key advantages to help the user make an informed judgement of the model suitability for the anticipated application
Constraints	An assessment of the key constraints to help the user make an informed judgement of the model suitability for the anticipated application
Used with climate projections	Info on whether the model has previously been used to make future projections - an established method may be preferable
Key Reference	A particularly useful reference to help the user understand and implement the model

Notes	Any additional notes that may be important for a user to consider

Results

Available approaches for water temperature modelling

The literature review identified 29 modelling approaches that may be suitable for developing national scale river water temperature projections (Table 2). Statistical (regression based) water temperature models were identified as the most established and widely used approach for modelling contemporary water temperature and making predictions (Table 2). These ranged from simple linear models of air-water temperature relationships, for example see Kelleher et al. (2012), to more complex generalized additive mixed effect models (Siegel & Volk 2019) and techniques emerging from the research domain (e.g. functional regression; Boudreault et al. 2019). Most of these approaches are only capable of making predictions at sites used in the model fit. However, in the case of mixed effect models with additional spatial covariates it is also possible to predict to new discrete points in the catchment, but with reduced accuracy. Spatial statistical river network models represent the current "state of the art" in statistical river temperature modelling; when a river network smoother is used, it can facilitate daily projections of mean/max water temperature but this requires sub-daily calibration data, a topologically correct digital river network with appropriate predictor variables and advanced statistical and programming expertise (Jackson et al. 2018).

Process-based modelling approaches are particularly well suited for prediction to unmonitored sites and projection (Dugdale et al. 2017). They are generally more transferable than statistical models as they represent the physical processes that control warming and cooling of river water. However, applications at larger spatial scales (e.g. greater than the river basin) were limited in the literature as data required for calibration becomes prohibitive (Table 3). *DynWat* a dynamical 1-D water energy routing model may be suitable for large scale water temperature projections (Wanders et al. 2019) but the errors associated with limited calibration are problematic and the coarse scale (10 km resolution) does not match river network maps used by the Environment Agency.

A number of emerging research orientated approaches were also identified (Tables 4 & 5) that may be suitable for large scale modelling once they become more accessible to non-specialists and have been applied more commonly to river temperature research thereby facilitating a more rigorous assessment of performance. Machine learning / artificial intelligence and hybrid approaches have mainly been used for prediction of current water temperature at specific sites (Zhu & Piotrowski 2020). Deep learning and hybrid wavelet-neural network models seem to hold the most potential for generating large scale projections (Rahmani et al. 2021).

Table 2. Summary table providing an overview of the statistical models used for water temperature modelling. Model N (number) is provided to aid cross-referencing with the decision trees. More detailed information on column criteria can be found in Table 1 in the methods section.

Model N	Model detailed description	Model approach	Spatial resolution	Prediction for unmonitored sites	Time step of input	Input data	Calibration requirements	Response metric	Computational requirements	Software available	Open source	Advantages	Constraints	Used with climate projections	Key references	Notes
1	Linear regression	Static	Site specific	Limited potential	*Has been used:* **daily - annual.** *Works best for:* **weekly - monthly**	Air temperature	Site specific water temperature and air temperature records for calibration	*Has been used:* **daily - annual mean or max** *Works best for:* **weekly - monthly mean or max**	Low -most basic statistical software can implement model calibration and fitting	R (lm function) SPSS MATLAB	Y	Well established technique that is widely used. Simple to implement and interpret	Site specific, linearity not always a valid assumption, autocorrelation not considered.	Yes	Stefan & Preudhomme (1993); Kelleher et al. (2012)	Most basic approach with limited potential for accurate future predictions. Need to correct for differences between air temperature station and water temperature station (e.g. altitude distance to the coast) - see Detenbeck et al (2016)
2	(Multiple) linear regression	Static	Site specific	Limited potential - however see Hrachowitz et al. (2010) and model (6) below for an extension for predication to unmonitored locations	*Has been used:* **daily - annual.** *Works best for:* **weekly - monthly**	Air temperature + Discharge + Other met. vars + Catchment descriptors	Site specific water temperature, air temperature and discharge records for calibration	*Has been used:* **daily - annual mean or max** *Works best for:* **weekly - monthly mean or max**	Low -most basic statistical software can implement model calibration and fitting (e.g. R or SPSS)	R (lm function) SPSS MATLAB	Y	Well established technique that is Widely used. Relatively Simple to implement and interpret	Site specific, linearity not always a valid assumption, autocorrelation not considered. Also need to consider collinearity and model parsimony. Constrained by calibration period	Yes	Ducharne (2008); Kelleher et al. (2012); Segura et al. (2015)	Good predictor variables: Discharge, lagged air temperature, snow melt solar radiation, humidity, riparian shading, river order, baseflow index, ground water , impervious land cover. Need to correct for differences between air temperature station and water temperature station (e.g. altitude distance to the coast)

Model N	Model detailed description	Model approach	Spatial resolution	Prediction for unmonitored sites	Time step of input	Input data	Calibration requirements	Response metric	Computational requirements	Software available	Open source	Advantages	Constraints	Used with climate projections	Key references	Notes
3	LASSO/ Ridge regression/support vector (extension of linear regression)	Static	Site specific	Limited potential	*Has been used:* **daily**	Air temperature + Catchment descriptors for groupings	Site specific water temperature, air temperature for calibration	*Has been used:* **daily max** *Works best for:* **daily - annual mean or max**	Low -most basic statistical software can implement model calibration and fitting (e.g. R or SPSS)	R (caret package)	Y	Established technique but not Widely used for water temperature modelling	Site specific, linearity not always a valid assumption, autocorrelation not considered. Also need to consider collinearity and model parsimony. Constrained by calibration period	Yes	St-Hilaire et al. (2018); Rehana (2019)	
4	Logistic regression	Static	Site specific	Limited potential	*Has been used:* **daily - annual.** *Works best for:* **weekly - monthly**	Air temperature	Site specific water temperature and air temperature records for calibration	*Has been used:* **daily - annual mean or max** *Works best for:* **weekly - monthly mean or max**	Low -most basic statistical software can implement model calibration and fitting (e.g. R or SPSS)	R (nls function) SPSS MATLAB	Y	Well established technique that is simple to implement and interpretation only slightly more difficult than linear regression	Parameters of model are site specific, sites do not always adhere to S-shaped curve. Autocorrelation not considered.	Yes	Mohseni et al. (1998); Koch and Grunewald (2010)	Good predictor variables: Weighted lagged air temperature. Need to correct for differences between air temperature station and water temperature station (e.g. altitude distance to the coast)
5	(multiple) Logistic regression extension	Static	Site specific	Limited potential	*Has been used:* **daily - annual.** *Works best for:* **weekly - monthly**	Air temperature + Discharge + Other met. vars + Catchment descriptors	Site specific water temperature, air temperature and discharge records for calibration	*Has been used:* **daily - annual mean or max** *Works best for:* **weekly - monthly mean or max**	Intermediate - statistical software can implement model calibration and fitting (e.g. R or SPSS). However user will need to have a good understanding of programming to implement as will not be possible from dropdown menu options	R (nls function) SPSS MATLAB - Captain toolbox	Y	Well established technique but requires some knowledge of statistics and programming. Interpretation is still relatively straight forward	Parameters of model are site specific, sites do not always adhere to S-shaped curve. Autocorrelation not explicitly considered.	Yes	Van Vliet et al. (2011); Johnson et al (2014); Piotrowski & Napirorkowski (2019)	Extension including declination angle of the sun

Model N	Model detailed description	Model approach	Spatial resolution	Prediction for unmonitored sites	Time step of input	Input data	Calibration requirements	Response metric	Computational requirements	Software available	Open source	Advantages	Constraints	Used with climate projections	Key references	Notes
6	Multiple regression models at single sites	Static	Site specific	Some potential	*Has been used:* **monthly**	Air temperature + Discharge + Other met. vars + Catchment descriptors	Site specific water temperature, air temperature	*Has been used:* **monthly max**	Intermediate - statistical software can implement model calibration and fitting (e.g. R or SPSS). However user will need to have a good understanding of programming to implement as will not be possible from dropdown menu options	R (various packages)	Y	Extension to a well-established technique but is moderately difficult to implement and requires some knowledge of statistics and programming.	Parameters of model need to be resampled so can lead to bias as spatial covariance is not included in model	Yes	Hrachowitz et al. (2010)	
7	Generalised linear modelling	Temporal (spatial as random effect)	Site specific	Some potential when using random effects	*Has been used:* **daily** *Works best for:* **daily - annual**	Air temperature + Discharge + Other met. vars + Catchment descriptors	Site specific water temperature, air temperature and discharge records for calibration	*Has been used:* **daily max** *Works best for:* **daily - annual mean or max**	Intermediate - statistical software can implement model calibration and fitting (e.g. R or SPSS). However user will need to have a good understanding of programming to implement as will not be possible from dropdown menu options	R (packages lme or lm4) SPSS MATLAB	Y	Established technique but not widely used for water temperature modelling. Enables temporal and spatial errors to be incorporated. Flexible - models can be nested with random effects at varying spatial and temporal scales.	Can be computationally demanding to fit and convergence can be an issue.	No	Wehrly et al. (2009); Moore et al. (2013); Siegel & Volk (2019)	

Model N	Model detailed description	Model approach	Spatial resolution	Prediction for unmonitored sites	Time step of input	Input data	Calibration requirements	Response metric	Computational requirements	Software available	Open source	Advantages	Constraints	Used with climate projections	Key references	Notes
8	Generalised additive modelling	Temporal (spatial as random effect)	Site specific	Some potential when using random effects	*Has been used:* **daily - weekly** *Works best for:* **any time step**	Air temperature + Discharge + Other met. vars + Catchment descriptors	Site specific water temperature, air temperature and discharge records for calibration	*Has been used:* **daily max and daily mean** *Works best for:* **daily - annual mean or max**	Intermediate - statistical software can implement model calibration and fitting (e.g. R or SPSS). However user will need to have a good understanding of programming to implement as will not be possible from dropdown menu options	R (mgcv package) SPSS	Y	Well established technique but not as easy to fit or interpret. Flexible and can account for non-linear relationship between air-water temperature. Flexible so can include temporal and spatial structure to the model. Need statistical knowledge and programming skills.	Can be computationally demanding to fit and prone to overfitting.	No	Wehrly et al. (2009); Laanaya et al. (2017); Jackson et al. (2017); Siegel & Volk (2019)	Can be used to establish breakpoints in air-water temperature relationship
9	Functional Regression Models	Static (can have temporal and spatial elements but not currently used for water temperature)	Site specific	New method so potential remains unknown	*Has been used:* **daily - monthly** *Works best for:* **daily - monthly**	Air temperature + Discharge + Other met. vars + Catchment descriptors	Site specific water temperature, air temperature, meteorological variables and discharge records for calibration	*Has been used:* **annual stream temperature curves** *Works best for:* **limited studies to make**	Intermediate computational demand. Statistical software can implement model calibration and fitting (e.g. R). However, user will need to have a good understanding of programming and background in statistics.	R (Fdboost package)	Y	New approach for water temperature modelling uses a curve instead of daily, weekly, or monthly metrics hence captures more of its variability. Flexible approach enables additional predictors to be incorporated into the model.	Difficult to interpret output and requires a high level of statistical expertise to implement.	No	Boudreault et al. (2019)	

Model N	Model detailed description	Model approach	Spatial resolution	Prediction for unmonitored sites	Time step of input	Input data	Calibration requirements	Response metric	Computational requirements	Software available	Open source	Advantages	Constraints	Used with climate projections	Key references	Notes
10	Autoregressive model	Temporal	Site specific	Limited potential	*Has been used:* **daily - monthly** *Works best for:* **daily - monthly**	Air temperature + discharge	Site specific water temperature and air temperature records for calibration. Long time series best (>15 years).	*Has been used:* **daily - monthly mean or max** *Works best for:* **weekly - monthly mean or max**	Intermediate - statistical software can implement model calibration and fitting (e.g. R or SPSS). However user will need to have a good understanding of programming required to implement as is not be possible from dropdown menu options	R (arima function, package forecast) SPSS MATLAB	Y	Well established technique that is relatively simple to implement. Accounts for temporal autocorrelation. Interpretation more difficult than linear regression but still relatively straight forward	Long time series are required for calibration. The transferability limited as functions need to be fitted for each new monitoring location. Stationarity is assumed so problematic for predicting for future climate scenarios. Spatial structure not considered.	Yes	Caissie et al. (2007); Benyahya et al. (2007)	
11	Periodic Autoregressive Models	Temporal	Site specific	Limited potential	*Has been used:* **daily - monthly** *Works best for:* **daily - monthly**	Air temperature + discharge	Site specific water temperature and air temperature records for calibration. Long time series best (>15 years).	*Has been used:* **daily - monthly mean or max** *Works best for:* **Daily - monthly mean or max**	Intermediate - statistical software can implement model calibration and fitting (e.g. R or SPSS). However user will need to have a good understanding of programming required to implement as is not be possible from dropdown menu options	R (package parts) SPSS MATLAB	Y	Established technique that is relatively simple to implement and interpretation more difficult than linear regression	Long time series are required for calibration. The transferability limited as functions need to be fitted for each new monitoring location. Prone to overfitting that can be an issue for future climate scenarios. Spatial structure not considered.	No	Benyahya et al. (2008); Graf (2018); Hague and Patterson (2014)	

Model N	Model detailed description	Model approach	Spatial resolution	Prediction for unmonitored sites	Time step of input	Input data	Calibration requirements	Response metric	Computational requirements	Software available	Open source	Advantages	Constraints	Used with climate projections	Key references	Notes
12	Linear Spatial Statistical Network models	Spatial	Distributed (predictions for the whole river network)	Good potential	*Has been used:* **monthly** *Works best for:* **monthly**	Air temperature + Discharge + Other met. vars + Catchment descriptors + topologically correct (unbroken, non-circuitous) Digital River Network	Spatially distributed water temperature records covering the environmental range required for prediction. Paired or gridded air temperature records also required for calibration.	*Has been used:* **monthly mean or max** *Works best for:* **summarized metrics (e.g. monthly max)**	High computational demand (e.g. many days to fit large model using 16 cores). Statistical software can implement model calibration and fitting (e.g. R or SPSS). Users will need a good understanding of programming to implement as is not be possible from dropdown menu options	R (SSN package) STARS toolset for geo processing in ARC Map OpenSTARS package for R (Kattwinkel et al 2020)	Y	Relatively new technique but with good package support. Potential to predict for unmonitored locations across the entire river network. Has been successfully used to predict summer temperature maxima	May only be effective when links between climate, groundwater, and topography is regionally constant. Computationally demanding and calibration requirements are data heavy. Can't incorporate temporal variability so is static - hence multiple models would be required for annual monthly prediction	Yes	Isaak et al. (2017); Lee et al. (2020)	Good potential for prediction of unmonitored sites however the GIS and calibration data requirements may be the limiting factor.
13	River network smoother models	Spatio-Temporal	Distributed (predictions for the whole river network	Good potential	*Has been used:* **daily - monthly** *Works best for:* **daily - monthly**	Air temperature + Discharge + Other met. vars + Catchment descriptors+ topologically correct (unbroken, non-circuitous) Digital River Network	Spatially distributed water temperature records covering the environmental range required for prediction. Lidar surveys may be possible see Lee et al (2020). Air temperature records for calibration.	*Has been used:* **daily - monthly mean or max** *Works best for:* **weekly - monthly mean or max**	High computational demand (e.g. many days to fit large model using 16 cores). Statistical software can implement model calibration and fitting. Users need a good understanding of programming to implement as is not be possible from dropdown menu options or currently developed packages	No dedicated package Can use Stars for preprep OpenSTARS package for R (Kattwinkel et al 2020). Fitting using existing packages to create river network smoother (mgvc)	Y	Relatively new technique that can be implemented using open source data analysis and statistical tools. Potential to predict for unmonitored locations across the entire river network. River network smoother more flexible than SSN Can incorporate space and time.	RNS not transferable between catchments. No direct package support. Significant data and computational requirements. Statistical and programming expertise required.	Yes - but not published	Jackson et al. (2018); O Donnell et al. (2014)	Good potential for prediction of unmonitored sites however the GIS and calibration data requirements may be the limiting factor.

Table 3. An overview of the process-based models used for water temperature modelling (see Table 1 in methods for details on column criteria). Met = Meteorological variables, GIS = spatial data including land cover, elevation, distance from source/sea etc, Hydro = hydrological variables (discharge or groundwater etc).

Model N	Model detailed description	Model approach	Spatial resolution	Prediction for unmonitored sites	Time step of input	Input data	Calibration requirements	Response metric	Computational requirements	Software available	Open source	Advantages	Constraints	Used with climate projections	Key references	Notes
14	BasinTemp or SnTemp (simplified heat budget)	Spatio-temporal	Distributed - Watershed	Good potential	Daily (for discharge data)	**GIS:** Digital elevation model (30m res), tree height, vector based stream network (minimum 1:24000), channel geometry, daily **Hydro:** mean daily discharge,	Spatially distributed water temperature monitoring stations to account for basin size, drainage density, and vegetation and lithological heterogeneity	Daily - monthly mean or max temperature	Computational requirements unclear for modelling at a scale larger than a single water shed.	Proprietary (Still Water Science)	N	Good support and well established. A simple hydrological model is included. No met data required as assumes that direct shortwave radiation drives summertime stream temperatures. So can calculate temperature based on latitude, aspect and riparian shading.	GIS data requirements are demanding (e.g. tree heights). The cost may be prohibitive. May need adaption for predictions based on future climate data as assumes solar radiation is the key drivers of heat budget	No	Allen et al. (2007)	May require further development to enable predictions based on air temperature
15	DHSVM-RBM (Distributed Hydrology Soil Vegetation Model coupled with semi-Lagrangian stream temperature model RBM) or VIC-RBM	Spatio-temporal	Distributed - Watershed	Good potential	Daily (for discharge data)	**Met variables:** precipitation, air temperature, down-ward shortwave and longwave radiation, wind speed, and relative humidity **Hydro**: discharge **GIS**: River network (slope and length) and vegetation cover for shading, soil data, land cover	Demanding as both the discharge and temperature components need to be calibrated	Daily - monthly mean or max temperature	Computationally demanding - state for space models. Requires highly specialised skill set to implement	Fortran Free download http://www.hydro.washington.edu/Lettenmaier/Models/RBM/index.shtml	Y	Characterization of the impacts of climate, landscape, and near-stream vegetation changes on stream temperature and allows modelling of spatially distributed water temperature for the entire stream network.	Computational requirements may prohibit use for large scale modelling	Yes	Sun et al. (2015); Yearsley et al. (2019); Van Vliet 2013	

Model N	Model detailed description	Model approach	Spatial resolution	Prediction for unmonitored sites	Time step of input	Input data	Calibration requirements	Response metric	Computational requirements	Software available	Open source	Advantages	Constraints	Used with climate projections	Key references	Notes
16	T-net model (equilibrium temperature)	Spatio-temporal	Distributed - Watershed	Good potential	Daily	**Met variables:** air temperature, specific humidity , wind velocity , global radiation and atmospheric radiation **Hydro**: discharge, GW flow, GW temperature **GIS**: River network (slope and length) and vegetation cover for shading	Spatially distributed water temperature and discharge monitoring stations to account for environmental heterogeneity	Daily - monthly mean or max temperature	Computationally demanding as discharge and groundwater flows need to be spatially distributed so coupling with a hydrological model required. Multiple steps required to solve the heat budget	N	N	Performs best for lower order streams. Proven to work across large catchments (e.g. Loire Basin)	Requires highly specialised skillset to implement (programming) . Seasonal bias due to fixed shading factor. Sensitive to variations in hydraulics	Yes	Beaufort et al. (2016)	
17	Dynamical 1-D water energy routing model (DynWat)	Spatio-temporal	Global (10km resolution)	Good potential	Daily	**Met variables**: precipitation, air temperature, down-ward shortwave and longwave radiation, wind speed, and relative humidity **Hydro**: 1. direct runoff or surface runoff;2. interflow;3. base flow or groundwater discharge; and 4. simulated or estimated temperature of these fluxes **GIS:** Land Processes Distributed Active Archive Centre, HYDRO1kElevation Derivative Database, http://eros.usgs.gov/#/Find_Data/Products_and_Data_Available/gtopo30/hydro	Spatially distributed water temperature and discharge monitoring stations to account for environmental heterogeneity	Daily - annual mean or max temperature. Works best for monthly/annual to assess long term trends	Computationally demanding as discharge needs to be spatially distributed hence coupling with a hydrological model required.	Model dynWat link: https://github.com/wande001/dynWat/tree/master/model Coupled hydrological Model PCR-Globwb2 https://github.com/UU-Hydro/PCR-GLOBWB_model	Y	Can provide daily estimates of water temperature across very large spatial scales. Based on GIS layers that are freely available with no need for pre processing.	Requires highly specialised skillset to implement (programming) . Coarse scale (10 km) and river network may not match requirements (i.e. hydrosheds network)	Yes	Wanders et al. (2019)	

Model N	Model detailed description	Model approach	Spatial resolution	Prediction for unmonitored sites	Time step of input	Input data	Calibration requirements	Response metric	Computational requirements	Software available	Open source	Advantages	Constraints	Used with climate projections	Key references	Notes
18	I Tree	Spatio-temporal	Reach - watershed	Good potential across small spatial scales	Hourly	Input data requirements are particular demanding and include: **Hydro** - discharge for river and lateral storm sewer inflows, groundwater and hyporheic exchange **Met -**precipitation, air temperature, down-ward shortwave and longwave radiation, wind speed, and relative humidity **GIS:** Land cover and shading data	Spatially distributed water temperature and discharge monitoring stations to account for environmental heterogeneity	Hourly mean	Computationally demanding.	Freely available code in C++ for VisualStudio ,thttp://www.itreetools.org/research_suite/coolriver.	Y	Can provide hourly stream temperature estimates. Can model urban impacts on heat budget and diel variability in riparian shading Useful for simulating river warming or cooling due to urban development or greening. Well documented source code so can be adapted/ extended if required.	Requires programming knowledge to implement. Only suitable for modelling reach to small basin scale due to input data requirements	No	Abdi et al 2020	Added as may be suitable for informing tree planting strategies in headwaters

Table 4. An overview of machine learning models used for water temperature modelling (see Table 1 in methods for details on column criteria).

Model N	Model detailed description	Model approach	Spatial resolution	Prediction for unmonitored sites	Time step of input	Input data	Calibration requirements	Response metric	Computational requirements	Software available	Open source	Advantages	Constraints	Used with climate projections	Key references	Notes
19	K-nearest neighbour	Static	Site specific	Limited potential	*Has been used:* **daily - monthly** *Works best for:* **daily - monthly**	Air temperature + Discharge + Other met. vars + Catchment descriptors	Site specific water temperature and air temperature records for calibration	*Has been used:* **daily max** *Works best for:* **daily - annual mean or max**	Intermediate - statistical software can implement model calibration and fitting (e.g. R or SPSS). However user will need to have a good understanding of programming to implement as will not be possible from dropdown menu options	Can be implemented in R using the tidymodels or caret package	Y	Established technique but not widely used for river temperature modelling. Flexible approach can include a multivariate dataset	Model tuning can be difficult. Long time series usually required for calibration.	No	Benyahya et al. (2008) St-Hilaire et al. (2012)	Models performed best when using lagged air and water temperature as predictors
20	Artificial Neural Network (feed forward)	Static	Site specific	Some potential	*Has been used:* **Hourly-monthly** *Works best for:* **daily - monthly**	Air temperature + Discharge + Other met. vars + Catchment descriptors	Site specific water temperature and air temperature records for calibration	*Has been used:* **daily - monthly max mean** *Works best for:* **daily - monthly mean or max**	Demanding - user will need to have a good understanding of programming to implement as will not be possible from dropdown menu options	See R package wateRtemp github.com/MoritzFeigl/wateRtemp	Y	Established technique that has been widely used in hydrology and specifically for water temperature modelling. Flexible approach that can incorporate a range of static and dynamic variables	Black box - difficult to identify relationship between predictor and response. Model tuning can be difficult. Long time series usually required for calibration.	Yes	Zhu et al. (2018) DeWeber & Wagner (2014)	
21	ANN and deep learning (long short-term memory)	Static	Site specific	Some potential	*Has been used:* **daily - monthly** *Works best for:* **daily - monthly**	Air temperature + Discharge + Other met. vars + Catchment descriptors	Site specific water temperature and gridded meteorological data	*Has been used:* **daily mean / max** *Works best for:* **daily - annual mean or max**	Demanding - user will need to have a good understanding of programming to implement as will not be possible from dropdown menu options	Can be implemented in Python using HYdroDL code (https://github.com/mhpi/hydroDL)	Y	Can outperform conventional statistical approches. in terms of accuracy Can be used to predict point scale temperature based on basin meteorological averages. Can predcit discharge for ungauged basins that can improve model accuracy.	Model tuning can be difficult and an experienced computer scientist is required. Black box model so can't extract physical basis. Still in the research phase so risky to implement.	Yes	Rahmani et al. (2021); Qiu et al. (2021)	

Model N	Model detailed description	Model approach	Spatial resolution	Prediction for unmonitored sites	Time step of input	Input data	Calibration requirements	Response metric	Computational requirements	Software available	Open source	Advantages	Constraints	Used with climate projections	Key references	Notes
22	GPR (Gaussian Process Regression)	Static	Site specific	Limited potential	*Has been used:* **daily** *Works best for:* **unclear due to limited studies**	Air temperature + Discharge + Other met. vars + Catchment descriptors	Site specific water temperature and air temperature records for calibration	*Has been used:* **daily mean / max** *Works best for:* **unclear due to limited studies**	Demanding - user will also need to have a good understanding of programming to implement as will not be possible from dropdown menu options	Can be implemented in R using the tidymodels or caret package	Y	Can outperform conventional statistical approaches in terms of accuracy. Can be used to predict point scale temperature. It combines various machine learning tasks, including model training, uncertainty estimation, and hyper parameter estimation, which is its major advantage over the other machine learning methods.	Model tuning and selection of prior can be difficult and an experienced computer scientist is required. Limited number of applications for river water temperature.	No	Zhu et al (2018) Grbic et al. (2013)	
23	Random Forest	Static	Site specific	Limited potential	*Has been used:* **daily** *Works best for:* **unclear due to limited studies**	Air temperature + Discharge + Other met. vars + Catchment descriptors	Site specific water temperature and air temperature records for calibration	*Has been used:* **daily mean** *Works best for:* **unclear due to limited studies**	Demanding - user will need to have a good understanding of programming to implement as will not be possible from dropdown menu options	Can be implemented in R using the tidymodels or caret package	Y	Insensitive to missing values	Model tuning can be difficult	No	Feigl et al (2021)	Paper still under open review in HESS
24	Extreme gradient boosting	Static	Site specific	Limited potential	*Has been used:* **daily** *Works best for:* **unclear due to limited studies**	Air temperature + Discharge + Other met. vars + Catchment descriptors	Site specific water temperature and air temperature records for calibration	*Has been used:* **daily mean** *Works best for:* **unclear due to limited studies**	Demanding - user will need to have a good understanding of programming to implement as will not be possible from dropdown menu options	Can be implemented in R using the tidymodels or caret package	Y	Insensitive to missing values	Model tuning can be difficult	No	Feigl et al (2021)	Paper still under open review in HESS

Table 5. An overview of hybrid models used for water temperature modelling (see Table 1 in methods for details on column criteria).

Model N	Model detailed description	Model approach	Spatial resolution	Prediction for unmonitored sites	Time step of input	Input data	Calibration requirements	Response metric	Computational requirements	Software available	Open source	Advantages	Constraints	Used with climate projections	Key references	Notes
25	Gallice-physics-derived statistical model	Hybrid	Point/ reach	Some potential but needs further validation	Monthly	**Met**: air temperature **GIS**:DEM (<10m), Corrected river network, land cover information **Hydro**: discharge	Site specific water temperature and air temperature records for calibration	*Has been used:* **Monthly mean** *Works best for:* Monthly mean	Intermediate - Can be implemented in many programming languages. User will need to have a good understanding of programming to implement and parameterise	No	N	Data requirements are minimal compared to physically based models. Model parameters have a physical basis so can be readily interpreted	Not tested outside Switzerland so would need to be parametrised for new locations	No	Gallice et al. (2015)	
26	Air2stream	Hybrid	Point/ reach	Some potential	Daily data	Air temperature and discharge	Site specific water temperature and air temperature records for calibration	*Has been used:* **daily - annual mean or max** *Works best for:* **weekly - monthly mean or max**	Demanding - can be implemented in Fortran with data prep and validation possible in other software in (e.g. MATLAB). User will need to have a good understanding of programming principals to implement as will not be possible from dropdown menu options.	Model source code available: https://github.com/marcotoffolon/air2stream. For Machine learning extensions for optimization MATLAB code available (see Piotrowski & Napiorkowski 2018)	Y	Can outperform traditional regression approaches and only requires minimal data to drive the model. Physical basis means predictions outside observed range possible.	Still in the research phase. Model optimization can be difficult with many different techniques available with no consensus on the best approach	No but has been used to hindcast long time series (see Islam et al., 2019)	Toffolon & Piccolroaz (2015) Piccolroza et al. (2016)	Lumped heat budget model. Can use gridded temperature data as an input. Uses single ordinary differential equation linearly dependent on air temperature, water temperature and discharge.
27	The Integrated Soil-Water-Balance and Artificial Neural Network version 1 (SWB-ANNv1)	Hybrid	Spatially distributed	Good potential	Daily	**Met variables:** air temperature and precipitation **Hydro**: discharge, groundwater delivery and ground water recharge **GIS**: Drainage area, sinuosity (corrected river network required), land cover	Site specific water temperature and air temperature records for calibration	*Has been used:* **daily mean , monthly mean (July)** *Works best for:* **daily mean**	Very Demanding - user will need to integrate the soil water model with a ANN model. A computer scientist is required to implement this model	No	N	Proven to work for spatially distributed future predications. Less demanding in terms of input data a than physically based models	Black box - difficult to interpret model. Computationally demanding so may not be feasible for large scale modelling	Yes	Stewart et al (2015)	

Model N	Model detailed description	Model approach	Spatial resolution	Prediction for unmonitored sites	Time step of input	Input data	Calibration requirements	Response metric	Computational requirements	Software available	Open source	Advantages	Constraints	Used with climate projections	Key references	Notes
28	Wavelet - AI model	Hybrid	point/ reach	Limited potential	Hourly - monthly	Air temperature	Site specific water temperature and air temperature records for calibration	*Has been used:* **daily mean** Works *best for:* **daily mean**	Demanding - can be implemented in MATLAB or R. Users will need to have a good grasp of programming to implement	*Caret* package in R for tuning ANN Multiple packages in R for wavelets including *wavelets*	Y	Performs well with just air temperature as the driver	Model tuning required for each new site. Long time series required (ideally >10 years)	No	Graf et al (2019) Qiu et al (2020)	
29	WT-MLR or Wavelet - fuzzy model	Hybrid	point/ reach	Limited potential	Hourly - monthly	Air temperature	Site specific water temperature and air temperature records for calibration	Has been used: **daily mean**	Demanding - can be implemented in MATLAB or R. Users will need to have a good grasp of programming to implement	*Caret* package in R for tuning ANN Multiple packages in R for wavelets including *biwavelets*	Y	Performs well with just air temperature as the driver	Model tuning required for each new site. Long time series required (ideally >10 years)	No	Zhu et al 2019	

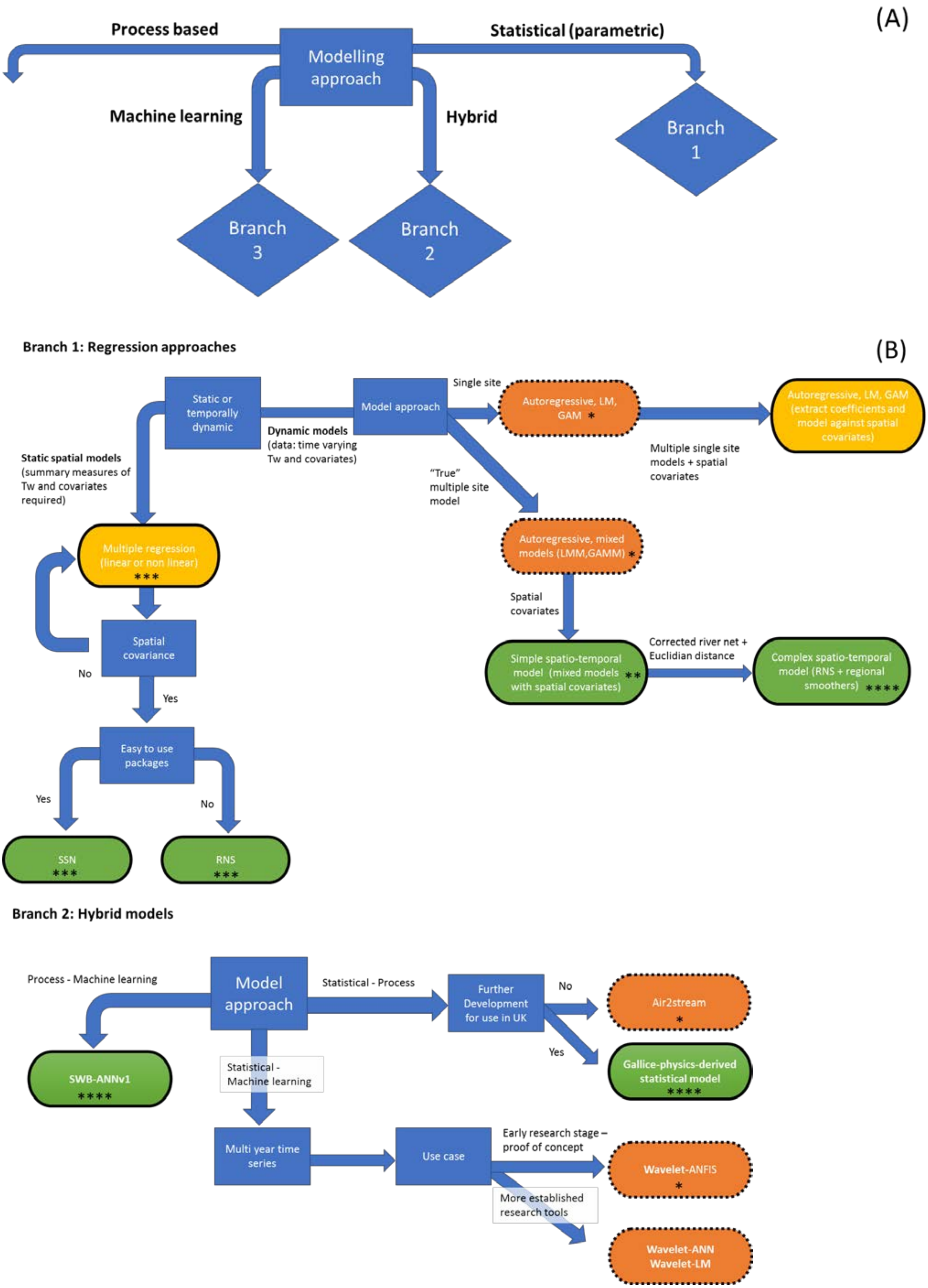
Decision trees for water temperature model selection

A series of decision trees were developed based on discussion with Environment Agency specialists focused around: (1) the information presented in Tables 2 – 5 and (2) the perceived challenges to implementation of a large-scale water temperature model with potential to make projections. A number of modelling approaches identified in Tables 2- 5 were not carried forward to the decision trees as they were deemed unsuitable due to the high data/calibration requirements (e.g. I-Tree or T-net) or lack of example use cases in the literature (e.g. functional regression).

The main goal of the report was to identify a suitable modelling framework based on data availability, analytical requirements, spatial/temporal scale and computational demand. In Figure 1 a set of decision trees is presented for selecting an appropriate modelling approach based first on the generic classification of the modelling approach (i.e. statistical, process based, machine learning or hybrid) and subsequently split by spatial and temporal scale of the predictions. This is particularly useful if a user has a preference for a particular modelling approach. For example if a statistical regression approach is selected (See Figure 1B) then a user can assess how the approaches are linked, the underlying data assumptions and potential to predict to unmonitored locations. An alternative series of decision trees are presented in Figure 2 with the primary split based on the data available for model fitting. Subsequent splits are then based on computational demands, prediction time step and statistical expertise required. This decision making approach is particularly useful when a user has a specific dataset and wishes to assess all the feasible modelling options.

The decision trees were worked through based on the likely data constraints and selection criteria outlined in the Methods section. Given the data limitations and need for an interpretable model it was clear that a statistical approach was required. Both the reach scale and entire river network outputs were not deemed feasible as the calibration/validation data available was not adequate to facilitate a river network model (SSN/RNS; Figure 1B) A mixed effect regression model was deemed the most feasible approach for producing temperature projections as it provided flexibility around the required model timestep (i.e. could be used with sub daily – monthly data) and has potential to predict to unmonitored locations.

The data requirements of a mixed-effect regression model are less demanding when compared to process based modelling approaches and model outputs/coefficients are interpretable, often with a physical basis (unlike black-box machine learning approaches), and there are a wide range of open source software applications available for implementation (Table 2). Furthermore, a mixed-effect regression model is flexible with potential for a wide range of use applications (e.g. station specific or multi-site) and also represents a building block towards a water temperature model for the entire river network (e.g. a spatial statistical model; Jackson et al., 2018).


(A)
Process based
Modelling approach
Statistical (parametric)
Machine learning
Hybrid
Branch 1
Branch 3
Branch 2
(B)
Branch 1: Regression approaches
Static or temporally dynamic
Model approach
Single site
Autoregressive, LM, GAM *
Autoregressive, LM, GAM (extract coefficients and model against spatial covariates)
Dynamic models (data: time varying Tw and covariates)
Multiple single site models + spatial covariates
Static spatial models (summary measures of Tw and covariates required)
"True" multiple site model
Autoregressive, mixed models (LMM,GAMM) *
Multiple regression (linear or non linear) ***
Spatial covariates
Spatial covariance
No
Yes
Simple spatio-temporal model (mixed models with spatial covariates) **
Corrected river net + Euclidian distance
Complex spatio-temporal model (RNS + regional smoothers) ****
Easy to use packages
Yes
No
SSN ***
RNS ***
Branch 2: Hybrid models
Process - Machine learning
Model approach
Statistical - Process
Further Development for use in UK
No
Air2stream *
Yes
Gallice-physics-derived statistical model ****
SWB-ANNv1 ****
Statistical - Machine learning
Multi year time series
Use case
Early research stage – proof of concept
Wavelet-ANFIS *
More established research tools
Wavelet-ANN Wavelet-LM

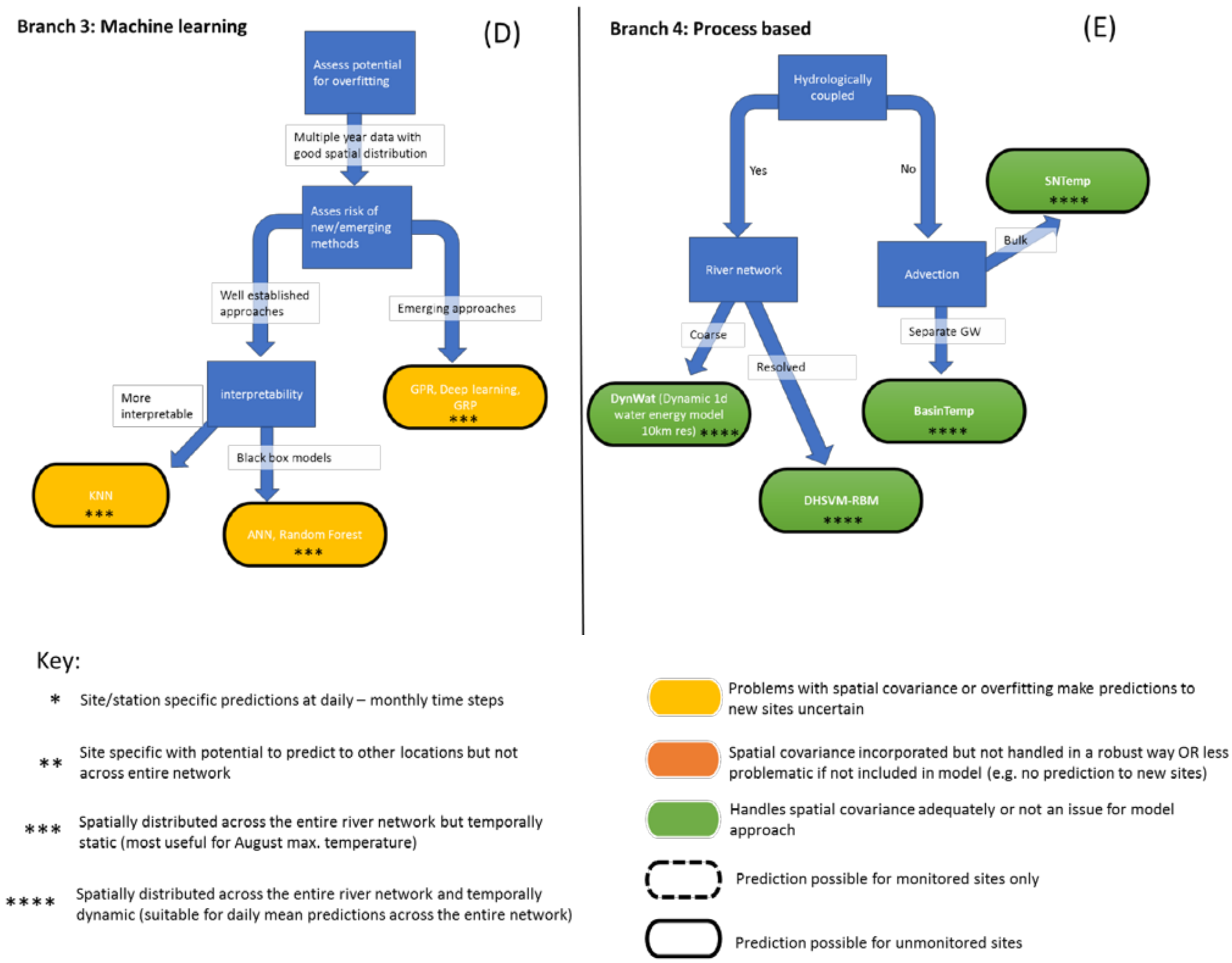
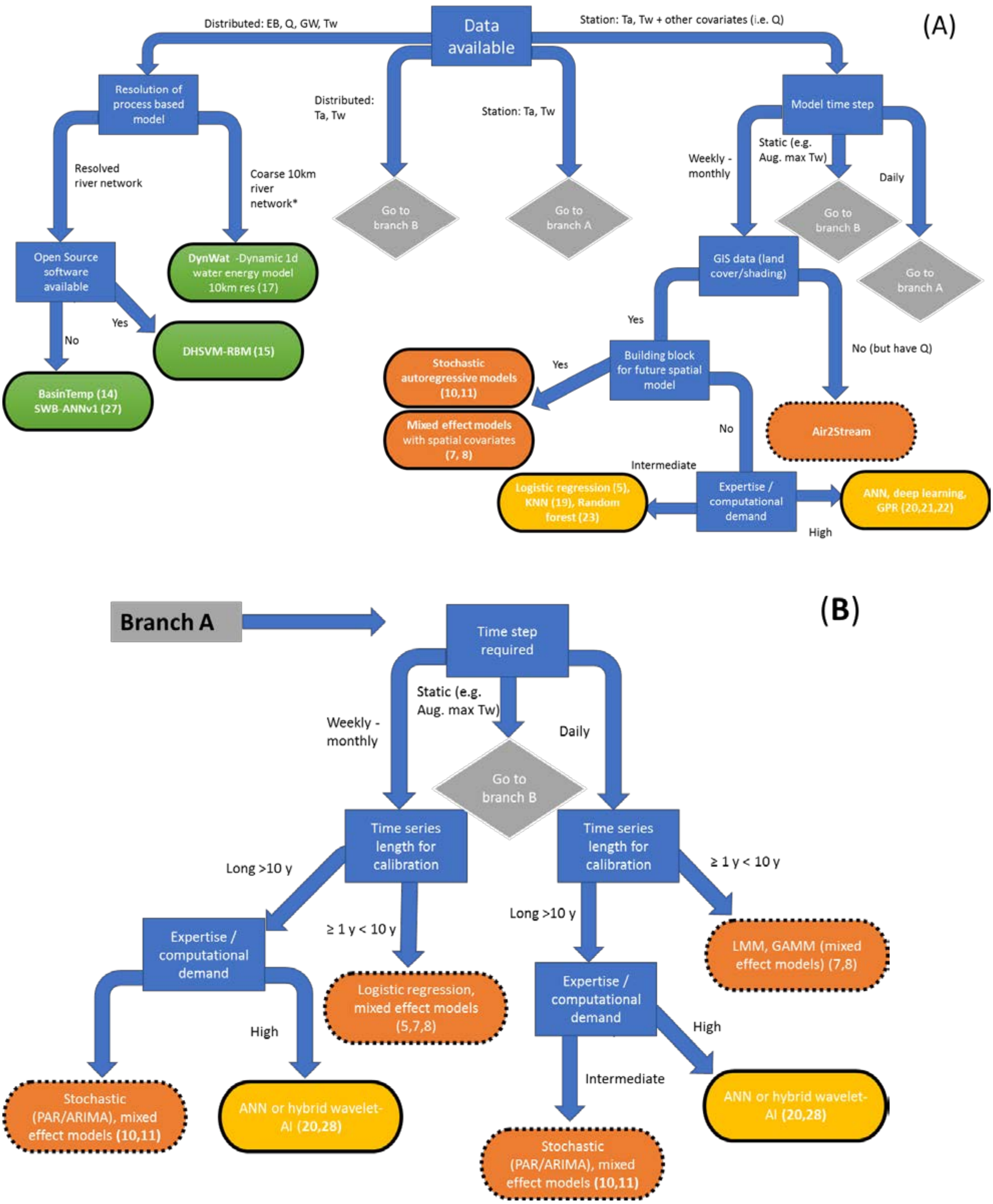


Figure 1. Decision tree for selecting modelling approaches based on the desired modelling approach (i.e. the primary split in the tree is based on the model approach (see A), for example process-based or statistical). Box colour denotes if a model can handle statistical problems associated with spatial covariance (see key). The dashed box outlines denote models that can only predict for monitored sites while solid box outlines are for models that can predict for unmonitored locations. The stars denote whether a model is site specific, spatially distributed or temporally dynamic (see key for detail). Distributed =*Water temperature sites at locations covering range of environmental conditions,* Station = *Location of monitoring stations haphazard (not covering range of env. conditions),* DRN = *Topologically correct (unbroken, non-circuitous) Digital River Network , Ta = Air temperature, Tw = Water temperature,* EB = *Meteorological data required for heat budget / energy balance (e.g. air temperature, humidity, wind speed, radiation, bed heat flux), Q = River flow/discharge, ANN = Artificial Neural Network, LMM/GAMM = Linear /generalized additive mixed effect model, SSN/RNS = Spatial Statistical Model/ River Network Smoother (specific type of SSN), KNN = K-Nearest Neighbour, GPR = Gaussian Process Regression.*


(A)
Data available
Distributed: EB, Q, GW, Tw
Station: Ta, Tw + other covariates (i.e. Q)
Distributed: Ta, Tw
Station: Ta, Tw
Go to branch B
Go to branch A
Resolution of process based model
Resolved river network
Coarse 10km river network*
Open Source software available
DynWat -Dynamic 1d water energy model 10km res (17)
Yes
No
DHSVM-RBM (15)
BasinTemp (14) SWB-ANNv1 (27)
Model time step
Weekly - monthly
Static (e.g. Aug. max Tw)
Daily
Go to branch B
Go to branch A
GIS data (land cover/shading)
Yes
No (but have Q)
Building block for future spatial model
Yes
No
Stochastic autoregressive models (10,11)
Mixed effect models with spatial covariates (7, 8)
Air2Stream
Intermediate
Expertise / computational demand
High
Logistic regression (5), KNN (19), Random forest (23)
ANN, deep learning, GPR (20,21,22)
(B)
Branch A
Time step required
Static (e.g. Aug. max Tw)
Weekly - monthly
Daily
Go to branch B
Time series length for calibration
Time series length for calibration
Long >10 y
≥ 1 y < 10 y
Long >10 y
≥ 1 y < 10 y
Expertise / computational demand
Logistic regression, mixed effect models (5,7,8)
LMM, GAMM (mixed effect models) (7,8)
Expertise / computational demand
High
High
Intermediate
Stochastic (PAR/ARIMA), mixed effect models (10,11)
ANN or hybrid wavelet-AI (20,28)
Stochastic (PAR/ARIMA), mixed effect models (10,11)
ANN or hybrid wavelet-AI (20,28)

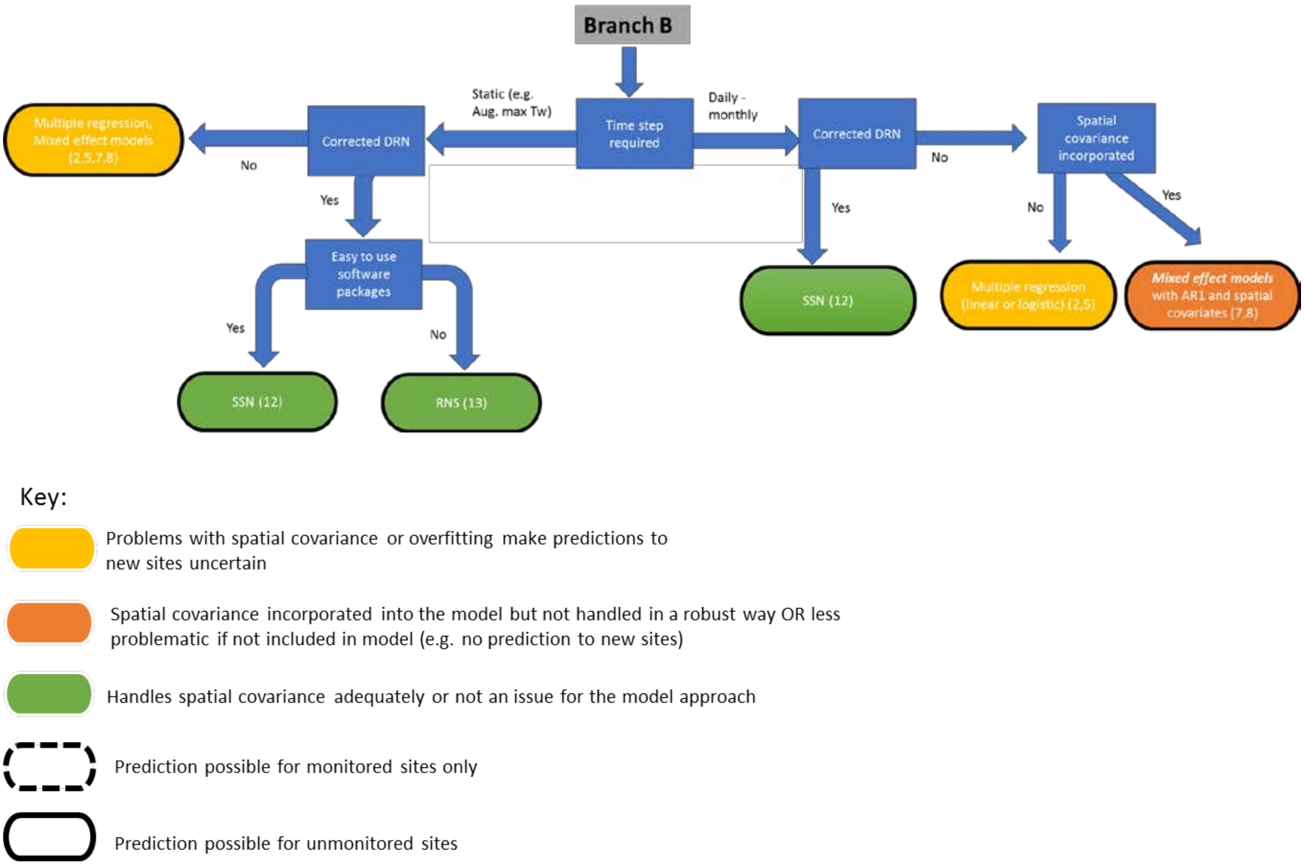


Figure 2. Decision tree for selecting water temperature modelling approaches depending on the availability of data (i.e. the primary split in the tree is based on the data available). Box colour denotes if a model can handle statistical problems associated with spatial covariance (see key). The dashed box outlines denote models that can only predict for monitored sites while solid lines are for models that can predict for unmonitored locations. Distributed =*Water temperature sites at locations covering range of environmental conditions,* Station = *Location of monitoring stations haphazard (not covering range of env. conditions),* DRN = *Topologically correct (unbroken, non-circuitous) Digital River Network , Ta = Air temperature, Tw = Water temperature,* EB = *Meteorological data required for heat budget / energy balance (e.g. air temperature, humidity, wind speed, radiation, bed heat flux), Q = River flow/discharge, ANN = Artificial Neural Network, LMM/GAMM = Linear /generalized additive mixed effect model, SSN/RNS = Spatial Statistical Model/ River Network Smoother (specific type of SSN), KNN = K-Nearest Neighbour, GPR = Gaussian Process Regression.* Note here the number displayed in parentheses relates to the model number in Tables 1 – 4, and is to aid cross-referencing.

Proposed framework for developing a flexible water temperature model

Development of methods for spatially distributed, daily projections of water temperature was deemed not feasible given the temporal resolution of the water temperature data available for model calibration and validation (See Methods section). Following the decision-making process outlined in the previous section a mixed effect regression model was identified as the approach that offered the greatest flexibility and scope for use in multiple applications (e.g. single station to multiple monitoring locations). While this modelling approach has some potential to predict to unmonitored locations any results should be treated with caution and only used when the calibration data covers the full range of environmental conditions within the river network. Furthermore, adequate data for robust validation of predictions is always required and it is still possible to overfit due to issues with spatial covariance (Figure 3). A useful property of a mixed effect regression model is that it represents a building block towards a fully distributed, river network water temperature model (see Figure 1B). Detailed instructions for developing a mixed effect regression model to make water temperature projections are provided in the appendices of this report. These instructions cover all the required steps, including: site/selection, data pre-processing, covariate extraction, exploratory analysis, model selection, model validation and developing projections.

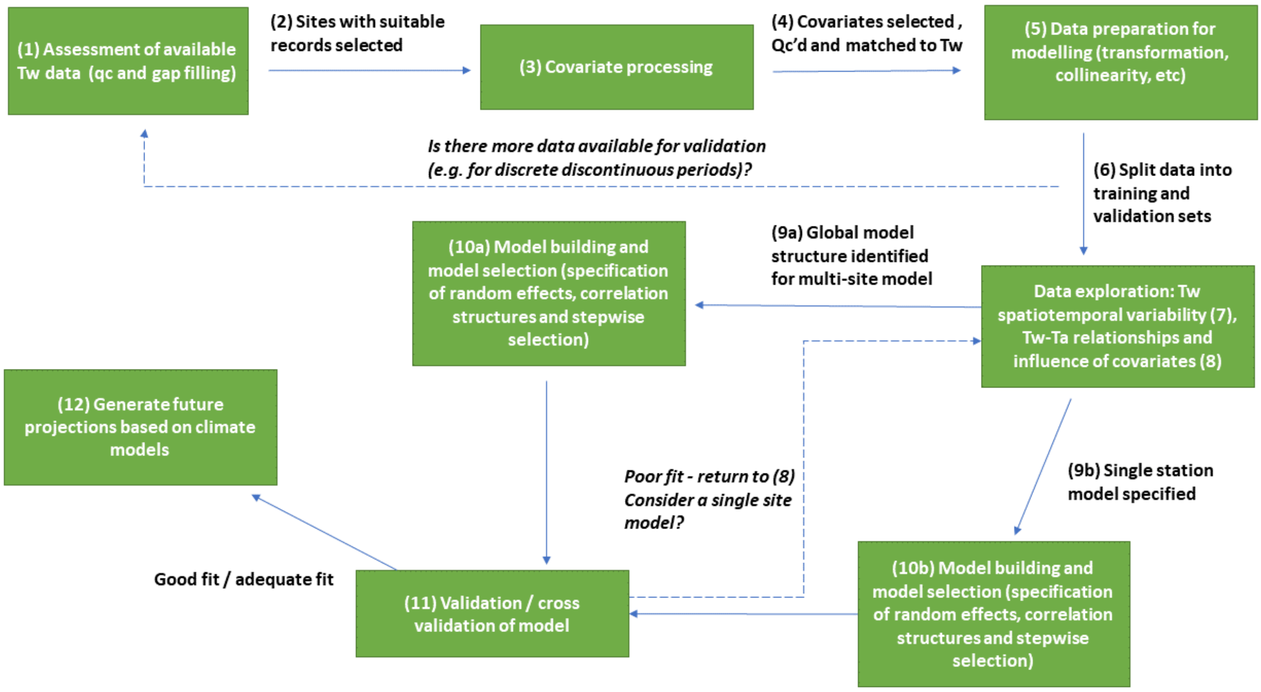


Figure 3. High-level schematic representation of the proposed regression based modelling approach to enable site specific water temperature predictions. The numbers relate to the steps outlined in detail in Appendix A and Appendix B. Note it is important that prior to undertaking any modelling exercise there is clear understanding of the decision context. For example, a user may wish to develop a

model for a well instrumented catchment. In this instance Figure 2 may identify a process based model is a suitable solution.

Further recommendations and considerations

The multi-site, mixed effect regression approach outlined above represents a building block on which a river network smoother model (RNS; Jackson et al. 2018) can be built, similar to existing models for Scotland. An RNS model would be temporally dynamic, facilitating prediction of any daily water temperature metric, and spatially distributed across the entire river network (i.e. England), whilst also accounting for spatial covariance (non-independence of data on river networks). To create an RNS model there are a number of additional steps required:

- A topologically correct (unbroken, non-circuitous) Digital River Network (DRN) for the whole of England needs to be generated and validated. Predictor variable also need to be available for all the nodes on the river network.
- At least one year of sub-daily water temperature data (preferably sub-hourly) needs to be generated for sites that cover the full range of potential environmental conditions within the network (Appendix C).
- Spatial data analysis similar to that outlined in Jackson et al. (2016) is required (Appendix C). This can be conducted for monitoring sites with historical data (i.e. those used in the mixed effect regression model above) to assess how well they cover the range of environmental conditions. This will enable optimisation of the site selection for additional high resolution water temperature monitoring - reducing redundancy and minimising the need to establish new monitoring sites.

Alternatively, a temporally static spatial statistical network model (SSNs) can be generated for a specific temperature metric and time period (e.g. summer maximum temperature or august mean temperature). These models still require sub-daily water temperature records (Isaak et al. 2017) but over a shorter time period (i.e. during time of interest) and recent research has highlighted the potential for using remote sensing data for calibration (Lee et al. 2020). While the calibration data requirements for SSN models can be less than RNS models, the trade-offs need to be considered as SSN models are only suitable for certain applications (e.g. assessing thermal maxima). RNS models have been aggregated spatially or temporally to provide a range of water temperature summary metrics (see Jackson et al. 2017).

As identified in Tables 2 – 5 there have been limited examples of water temperature models being driven by climate models to generate projections. Hence, there are not enough examples to facilitate a rigorous assessment and thus advise on best practise in the context of water temperature modelling. However, it is important to consider the spatiotemporal scale required as this will dictate the choice of climate model product (see appendix B) For example, a static spatial model may be best driven by a probabilistic climate projection with a monthly temporal resolution, while a dynamic river network smoother model by a regional or derived climate projection (daily time step). Another important consideration relates to the choice of bias correction which can have implications for the ability to quantify extremes (see appendix B). Furthermore, it is worth considering the properties of any future climate scenario that are required for the particular application (i.e. means vs extremes/ change in seasonality). For example, in certain situations an approach similar to that outlined by Isaak et al. (2017) may be feasible where future scenarios are driven by simple change factors (i.e. the current air temperature series; +2 °C, +4 °C +6 °C).

Summary

In this report we have reviewed available approaches for modelling river temperature across a range of spatial and temporal scales. A number of promising emerging research approaches were identified that may be suitable for large scale modelling. Machine learning / artificial intelligence hold promise for future development but spatial network models represent the current “state of the art” for water temperature modelling. Decision trees were developed for selecting water temperature models based on: (a) methodological approach (e.g. statistical, process based, etc) (b) data availability / spatio-temporal scale. A potential modelling approach (mixed effect regression) was identified for making water temperature projections primarily based on constraints in data availability and the spatio-temporal scale required for model predictions. Finally, further considerations are presented around the available climate projections, how these could be used to drive future temperature predictions and the additional steps required to develop a water temperature model for the entire river network.

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List of abbreviations

AIC	Akaike Information Criterion
ANN	Artificial Neural Network
AI	Artificial Intelligence
BIC	Bayesian Information Criterion
DRN	Digital River Network
EB	Energy Balance
GAM	Generalized Additive Model
GAMM	Generalized Additive Mixed effect Model
GPR	Gaussian Process Regression
KNN	K-Nearest Neighbour
LMM	Linear Mixed effect Model
Q	River flow/discharge
RPCs	Representative Concentration Pathways
GCMs	Global Circulation Models
RNS	River Network Smoother
SAGIS	Source Apportionment Geographical Information System
SIMCAT	Environment Agency’s stochastic water quality river mode
SSN	Spatial Statistical Model
Ta	Temperature of the air

Tw	Temperature of the water

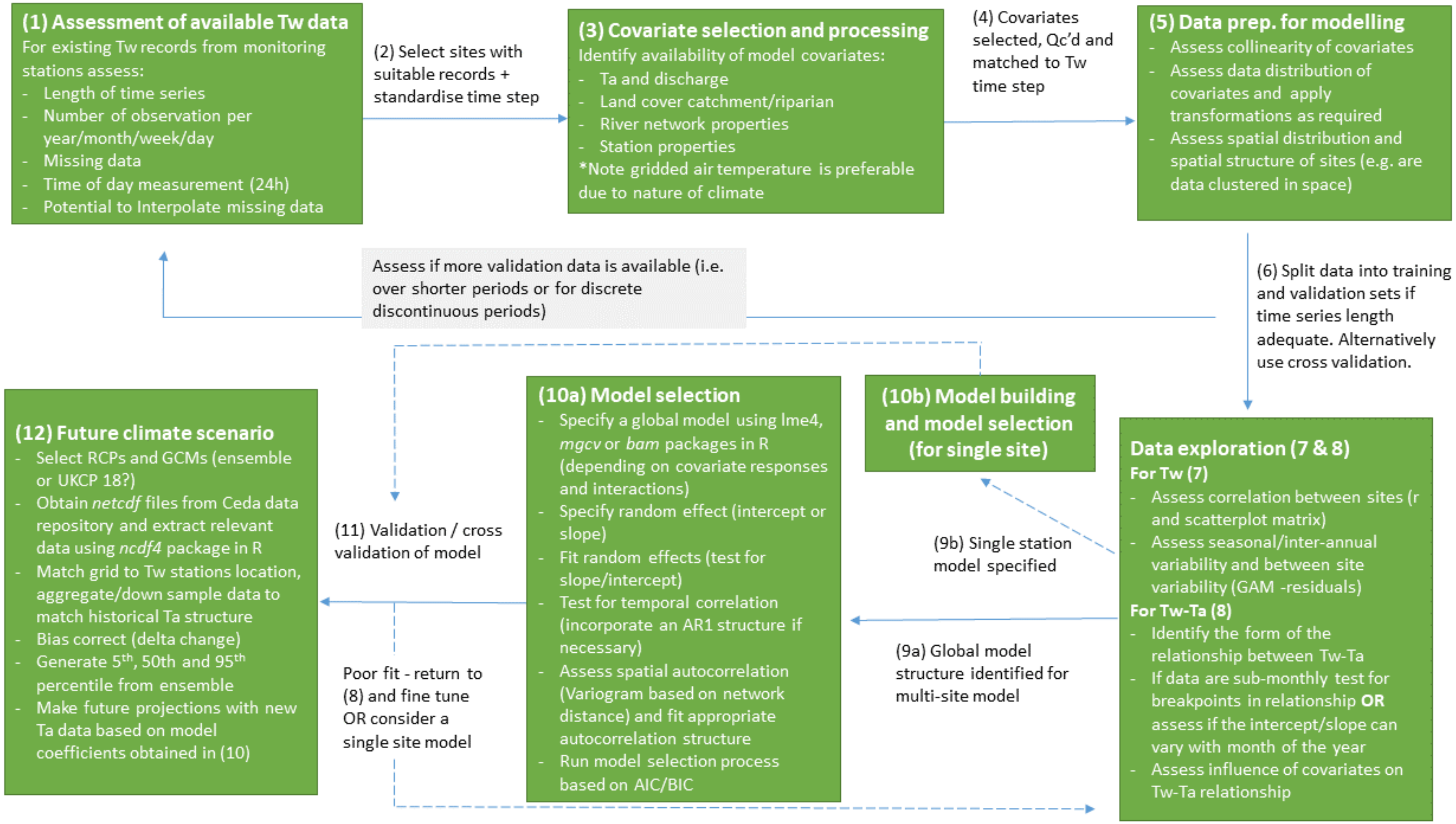
Glossary

Akaike Information Criterion	A single number score that can be used to determine which of multiple models is most likely to be the best model for a given dataset
Artificial intelligence	Computer systems able to perform tasks normally requiring human intelligence
Artificial Neural Network	Computer systems based on biological neural networks in brains
Autocorrelation	A mathematical representation of the degree of similarity between a given time series and a lagged version of itself over successive time intervals.
Bayesian Information Criterion	A single number score that can be used to determine which of multiple models is most likely to be the best model for a given dataset
Calibration data	Data used to provide correction of measured data or perform uncertainty calculations.
Collinearity	When one predictor variable has a linear relationship with another, which in turn reduces their statistical significance
Covariates	A possible predictive or explanatory variable of the dependent variable
Deep learning models	A type of machine learning
Digital River Network	A digitised map of the entire river network that should be topologically correct (unbroken, non-circuitous)
Distributed	Water temperature sites or modelling points are spread across the entire river network at a spatial resolution suitable for the purposes of the modelling exercise
DynWat	A dynamical 1-dimensional water energy routing model

Energy balance	Meteorological data required for heat budget / energy balance (e.g. air temperature, humidity, wind speed, radiation, bed heat flux)
Functional regression	A version of regression analysis when responses or covariates can be functions (e.g. information about the shape of a curve)
Gaussian Process Regression	A nonparametric, Bayesian approach to regression
Generalized additive mixed effect model	An extension of linear mixed models to allow response variables from different distributions
Generalized additive model	A modelling technique where the impact of the predictive variables is captured through smooth functions which can be nonlinear
Global Circulation Model	A mathematical type of climate model of the general circulation of a planetary atmosphere or ocean
Heterogeneous	Diverse in character or content
Hybrid wavelet-neural network models	A type of machine learning
K-Nearest Neighbour	A machine learning algorithm
Linear mixed effect model	An extension of simple linear models particularly used when the data have temporal or spatial structure that needs to be considered to ensure assumptions of independence are not violated.
Linear models	A linear approach to modelling the relationship between a response and one or more explanatory variables
Logistic regression	A modelling approach used to describe data and to explain the relationship between one dependent variable and one or more explanatory variables.

Machine learning	A field of artificial intelligence where a computer program can learn and adapt to new data without human intervention
Overfitted	A modelling error occurring when there is limited variation within the model reducing its predictive power
Process-based models	A water temperature modelling approach that attempts to recreate the physical phenomena that cause warming or cooling.
Regression based models	A model exploring the relationship between one variable (the dependent variable), and several other variables (independent variables)
Representative Concentration Pathways	A greenhouse gas concentration (not emissions) trajectory adopted by the Intergovernmental Panel on Climate Change
Residuals	An estimate of the unobservable statistical error
River Network Smoother	A statistical model with potential to predict for unmonitored locations across an entire river network.
Spatial Statistical Model	A model based on statistical tools that are used to characterize the distribution of something across space
Station	A monitoring location
Sub-daily	At a frequency of smaller periods than days
Sub-hourly	At a frequency of smaller periods than hours
Topology	The shape of the land

APPENDIX A: Detailed schematic representation of the modelling approach.



APPENDIX B: Development of spatio-temporal river temperature model using "spot" river temperature measurements in the absence of a corrected digital river network

Prerequisites

The minimum data requirement for a site-specific (i.e. not distributed across the entire network) regression based river temperature model is water and air temperature records. These can either be paired stations (models may need to be developed to apply transfer functions if the distance is > 2km) or based on gridded temperature products available from the Met Office. The recommended regression based model described here assumes it is unlikely that the Environment Agency will have access to sub-daily water temperature data from enough sites to develop a spatially distributed and temporally dynamic regression model. Hence, it is recommended that sites with long term and sub-monthly water temperature time series based, on spot sampling, are used to develop a mixed effect regression model. This approach provides some potential to predict for new unmonitored sites providing there is no bias in the calibration data, and the new locations are within the environmental range of sites used to calibrate the model. A useful first step before model fitting would be to investigate the consequences of using spot sample data (collected during regular working hours) to characterise daily temperature metrics and investigate to what extent biases could vary between sites and consider the consequences for regression models. This could be based on resampling of existing high-frequency (hourly) records to simulate the spot sampling resolution (weekly – monthly). Other covariates are recommended to improve the model accuracy and also to increase the potential to make predictions for unmonitored sites. It is assumed that all data (particularly water temperature and air temperature) used have undergone quality control procedures to identify and remove spurious values associated with operator or instrument error (see Orr et al. 2015). It is beyond the scope of this document to outline suitable methods for the quality control step in the procedure. Finally, the following method is only appropriate for circumstances where spot samples are collected at random times of day to ensure on temporal biases within or between sites.

Step by Step Instructions

STEP 1. A thorough assessment of the available water temperature (Tw) data is required. Identification of missing records can be done using the R software environment which offers useful tools for graphing (ggplot2) and summarising (skimr) large data sets.

```
> skim(mtcars)
Numeric Variables
# A tibble: 11 x 13
     var    type missing complete     n       mean          sd    min `25% quantile`  median `75% quantile`     max  hist
   <chr>   <chr>   <dbl>    <dbl> <dbl>      <dbl>       <dbl>  <dbl>          <dbl>   <dbl>          <dbl>   <dbl> <chr>
1     am numeric       0       32    32   0.406250   0.4989909  0.000        0.00000   0.000           1.00   1.000
2   carb numeric       0       32    32   2.812500   1.6152000  1.000        2.00000   2.000           4.00   8.000
3    cyl numeric       0       32    32   6.187500   1.7859216  4.000        4.00000   6.000           8.00   8.000
4   disp numeric       0       32    32 230.721875 123.9386938 71.100      120.82500 196.300         326.00 472.000
5   drat numeric       0       32    32   3.596563   0.5346787  2.760        3.08000   3.695           3.92   4.930
6   gear numeric       0       32    32   3.687500   0.7378041  3.000        3.00000   4.000           4.00   5.000
7     hp numeric       0       32    32 146.687500  68.5628685 52.000       96.50000 123.000         180.00 335.000
8    mpg numeric       0       32    32  20.090625   6.0269481 10.400       15.42500  19.200          22.80  33.900
9   qsec numeric       0       32    32  17.848750   1.7869432 14.500       16.89250  17.710          18.90  22.900
10    vs numeric       0       32    32   0.437500   0.5040161  0.000        0.00000   0.000           1.00   1.000
11    wt numeric       0       32    32   3.217250   0.9784574  1.513        2.58125   3.325           3.61   5.424
```

Figure A1. Example of the summary output that can be generated using Skimr.

Depending on gap length and timestep, operators must decide if interpolation is a viable option. Linear interpolation is the best option for short gaps while splines or polynomials are better suited to longer gaps (Gnauck 2004, Lepot et al. 2017). More complex methods are available (e.g. machine learning and autoregressive models) but require longer timeseries to be reliably implemented. There are a number of R packages available for univariate time series interpolation, however ImputeTS is a recommended staring point.

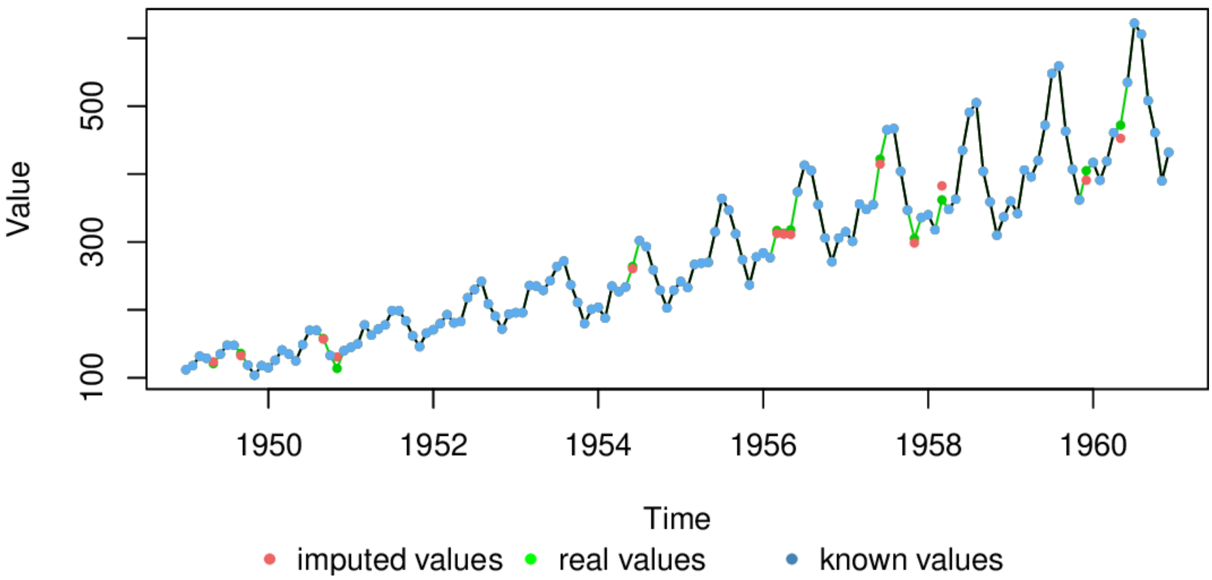


Figure A2. Example of a test time series (monthly resolution) with missing data filled using ImputeTS. The imputed values are those filled by the statistical function with "real values" representing the actual value for the filled data point. The advantage of ImputeTS is that the fill function performs well even when data are trending.

An assessment of the number of samples per year/month/week/day is required to decide on feasible model time step. A rough guide is that: i) *daily models* require hourly records, ii) *weekly models* require daily data, iii) *monthly models* require sub-weekly records. The time of day that the measurement was collected is also important as this can bias estimates of maximum or mean due to peak water temperature generally occurring in the afternoon during summer. Advection and site/ catchment specific properties makes it difficult to create models for deriving daily peak water temperature from a spot sample. However, bias in the calculation of weekly/monthly mean Tw is reduced, if sites with >3 year record length and a degree of variability in the time of day that the water temperature was measured are selected for modelling. ***NOTE:*** for models at the monthly time step data longer time series are recommended to build robust models. If there is limited variability in the time of measurement and an unbiased mean cannot be generated then a judgment must be made as to whether modelling relative change in water temperature is a suitable compromise.

STEP 2. Water temperature and air temperature need to be available at the same temporal resolution, so a data aggregating may be required if this is not the case. The xts package in R provides 'downsampling' or aggregating functions. Alternatively, if adequate data is available calculation of a water temperature metric (e.g. mean Tw) can be conducted. Interpolation from coarse monitoring time steps (e.g. monthly or weekly) to daily time steps is not advisable as the uncertainty associated can be significant. However, there are promising approaches being developed for hydrographs and groundwater level observations see the tool box for TFN models (multiple site linear transfer function noise) - http://peterson-tim-j.github.io/HydroSight/.

STEP 3. The availability of covariates for model fitting needs to be assessed. Following Jackson et al. (2018) the following suite of covariates provide good predictive power: air temperature data (station or gridded), discharge data records (river flow archive), land cover data (CEH land cover map 2019), riparian shading (e.g. woodland in a 25 m buffer width extending 1000 m upstream), upstream catchment area, Strahler river order, channel orientation, altitude, summer and winter hill shading, channel width, channel gradient, distance to coast and distance to the sea along the river. A decision on the use of station specific vs gridded air temperature records is required at this stage. Gridded data is recommended as it is directly comparable to climate model outputs. All covariates need to be collated and the quality assessed before including them in the model. In addition all spatial data used must cover the spatial scale to be predicted over as you have matched covariates for all of the prediction locations.

STEP 4. If a water temperature metric (e.g. Mean Tw) was calculated in (2) then the same must be done for covariate time series data (air temperature and discharge). Time steps should be aligned and checked for consistency. It is assumed that all data taken to this stage have been quality controlled. Screening for outliers is advised and missing data should be filled where it is feasible.

STEP 5. Data preparation prior to modelling. An assessment of collinearity between covariates is required. This can be carried out using a combination of visual tools, correlation coefficients and variance inflation factors (vif) - see Zurr et al. (2010) for a detailed guide. Correlation coefficients (r) > 0.8 and vif >3 are reasonably conservative indictors of problematic combinations of variables. To avoid issues later in the model fitting process the variables that are highly correlated need to be carefully considered and removed from the analysis based on either data quality/record length or physical principles*. Following this a visual assessment of data distributions is advised with subsequent transformation if required. This is particularly important if data are highly skewed or non-normal (square-root and log transformations are good starting points the bestNormalize package in R is also a useful tool). An assessment of spatial distribution and spatial structure of sites (e.g. are data clustered in space) is advised.

*An alternative option is to undertake a principal component analysis (PCA) to reduce the dimensionality of the dataset and overcoming any issues associated with collinearity.

STEP 6. To ensure models are robust and not overfitted to the available data it is advisable to conduct model training and model validation on different data fractions (i.e. spatially or temporally). The traditional method requires partitioning data into training and validation sets (training data needs to be continuous and evenly distributed across the year, while validation data need not be temporally continuous). If the time series length is short (<3 years) cross validation approaches represent a more robust alternative and can be applied once the model is specified (Kuhn & Others 2008, Kuhn & Johnson 2013).

STEP 7. A phase of data exploration is required before model fitting and selection. The water temperature time series should be the focus in the first instance. Visualisation of the Tw time series (ggplot2) can help identify sites/regions with differing thermal regimes. This can be further aided by a statistical assessment of similarity between sites (e.g. Pearson's correlation coefficient). A GAM smoother should be fitted to assess relationship between time step (e.g. week or month of the year) and water temperature. This can be done using the mgcv package in R. Temporal structure in the residuals can be assessed to identify periods when thermal patterns are most heterogeneous, spatial structure can also be assessed (x-y coordinates, elevation, distance from sea, etc). This information will help guide the operator towards the most important covariates for model building and the need for spatial covariance structure in the final model.

STEP 8. A second phase of data exploration is required to explore the form of the relationship between Tw-Ta. A first step is to asses is the relationship is linear or non-linear fit (e.g. logistic regression) which will then be taken forward for subsequent modelling steps. Note that a seasonally varying linear relationship can look non-linear (e.g. Jackson et al., 2018). Failure to capture seasonal variability would introduce temporal bias in predictions If data are sub-monthly test for breakpoints in relationship between Tw- Ta (see Letcher et al. 2016) and only model for periods when Tw – Ta are synchronised. If predication across the full year is required then assess the monthly variability in intercept and slope of the Tw-Ta relationship. If this is significant then incorporate a term to account for variation (see Jackson et al. 2018). Assess site specific variability in the Tw-Ta relationship and consider adding a random effect to allow the intercept and slope to vary between sites. Assess influence of covariates on Tw-Ta relationship - coplots in R are a recommended starting point for this.

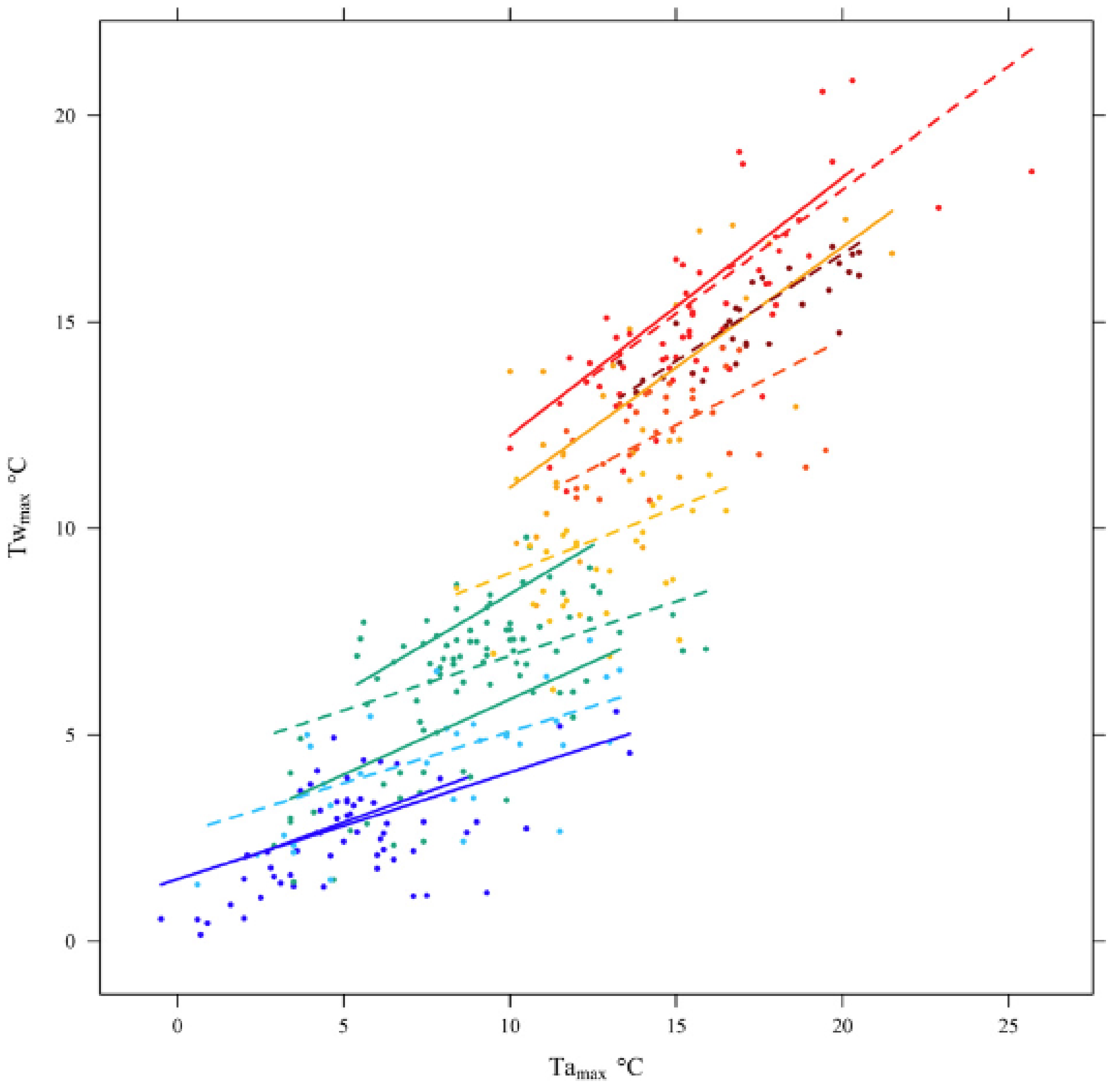


Figure A3. Example of the seasonal relationship between air and water temperature for an example sites in Scotland. Solid lines represent the first six months of the year (January–June) and dashed lines the second six months (July–December). The colour range is between blue (cool) and red (warm) and vary according to the maximum observed daily temperature in each month. After Jackson et al. (2018).

STEP 9. The structure of the fixed effects required in the model should be apparent if sufficient time was spent exploring relationships during step (step 8). If the operator is satisfied that no further exploration of the water temperature and covariate relationships is required then the model selection process can be undertaken.

STEP 10. Specify the global model – i.e. the most complex model including all variables and interactions identified in steps (step 5) and (step 8). Fit the model mgcv package in R with smooth terms for non-linear effects. If no no-linear terms are apparent then a linear mixed effect model can be fitted using the lme4 package. The operator must decide on the random effect structure (e.g. allow intercept and slope for Tw-Ta relationship to vary by site) then test for temporal autocorrelation (incorporating an AR1 structure if necessary – see Jackson et al. (2018). The spatial autocorrelation structure must then be assessed. Ideally this would be done using a variogram based on network distance and "as the crow flies" distance but if a corrected river network is not available then just use Euclidean distance. Detailed information regarding spatial autocorrelation, variograms and fitting appropriate correlation structure to mixed models can be found in Zuur et al. (2009) and Zimmerman & Ver Hoef (2017). Once the random effect structure and temporal/ spatial correlation structure(s) have been specified a stepwise model selection process-based on AIC or BIC can be conducted (see Jackson et al. 2018). The aim is achieve a parsimonious model with normally distributed residuals.

STEP 11. Once the final model has been selected the performance of the model should be assessed using the validation data set or via a suitable cross validation approach (see below). It is generally good practice to assess multiple indicators of model performance – Root mean Square error (RMSE), Coefficient of variation (R^2) and percent bias. The hydroGOF package in R provides a variety of functions to facilitate the calculation of these goodness of fit indicators. If the record length was too short for a data partition then 10-fold cross-validation should be used. This is a resampling approach that splits the training/calibration dataset into k-folds, refits the model and predicts for the data left out (Kuhn & Others 2008, Kuhn & Johnson 2013). If the performance is not satisfactory return to (step 8) and refine the model or collect more data. If the performance is good the potential to predict to unmonitored sites can be further explored using new sites not included in the training/validation set.

Alternatively, the operator can decide to return to (step 8) and then fit single station models. This would involve the operator specifying a global model with the temporally dynamic data available for each site (i.e. 9b in Appendix A). Then a regression model can be fitted for each site in the dataset at step 10 (i.e. 10b in Appendix A) and the coefficients generated used to predict or generate projections into the future for that particular site.

STEP 12. Once the final model has been selected and validated it can be used for water temperature projection. The first step required is a decision Global Circulation Model (GCMs) to be used (UKCP 18 is recommended). A useful starting point is the series of factsheets available for UKCP18. In the first instance users need to decide on the spatio-temporal resolution as this can limit the climate products available - i.e. GCM, RCMs, probabilistic (see Table A1). If a probabilistic projection is chosen then a decision must be made on the Representative Concentration Pathways (RCPs) to be used (See Table A2. Generation of ensembles that sample key uncertainties in the different types of climate models are required for robust future projections. Once the GCMS and RCPs have been selected the required *netcdf* files should be obtained from the Ceda data repository (www.ceda.ac.uk). The operator will then need to extract relevant grid cells and meteorological data - this can be done using the *ncdf4* package in R. The time series for the particular location must be aggregated/down sampled to match the time step of the water temperature model. Then the outputs from each climate model need to be bias corrected. The delta change approach is well established and has been widely used (see Hay et al. 2000). Briefly, this approach uses the GCM response to climate change to modify observations of Ta. For example if the climate model predicts +3°C, then 3°C is added to all historic observations to construct a new time series for the future climate. There are other delta change methods available including variance scaling, quantile mapping and trend-preserving quantile mapping (See Table A3) If the operator has used an ensemble or a probabilistic product the 5^{th}, 50th and 95^{th} percentiles can then be taken forward to make future Tw projections based on model coefficients obtained in (step 10).

Table A1 summary of the key characteristics of each of the three strands of information for the UKCP18 land projections. Taken from the [UKCP18 guidance document]

	Probabilistic projections	Global (60km) projections	Regional (12km) and Local (2.2km) projections	Derived projections
Description	Probabilistic changes in future climate based on a assessment of model uncertainties	A set of 28 climate futures with detailed data on how it may evolve in the 21st century ▪ 15 x Hadley Centre Model variants HadGEM3-GC3.05 (PPE-15)‡ ▪ 13 x Other climate models (CMIP5-13)‡	Two sets of 12 climate futures at high resolution: ▪ 12km over Europe, downscaled from the global projections (PPE-15) using Hadley Centre model HadREM3-GA705 ▪ 2.2km for the UK, providing further downscaling from the 12km simulations using HadREM3-RA11M	A set of climate futures derived from the global projections for a lower emissions scenario and global warming levels
Period	1961-2100	1900-2100	1981-2080 for 12km 1981-2000, 2021-2040, 2061-2080 for 2.2km	1900-2100
Temporal resolution	Monthly Seasonal Annual	Daily Monthly Seasonal Annual	Subdaily for 2.2km Daily Monthly Seasonal Annual	Daily Monthly Seasonal Annual
Spatial resolution	25km	60km	12km 2.2km	60km
Geographical extent	UK & regions	UK & regions Global	UK & regions Europe for 12km	UK
Emissions scenarios	RCP2.6 RCP4.5 RCP6.0 RCP8.5 SRES A1B	RCP8.5	RCP8.5	RCP2.6 2°C world 4°C world
Why should you use it?	▪ Explores emissions scenario uncertainty ▪ Explores uncertainty in key processes in climate models ▪ Helps characterise future extremes in risk assessment	▪ Long time series ▪ Spatially and temporally coherent* ▪ Direct access to 'raw' climate model data ▪ Met Office Hadley Centre global climate model HadGEM3-GC3.05	▪ Enhanced spatial detail ▪ Spatially and temporally coherent* ▪ Improved extremes ▪ Direct access to 'raw' climate model data ▪ CPM projections uses climate model featuring explicit dynamical representation of large convective storms	▪ Long time series ▪ Spatially and temporally coherent* ▪ Explore emissions scenario uncertainty when used with global projections ▪ Explore global warming levels

Table A2 1 The increase in global mean surface temperature averaged over 2081-2100 compared to the pre-industrial period (average between 1850-1900) for the RCP pathways (best estimate, 5-95% range). From IPCC AR5 WG1.

RCP	Mean change in Ta by 2081-2100 (°C)
RCP2.6	**1.6**
RCP4.5	**2.4**
RCP6.0	**2.8**
RCP8.5	**4.3**

Table A3: Information on some of the most commonly used bias correction methods used for climate data. Taken from the UKCP18 how to bias correct document.

	Linear scaling	Variance scaling	Quantile mapping	Trend-preserving quantile-mapping
Description	Simple method that only adjusts for mean bias	A popular method that adjusts mean and variance bias	A method often used for precipitation as it preserves the distribution and can inform extreme values	A method endorsed by the ISIMIP project (www.isimip.org). It combines two steps: (1) linear scaling approach for the long-term trend and (2) quantile mapping approach for variability
Pros	Simple method	▪ Simple method that many have previously used ▪ Retains climate change signal	▪ Considers entire distribution ▪ Useful for changes in extreme values and where variability is important	Same as quantile mapping method but also preserving climate change signal
Cons	Only corrects for the mean	▪ Variability follows that of observed ▪ Restricted to range of observed anomalies	▪ Climate change signal can be altered ▪ Assumes correction increments are the same as in the current climate ▪ Extreme values restricted to observed	▪ As with other methods, variables corrected independently. Can lead to physical inconsistency ▪ Many more steps involved
When to use it	▪ Not often used on its own. See Trend-Preserving Quantile Mapping column ▪ Unsuitable for extreme events such as floods	▪ Often used for any variable at monthly to annual timescales ▪ Unsuitable for extreme events such as floods	▪ Often used for precipitation when considering hydrological applications	▪ Often used in hydrological applications
UK examples	Lafon et al, (2013), Guillod et al, (2018)	Dutch example available from Leander and Buishand (2017)	Prudhomme et al, (2012), Lopez et al, (2009), Brown et al, (2009)	Hutchins et al, (2018) who used ISIMIP data (Hempel et al, 2013)
Formulae	For additive adjustments (e.g. for temperature): $X(t) = \overline{O_{base}} - \overline{X_{base}} + X_{fut}(t)$ For relative adjustments (e.g. for precipitation): $X(t) = \frac{\overline{O_{base}}}{\overline{X_{base}}} \cdot X_{fut}(t)$	$X(t) = \frac{\sigma_{X_{fut}}}{\sigma_{X_{base}}} \cdot (O_{base}(t) - \overline{X_{base}}) + \overline{X_{fut}}$	$X(t) = F_O^{-1}\left(F_X\left(X_{fut}(t)\right)\right)$	$X(t) = C + X_{fut}(t) + \Delta\tilde{X}_{fut}(t)$ Step 1: $C = \overline{O}_{base} - \overline{X}_{base}$ Step 2: $\Delta\tilde{X}_{fut}(t) = \overline{B} \cdot \Delta X_{fut}(t)$

where X is the bias-corrected model data, O are observations, subscripts refer to baseline and future periods, t is time, σ is the variance, F is the cumulative distribution function mapping modelled data to observations, C is the long term trend, $\Delta\tilde{x}$ is the anomaly, B is the slope of the quantile mapping curve

APPENDIX C: Spatial data analysis example.

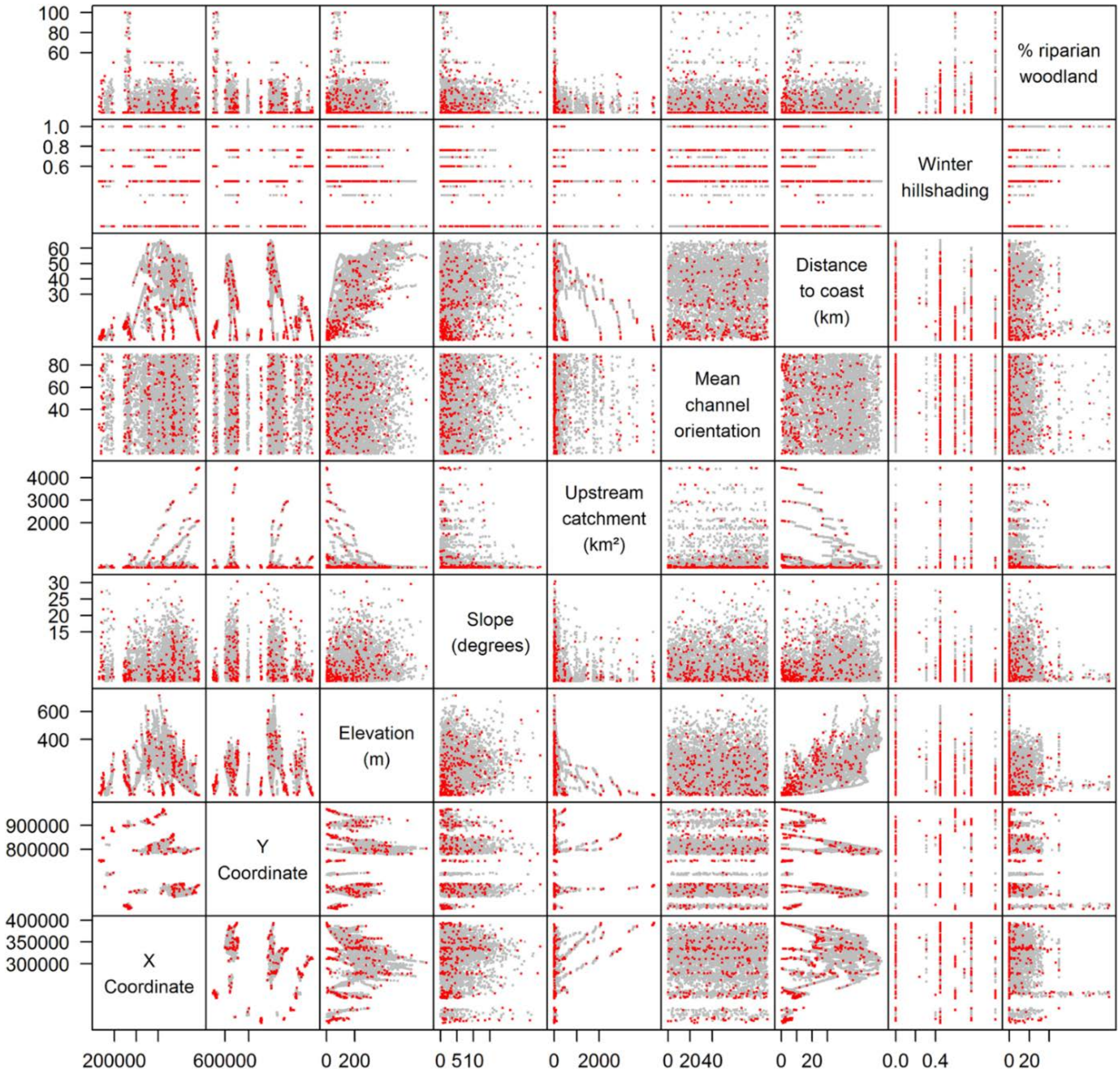


Figure C1: From Jackson et al. (2016) – Coverage of the environmental parameter space (grey dots) sites selected for the Scotland river temperature monitoring network (red dots) and subsequently used to build an RNS model.

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