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Stream temperature prediction in ungauged basins

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Stream temperature prediction in ungauged basins: review of recent approaches and description of a new physically-based analytical model

A. Gallice¹, B. Schaefli¹, M. Lehning^{1,2}, M. P. Parlange^{1,3}, and H. Huwald¹

¹School of Architecture, Civil and Environmental Engineering (ENAC), École Polytechnique Fédérale de Lausanne (EPFL), Switzerland

²SLF, WSL Institute for Snow and Avalanche Research, 7260 Davos, Switzerland

³Faculty of Applied Sciences, University of British Columbia, Vancouver, Canada

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Correspondence to: A. Gallice (aurelien.gallice@epfl.ch)

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Abstract

The development of stream temperature regression models at regional scales has regained some popularity over the past years. These models are used to predict stream temperature in ungauged catchments to assess the impact of human activities or climate change on riverine fauna over large spatial areas. A comprehensive literature review presented in this study shows that the temperature metrics predicted by the majority of models correspond to yearly aggregates, such as the popular annual maximum weekly mean temperature (MWMT). As a consequence, current models are often unable to predict the annual cycle of stream temperature, nor can the majority of them forecast the interannual variation of stream temperature. This study presents a new model to estimate the monthly mean stream temperature of ungauged rivers over multiple years in an Alpine country (Switzerland). Contrary to the models developed to date, which mostly rely upon statistical regression to express stream temperature as a function of physiographic and climatic variables, this one rests upon the analytical solution to a simplified version of the energy-balance equation over an entire stream network. This physically-based approach presents some advantages: (1) the functional form linking stream temperature to the predictor variables is directly obtained from first principles, (2) the spatial extent over which the predictor variables are averaged naturally arises during model development, and (3) the regression coefficients can be interpreted from a physical point of view – their values can therefore be constrained to remain within plausible bounds. The evaluation of the model over a new freely available data set shows that the monthly mean stream temperature curve can be reproduced with a root mean square error of $\pm 1.3^{\circ}\text{C}$, which is similar in precision to the predictions obtained with a multi-linear regression model. We illustrate through a simple example how the physical basis of the model can be used to gain more insight into the stream temperature dynamics at regional scales.

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1 Introduction

Among the parameters affecting the ecological processes in streams, temperature occupies a predominant role. It influences the concentration of chemicals, such as dissolved oxygen, and may increase the toxicity of dissolved substances (Langford, 1990). It also affects the life cycle of many fish species, particularly the salmonids whose rate of spawning, timing of birth and rate of death are directly influenced by stream temperature (Caissie, 2006; Benyahya et al., 2007). Water temperature is also a relevant factor for many thermal power plants which rely on cooling by river water, and whose electricity production decreases when water temperature exceeds a certain limit (Haag and Luce, 2008).

Stream temperature modeling has regained some interest over the past 10–15 years, which led to the development of many stochastic and deterministic models (e.g. Mohseni et al., 1998; Segura et al., 2014; Chang and Psaris, 2013; DeWeber and Wagner, 2014; Meier et al., 2003; Westhoff et al., 2007). The former type relies on a statistical analysis to empirically relate stream temperature to climatic and physiographic variables, such as air temperature, discharge, altitude or channel width (see Benyahya et al., 2007, for a complete review of this subject). Deterministic models, on the other hand, rely on a physically-based formulation of the stream energy conservation to compute water temperature (Caissie, 2006). Both model types have usually been applied to a single stream reach or a limited number of catchments (e.g. Sinokrot and Stefan, 1993; Roth et al., 2010; Caissie et al., 2001; Caldwell et al., 2013; Grbić et al., 2013). However, some studies have recently attempted at developing regionalized stream temperature models. This effort was certainly fostered by the incentive of the International Association of Hydrological Sciences (IAHS), which set the focus of the last decade on hydrological prediction in ungauged basins (Sivapalan et al., 2003; Hrachowitz et al., 2013). In the case of stream temperature, authors relied on statistical approaches to make predictions in ungauged catchments; to the best of our knowledge, no study has investigated the regionalization of a deterministic model to

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Regarding the modeling approach, Wehrly et al. (2009) investigated four different statistical model types and showed that their difference in prediction accuracy was relatively small. The same conclusion was reached by Daigle et al. (2010), who compared four other modeling approaches. Isaak et al. (2010) found that networked kriging regression performed better than multi-linear regression over the calibration data set, but this assertion became much less evident over the validation set. Similarly, Pratt and Chang (2012) and Chang and Psaris (2013) concluded that geographically weighted regression is slightly more accurate than multi-linear regression, but they did not validate their results on an independent data set. As such, no significant decrease in the prediction errors should be awaited from a change in the statistical modeling technique.

Further comparisons between the different models reported in the literature is unfortunately hindered by the diversity of temperature metrics and error measures used by the authors. As mentioned in several studies already, we advocate here the systematic use of the different error measures that are RMSE, bias and coefficient of determination R^2 for the evaluation of the model precision, possibly combined with a benchmark model (Schaeffli and Gupta, 2007). It should be noted that R^2 is also referred to as Nash–Sutcliffe efficiency by the hydrological community (Nash and Sutcliffe, 1970), and is defined as one minus the ratio of the model error variance over the variance of the observed data.

1.2 Few models can predict the stream temperature annual cycle

Inspecting Table 1, it can be seen that most regionalization efforts have concentrated on some particular periods of the year. For example, Jones et al. (2006), Isaak et al. (2010) and Chang and Psaris (2013) focused on the annual maximum of the 7 day moving average of the daily maximum temperature (MWMt). Similarly, both Pratt and Chang (2012) and Hill et al. (2013) aimed at estimating mean stream temperature in summer and winter. Very few studies have actually attempted at deriving regional

models to compute the complete annual cycle of stream temperature over several years.

Miyake and Takeuchi (1951) and Stefan and Preud'homme (1993) were probably the first authors to address this issue; they relied on linear regression against air temperature to simultaneously estimate stream temperature at multiple sites. However, their respective works are restricted to a limited number of rivers (20 and 11, respectively) and could probably not be applied to larger areas. In an attempt at generalizing these models, Ozaki et al. (2003) and Kelleher et al. (2012) separately regressed stream temperature against air temperature in each one of the catchments they considered, and subsequently regionalized the slopes of the regression lines. However, both studies were only partly successful in completing the regionalization step, since the modeled regression slopes had large prediction errors. They would additionally have had to model the intercepts of the regression lines to completely regionalize the stream–air temperature relationship. In a similar fashion, Johnson et al. (2014) relied on the logistic equation introduced by Mohseni et al. (1998) to relate stream temperature to air temperature in each catchment. Also they faced difficulties to regress the equation parameters against geomorphological properties of the catchments. The two most complete works on the regionalization of the linear stream–air temperature relationship were recently conducted by Ducharne (2008) and Segura et al. (2014). These two studies attempted at regionalizing both the slopes and intercepts of the regression lines between stream and air temperature. To this end, Ducharne grouped the streams according to their Strahler order and fitted a single line in each group. Segura et al., on the other end, expressed the slopes and intercepts as linear combinations of climatic and physiographic variables. The model of Ducharne had nominally a higher explanatory power ($R^2 = 0.88\text{--}0.96$ depending on the Strahler order) than Segura et al.'s model ($R^2 = 0.79$), but was effectively based on about 10 times fewer rivers.

Instead of using air temperature as independent variable, Bogan et al. (2003) relied on equilibrium temperature. This variable corresponds to the stream temperature at

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which the net energy flux at the air–water interface vanishes (e.g. Edinger et al., 1968). It was shown by Bogan et al. to be a fairly good estimator of stream temperature for almost 600 rivers in the Eastern and Central United States, with a prediction error of about 3°C.

As an alternative to the above-mentioned studies, the annual cycle of stream temperature has been modeled by some authors as a function of time directly, rather than air or equilibrium temperature. Hrachowitz et al. (2010), Imholt et al. (2013) and Rivers-Moore et al. (2012) expressed water temperature as a linear combination of climatic and physiographic variables for each month of the year separately. Their models were derived for a particular year, but can be transferred to other years by estimating stream temperature at a few measurement points using Mohseni's logistic equation and fitting the multi-linear regression model to the resulting values (Hrachowitz et al., 2010). Based on a similar approach, Macedo et al. (2013) succeeded to derive one single regression model to estimate daily mean stream temperature at 12 different sites in Brazil over 1.5 years. The performance of their model was not tested using data from subsequent years, though.

Johnson (1971) relied on a yet different technique to estimate the thermal regime of 6 rivers in New Zealand. He first fitted the stream temperature annual cycles with sine curves. In a second step, he identified the physiographic properties of the catchments which best correlated with the fit coefficients. The focus of his study being on the investigation of these physiographic properties, he did not evaluate the prediction error of his model. Although not intended for this purpose, the work of Garner et al. (2014) is based on a somewhat similar approach and may be used to get a first estimate of the annual cycle of temperature in UK streams. The authors classified rivers into several groups according to the shape and magnitude of their respective thermal regimes. Then, they investigated the similarities and dissimilarities of some geomorphological properties among and between the groups. This processing could be inverted to infer the thermal regime from the physiographic properties of the catchments.

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Finally, some studies have evaluated the possibility of modeling the time evolution of stream temperature using machine learning techniques. For example, DeWeber and Wagner (2014) trained an artificial neural network to reproduce daily mean temperature values from May to October over more than 30 years for 1080 streams in the Eastern United States. Their approach could be easily extended so as to model the complete annual cycle of stream temperature each year.

1.3 Space-averaging of the predictor variables

Some of the reviewed publications on regional stream temperature modeling addressed the question of the spatial scale over which the predictor variables should be averaged. It is common knowledge that stream temperature is not only affected by local environmental conditions, but also by the conditions prevailing upstream. However, the exact extent of the area controlling the stream energy-balance at a given point is not clear (Moore et al., 2005).

Due to this uncertainty, different approaches have been used in the literature to average the predictor variables. Based on studies of the effect of forest harvesting on stream temperature (e.g. Moore et al., 2005), some authors considered riparian buffer zones of various widths and lengths as averaging areas. This approach was usually applied to average the land-cover characteristics only, particularly forest coverage (e.g. Sponseller et al., 2001; Scott et al., 2002; Macedo et al., 2013; Segura et al., 2014), but also in some cases to average most of the predictor variables, including elevation or slope (Hrachowitz et al., 2010; Imholt et al., 2013). Other authors considered larger portions of the catchments as averaging areas, sometimes extending far beyond the riparian zone. For example, Wehrly et al. (2009) used the whole area drained by the stream segment located directly upstream of the temperature measurement point. Whereas most studies relied on simple spatial averaging, a few of them applied a weighting scheme to give more emphasis to the conditions prevailing near the gauging point. As such, Isaak et al. (2010) and Hill et al. (2013) applied a weight w

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(Beyeler, 2007; Hari and Zobrist, 2003; Hari and Güttinger, 2004; Jakob, 2010). Finally, other authors relied on physically-based models to simulate water temperature dynamics in single stream reaches or catchments (Meier et al., 2003; Roth et al., 2010; Magnusson et al., 2012; Carlier, 2013), which is not the subject of the present study.

1.5 Investigation of a new modeling approach

The above literature review revealed two subjective choices that are faced by all authors: (a) the selection of the predictor variables, and (b) the choice of the statistical approach to link these predictor variables to stream temperature. The choice of predictor variables varies quite significantly from one model to the other. Some studies consider only physiographic variables (e.g. Scott et al., 2002; Jones et al., 2006; Nelson and Palmer, 2007; Hrachowitz et al., 2010), while others also include climatic variables (e.g. Isaak et al., 2010; Ruesch et al., 2012; Moore et al., 2013), stream morphological factors such as channel width or bed gravel size (e.g. Hawkins et al., 1997; Arscott et al., 2001; Daigle et al., 2010), or even markers of anthropogenic activities (e.g. Pratt and Chang, 2012; Hill et al., 2013; Macedo et al., 2013). Similarly, the range of used statistical methods is rather broad. It encompasses traditional methods such as multi-linear regression (e.g. Arscott et al., 2001; Mayer, 2012; Imholt et al., 2013) or linear mixed modeling (Macedo et al., 2013), but also more advanced techniques such as geographically weighted regression (Pratt and Chang, 2012; Chang and Psaris, 2013), networked kriging models (Gardner and Sullivan, 2004; Isaak et al., 2010; Ruesch et al., 2012) or machine learning techniques (e.g. Westenbroek et al., 2010; Hill et al., 2013; DeWeber and Wagner, 2014).

We advocate here that the statistical modeling approach suffers two drawbacks. First, the selection of the predictor variables relies on the training and experience of the author(s); as such, it is not a deterministic procedure. This explains the fact that, despite some similarities, all lists of predictor variables are different among the reviewed articles. Secondly, the choice of the statistical model directly dictates the functional form of the relationship between the predictand (stream temperature) and

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predictor variables. For example, a multi-linear model assumes that the predictand can be expressed as a linear combination of the predictors. This fact is also true for non-parametric methods such as the artificial neural networks, which implicitly impose some (flexible) functional form. The selection of one type of model over another one is generally a heuristic decision.

We acknowledge that the statistical approach cannot be avoided in many disciplines, such as in Social Sciences or Economics, where the interactions between the different variables of interest are so complex that no functional form prevails in practice. Yet stream temperature is known to obey the energy conservation law. Our aim is to investigate whether the consideration of this physical law leads to the development of a more general and justifiable model. This approach is strongly inspired from the physically-based models which have been used for decades to predict water temperature along stream reaches (e.g. Brown, 1969; Sinokrot and Stefan, 1993; Westhoff et al., 2007). However, it differs from these models in the sense that we seek a much simpler expression for stream temperature, expressed as a function of variables which are readily available at the regional scale.

Our method requires analytically solving the energy-balance equation using some simplifying assumptions (see Sect. 2.1). The resulting expression for stream temperature is in theory not subject to the two above-mentioned drawbacks pertaining to the statistical approach. As a matter of fact, the predictor variables do not need to be specified a priori, as they naturally appear during the derivation of the expression. Moreover, the analytical formula directly provides the functional form of the relationship between stream temperature and the predictor variables. In practice these two assertions have to be moderated, since some of the predictor variables appearing in the analytical expression are not available in ungauged catchments – such as the long-wave radiation emitted by the stream. So as to keep our model as simple as possible, we choose to express these unknown quantities as linear functions of the available data. Although this step involves the selection of predictor variables and assumes a linear relationship with the unknown quantities, we do not think that it

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entirely questions our incentive to base our work on physical grounds. Indeed, only the unknown variables are replaced in the analytical formula, letting the global form of the relationship unaffected. Moreover, our approach attributes a physical meaning to the terms appearing in the formula. These terms can be constrained to remain within physical bounds, hereby restricting the range of values that the calibration parameters can adopt.

The objectives of the present work are three-fold: (1) describe a new analytical expression for the prediction of stream temperature in ungauged basins, allowing for the computation of the monthly resolved annual cycle and capturing inter-annual variability; (2) through proper calibration of the model, determine the length of the upstream area which controls stream temperature at a given point; and (3) compare the analytical model with a more standard statistical approach over a set of various Swiss catchments. The models are described in Sect. 2. The characteristics of the Swiss catchments are presented in Sect. 3, and the stream temperature data set in Sect. 4. Results are detailed in Sect. 5 and discussed in Sect. 6, followed by the conclusion.

2 Formulations of the stream temperature models

The new analytical expression for stream temperature prediction is derived in the following subsection. The statistical model used for comparison is presented in Sect. 2.2.

2.1 Physically-based stream temperature model

As mentioned above, the physically-based stream temperature model presented in this paper is based on the analytical solution to the stream energy-balance equation. This topic has been investigated extensively in the literature (e.g. Edinger et al., 1968; Theurer et al., 1984; Gosink, 1986; Polehn and Kinsel, 2000; Toffolon et al., 2010), although used only once for stream temperature prediction in ungauged basins (Bogan

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et al., 2003). In order to analytically solve the energy-balance equation, all studies relied on the linearization of the heat flux σ at the air–water interface as a function of stream temperature T : $\sigma = -k(T - T_e)$. Some of them assumed the heat transfer coefficient k to be constant and used prescribed functions of time, space or both to express the equilibrium temperature T_e (e.g. Gosink, 1986; Polehn and Kinsel, 1997; Daly, 2005). Other studies derived analytical formulations for k and T_e based on the physical expressions of the heat fluxes occurring at the stream–air interface (e.g. Edinger et al., 1968; Bogan et al., 2003; Caissie et al., 2005; Bustillo et al., 2014). While a minority of authors considered the temperature distribution to be spatially homogeneous (Edinger et al., 1968; Caissie et al., 2005; Bustillo et al., 2014), most of them assumed the stream to be in a steady-state or, equivalently, the stream celerity to be constant. In addition, they all imposed the river width to remain constant along the stream so as to analytically solve the energy-balance equation. Very few studies accounted for the heat exchange with the stream bed or the heat advected by lateral inflow of water (Bogan et al., 2004; Herb and Stefan, 2011). Bogan et al. (2003) were the only authors to evaluate their analytical expression over ungauged basins. They tested their model in the Central and Eastern United States, since this region has a topography flat enough for a meteorological station located even at more than 100 km from a given point to be still representative of the climate at that point. Their work is therefore hardly transferable to Switzerland, where the mountainous landscape prevents the proper interpolation of variables such as air humidity or wind speed, which are required as input by the model.

2.1.1 Derivation of the analytical solution to the energy-balance equation

Assuming a well-mixed water column and a negligible longitudinal heat dispersion, the mass and energy-balance equations along a stream reach read (adapted from

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where ϕ_r [W m^{-2}] denotes the net radiative heat flux, incorporating both the shortwave and longwave components. The second term on the right-hand side accounts for both the latent and sensible heat fluxes (e.g. Polehn and Kinsel, 1997; Toffolon et al., 2010), where the bulk heat transfer coefficient k [$\text{W m}^{-2} \text{°C}^{-1}$] between water and air is assumed to be constant, and T_a [$^{\circ}\text{C}$] refers to the air temperature.

- iii. The energy flux at the stream–bed interface is neglected, i.e. $\phi_b = 0$ (e.g. Bogan et al., 2003; Caissie et al., 2005; Bustillo et al., 2014).
- iv. The lateral inflow of water q_ℓ is assumed to be spatially constant (e.g. Biswal and Marani, 2010; Mutzner et al., 2013).
- v. The ratio of stream width to discharge w/Q is assumed to be spatially constant. This approximation is different from the one of Theurer et al. (1984) and Polehn and Kinsel (2000), who both assumed a constant stream width. It allows for the definition of a characteristic stream length L_c [m],

$$L_c = \frac{c_p \rho Q}{w k}. \quad (4)$$

- vi. All sources in the network are supposed to have the same discharge, denoted as Q_s in the following. This approximation is discussed in more details in Sect. 2.1.2.

Using the above assumptions, the mass and energy-balance equations simplify to Eqs. (5)–(6),

$$\frac{dQ}{dx} = q_\ell, \quad (5)$$

$$\frac{dT}{dx} = \frac{1}{L_c} (\gamma \phi_r + T_a - T) + \frac{q_\ell}{Q} (T_\ell - T) - \frac{g}{c_p} \frac{dz}{dx}, \quad (6)$$

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The two factors δ_s and δ_ℓ are defined as

$$\delta_s = \frac{1}{n_s} \sum_{i=1}^{n_s} e^{-d_{s,i}/L_c}, \quad (13)$$

$$\delta_\ell = \frac{L_c}{L_{\text{tot}}} \sum_{k=1}^{n_r} e^{-d_k/L_c} (1 - e^{-L_k/L_c}), \quad (14)$$

where n_r denotes the number of reaches in the stream network, d_k the streamwise distance between the downstream point of stream reach k and the catchment outlet, and L_k the length of stream reach k . The factor δ_s corresponds to the average of the weight $\exp(-d(x)/L_c)$ over all the network sources, and the factor δ_ℓ refers to the average of the same weight over the set of all stream reaches in the catchment. It follows that both δ_s and δ_ℓ decrease roughly exponentially as a function of the network length.

Equation (8) expresses stream temperature as a linear function of air temperature, the slope of the regression line between the two being equal to $\omega_3 = 1 - \omega_1 - \omega_2$. Assuming η to vary only slightly along the network, it can be seen from Eqs. (9)–(10) that ω_1 and ω_2 decrease roughly exponentially with the stream network length. As a consequence, the present model predicts ω_3 to tend towards 1 as the catchment size increases, a fact which has been observed at many locations (e.g. Ozaki et al., 2003; Ducharne, 2008; Kelleher et al., 2012; Chang and Psaris, 2013; Segura et al., 2014).

The present expression for T_{out} differs from those reported previously in the literature in at least two aspects (see Sect. 1 for a review of the analytical solutions to the energy-balance equation published to date). First, the terms on the right-hand side of Eq. (6) were not assumed to be spatially homogeneous when integrating them. This explains the presence of the spatial averaging operator $\langle \cdot \rangle_L$ in Eq. (8), which in turn translates the fact that stream temperature is not impacted by local conditions only. This operator has already been used for the computation of predictor variables in regression-based stream temperature models (Isaak et al., 2010; Hill et al., 2013), but

25 000 (for more information on this map, see <http://www.swisstopo.admin.ch/internet/swisstopo/en/home/products/maps/national/25.html>) and is freely available on the website of the Swiss Federal Office for the Environment (see <http://www.bafu.admin.ch/hydrologie/01835/02118/02120/index.html?lang=fr>; description available only in German, French or Italian). This map was overlaid with a digital elevation model of Switzerland with 2 m horizontal resolution produced by the Swiss Federal Office of Topography (see <http://www.swisstopo.admin.ch/internet/swisstopo/en/home/products/height/swissALT13D.html>) in order to extract the altitude of each point. As an alternative approach, a geomorphological analysis of the stream watersheds could have been performed so as to automatically extract the stream networks. However, it was observed that the results of this analysis did not match with the land cover map in some basins (not shown).

The monthly mean air temperature T_a along the streams is assumed to be a linear function of altitude. The slope and intercept of this function are computed every month and for each catchment i separately (see Sect. 4.1 for a description of the selected catchments),

$$T_{a,i}(z) = a_{l,i}(z - z_i) + b_{l,i}, \quad (15)$$

where z_i [m] refers to the altitude of the gauging station. The lapse rate $a_{l,i}$ [$^{\circ}\text{C m}^{-1}$] is derived using the air temperature measurements of all the meteorological stations located at less than 20 km from the catchment outlet – or the 3 closest meteorological stations if less than 3 are located within a 20 km radius. In case the coefficient of determination R^2 of the regression line between the air temperature values and the altitudes of the meteorological stations is lower than 0.6, $a_{l,i}$ is set equal to zero. The intercept $b_{l,i}$ [$^{\circ}\text{C}$] is computed as the inverse-distance weighted average of the air temperature values measured by the same neighbouring stations. Before computing their average, these values are corrected for the altitude effect by virtually transferring them to altitude z_i using the lapse rate $a_{l,i}$.

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The monthly mean net radiation heat flux at the water surface ϕ_r is mostly dominated by incoming solar radiation, particularly in summer (Caissie, 2006; Webb et al., 2008). In order to keep our model simple, and because ϕ_r eventually has to be distance-averaged using the operator $\langle \cdot \rangle_{\mathcal{L}}$, we express the unknown quantity $\gamma\phi_r$ as a linear combination of the measured incoming solar radiation $\phi_{sw,inc}$, an index quantifying the shading by topography f_s , the stream orientation θ and the fraction f_{rc} of the riparian zone covered with forests,

$$\gamma\phi_r = a_{\phi,sw}\phi_{sw,inc} + a_{\phi,s}f_s + a_{\phi,\theta}\theta + a_{\phi,f}f_f + b_{\phi}. \quad (16)$$

The above equation requires the calibration of 5 unknown coefficients, namely $\{a_{\phi,x}\}_{x=sw,s,\theta,f}$ and b_{ϕ} . In order to avoid equifinality issues (see e.g. Beven, 1993), this expression is not directly used as is. Instead, more parsimonious formulations are evaluated by setting at least two of the coefficients $\{a_{\phi,x}\}_{x=sw,s,\theta,f}$ to zero. Considering all possible combinations of these coefficients, 11 different models are tested for $\gamma\phi_r$ in total – including the constant expression with only b_{ϕ} as calibration parameter. In Eq. (16), the monthly mean incoming solar radiation $\phi_{sw,inc}$ is approximated as a linear function of altitude, whose slope and intercept are computed every month and for every catchment using the same procedure as described above for air temperature (see Eq. 15). Shading by topography f_s is expressed at each point along the stream network as a value between 0 and 1, 1 indicating complete shading. It is derived from the above-mentioned 2 m digital elevation map of Switzerland at nine different hours of day time – corresponding to the fractions 0.1–0.9 of the day-time length – on the 15th day of each month of the year. These values are then averaged at each grid cell and in each season to obtain the spatial distribution of f_s . The stream orientation θ is computed as the cosine of the angle between the North and the stream direction at the point of interest along the network. It follows that θ is a measure of northing, i.e. values close to 1 (resp. -1) indicate a catchment that is oriented towards the North (resp. the South). The fraction f_f of the riparian zone covered with forests is extracted from the same national land cover map at scale 1 : 25 000 which is also used to derive

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the stream network (see above). As the extent of the riparian zone affecting stream temperature is unclear (Moore et al., 2005), the forest cover fraction is computed over riparian buffers with different widths: 25, 50 and 100 m on each side of the center line of the streams (total buffer widths are 50, 100 and 200 m, respectively). The map does unfortunately not allow for the distinction between coniferous and deciduous forests.

The two weights ω_1 and ω_2 cannot be readily estimated from Eqs. (9)–(10). While the values of the factors δ_s and δ_ℓ can be easily derived from the vector representation of the stream network described above, the parameter η requires additional assumptions. It should be reminded that this parameter corresponds to the fraction of the outlet discharge which originates from lateral inflow. Assuming a typical power-law relationship between drainage area and discharge (e.g. Mutzner et al., 2013), η could in principle be approximated as the ratio between the area A_{net} drained by the network (excluding the area drained by the sources) and the total catchment area A_{tot} , raised to some power α : $\eta \sim (A_{\text{net}}/A_{\text{tot}})^\alpha$. However, the computation of A_{net} would require a geomorphological analysis, which was discarded based on the discrepancy between the stream network predicted by this analysis and the observed one (see above). As alternative methods, we consider two different techniques for estimating η . The simplest approach assumes a constant single value for η , calibrated over all catchments. The second approach relies on the analytical expression for η presented in Eq. (12), in which the ratio Q_s/Q_{tot} is replaced with $(A_s/A_{\text{tot}})^\alpha$:

$$\eta = 1 - n_s \left(\frac{A_s}{A_{\text{tot}}} \right)^\alpha. \quad (17)$$

The calibration parameters of this second method correspond to the area A_s drained by a single source and the exponent α .

In order to compute $\overline{T_s}$ and $\langle T_\ell \rangle_L$ in Eq. (8), two different methods for the estimation of the source and lateral inflow temperatures are considered. In a first approximation, these two temperatures are assumed to be both constant and equal. The second method considers them to be linearly related to air temperature as measured at their

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respective altitudes. In other words, it expresses the temperature $T_{s,i}$ of each source $i = 1 \dots n_s$ and the lateral inflow temperature $T_\ell(z)$ at any point with altitude z along the network as

$$T_{s,i} = a_w T_a(z_{s,i}) + b_w, \quad (18)$$

$$T_\ell(z) = a_w T_a(z) + b_w, \quad (19)$$

where $z_{s,i}$ [m] denotes the altitude of source i , and a_w [$^{\circ}\text{C}^{\circ}\text{C}^{-1}$] and b_w [$^{\circ}\text{C}$] are two parameters to be calibrated over the set of all catchments. Notice that the same slope a_w and intercept b_w are used to derive both $T_{s,i}$ and T_ℓ from air temperature, hereby assuming that the source and lateral inflows originate from the same hydrological processes. Moreover, since these two parameters are the same for all catchments, it is implicitly supposed that the ratio of surface runoff to subsurface runoff is the same in all watersheds. As discussed in Sect. 4.2, this requires catchments to be classified by hydrological regime before a_w and b_w can be calibrated separately for each regime. In Eqs. (18)–(19), the monthly mean air temperature is computed in each catchment using Eq. (15).

The distance-average of variables T_ℓ , $\gamma\phi_r$, T_a and dz/dx are computed by discretizing the operator $\langle \cdot \rangle_{\mathcal{L}}$ over the stream segments,

$$\langle f \rangle_{\mathcal{L}} = \frac{\sum_{k \in \Gamma} e^{-(d_k + L_k/2)/L_c} L_k f_k}{\sum_{k \in \Gamma} e^{-(d_k + L_k/2)/L_c} L_k}, \quad (20)$$

where f_k denotes the unweighted mean value of variable f along stream segment k ; the other quantities have been defined previously in Sect. 2.1.1. Except for the riparian forest cover f_f which is derived over buffers of widths 25, 50 and 100 m, the unweighted mean of all other quantities (namely $\phi_{\text{sw,inc}}$, f_s , T_a and dz/dx) along each stream segment are computed over a 20 m wide buffer centered around the center line of the segment, as extracted from the vector representation of the stream network at scale 1 : 25 000 (see above). The value of 20 m is considered as being typical for the width of

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the streams investigated in the present study; although only this value has been tested, it is expected to have little impact on the computed averages. It should be noted that the expressions for $\langle T_a \rangle_L$ and $\langle \phi_{sw,inc} \rangle_L$ both reduce to linear functions of the distance-weighted average of altitude along the stream network $\langle z \rangle_L$ as per Eqs. (15) and (16).

5 The length L_k of stream reach k and the distance d_k between the downstream end of reach k and the catchment outlet are derived from the vector map of the stream network.

Replacing the terms in Eq. (8) by their above expressions, the stream temperature model reads

$$10 \quad T_{out} = (1 - \eta)\delta_s(a_w \bar{T}_a + b_w) + \eta\delta_\ell(a_w \langle T_a \rangle_L + b_w) \\ + (1 - \delta_s - \eta\delta_s - \eta\delta_\ell)\langle T_{eq} \rangle_L, \quad (21)$$

where

$$15 \quad T_{eq} = a_{\phi,sw}\langle \phi_{sw,inc} \rangle_L + a_{\phi,s}\langle f_s \rangle_L + a_{\phi,\theta}\langle \theta \rangle_L + a_{\phi,f}\langle f_f \rangle_L + \langle T_a \rangle_L \\ - L_c \frac{g}{c_p} \left\langle \frac{dz}{dx} \right\rangle_L + b_\phi. \quad (22)$$

15 The calibration parameters of the model are listed in Table 2. When testing a constant parametrization for the source and lateral inflow temperatures, a_w should be set to zero. Similarly, at least two of the coefficients $\{a_{\phi,x}\}_{x=sw,s,\theta,f}$ are assumed equal to zero as per the parametrization of the radiation term discussed above. As such, between 3 and 8 parameters must be calibrated depending on the methods used to approximate the respective unknown variables in Eq. (8). Advantage is taken of the fact that each parameter can be interpreted from a physical point of view to restrict its associated calibration range (see Table 2). For example, η is imposed to adopt a value between 0 and 1 as per Eq. (12), and only positive values are considered for $a_{\phi,sw}$ based on the fact that solar radiation is contributing positively to the net radiation heat flux. Moreover, 20 six different values are tested for the characteristic length L_c used in the definition of

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$\langle \cdot \rangle_L$: 1, 2, 4, 8, 16 and 32 km (see Sect. 5.2). All possible combinations of the different parametrizations of the model terms are tested for each one of these values of L_c . The model associated with the lowest value of the modified Akaike information criterion (AICc) is considered to be the best one among the tested set (e.g. Burnham and Anderson, 2002). As mentioned in Sect. 2.1.1, the model is calibrated in each season separately to account for the fact that the value of the parameter L_c varies over the year.

2.2 Regression model

In order to assess its performances, the physically-based model described by Eq. (21) is compared with a regression model which we developed based on a combination of some of the standard statistical approaches reviewed in Sect. 1. The regression model takes advantage of the fact that most stream temperature curves have a similar shape (see Sect. 4.2). This shape is first estimated by the model based on air temperature, before being mapped to the respective stream temperature curves of the catchments using a linear transformation.

The model assumes all streams to have the same z-scored (i.e. standardized) temperature \hat{T} [-]. The latter is related to the monthly mean temperature T_i of each individual catchment i through (see e.g. Garner et al., 2014)

$$T_i = \sigma_i \hat{T} + \bar{T}_i, \quad (23)$$

where \bar{T}_i [°C] and σ_i [°C] correspond to the annual mean and standard deviation of monthly mean stream temperature in catchment i , respectively. These two quantities are estimated each year independently using multi-linear regression models (MLR). Although more sophisticated techniques could have been used, Wehrly et al. (2009) and Daigle et al. (2010) showed that MLR performs at least as good as several more complicated statistical methods for stream temperature prediction. The MLR models were constructed using similar predictor variables as in the physically-based model,

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namely the annual mean and standard deviation of both air temperature and incoming short-wave radiation, the riparian forest cover fraction, stream channel slope, stream orientation, the difference in topographical shading between summer and winter, the number of sources in the network and the watershed area. All multi-linear models based on any possible subset of these variables were tested, with a maximum number of terms per model arbitrarily fixed to 6 to prevent over-parametrization. Multicollinearity issues were avoided by discarding models whose variance inflation factor (VIF) exceeded 5. Each predictor variable was distance-averaged over the stream networks using the operator $\langle \cdot \rangle_{L_c}$, as in the case of the physically-based model. Different values of L_c were considered when applying this operator as per Eq. (20): 1, 2, 4, 8, 16 and 32 km. The best predicting MLR models for \bar{T}_i and σ_i were selected based on AICc.

In Eq. (23), the z-scored stream temperature is computed each month by the model based on a non-linear relationship with air temperature,

$$\hat{T} = \mu + \frac{\alpha - \mu}{1 + \exp(-\kappa(\hat{T}_a - \beta))}, \quad (24)$$

where μ [°C], α [°C], β [°C] and κ [°C⁻¹] are coefficients obtained through ordinary least squares regression, and \hat{T}_a [-] denotes the mean z-scored air temperature over Switzerland. \hat{T}_a is obtained by averaging the z-scored measurements of 14 reference meteorological stations, which are considered by the Swiss Meteorological Office to be representative of the climate diversity in Switzerland (see http://www.meteosuisse.admin.ch/web/fr/climat/climat_aujourd'hui/donnees_mensuelles_homogeneisees.html; description only available in German, French or Italian),

$$\hat{T}_a = \frac{1}{14} \sum_{k=1}^{14} \frac{T_{a,k} - \bar{T}_{a,k}}{\sigma_{a,k}}. \quad (25)$$

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In the above equation, $T_{a,k}$ [°C] denotes the monthly mean air temperature measured at station k , and $\bar{T}_{a,k}$ [°C] and $\sigma_{a,k}$ [°C] refer to the annual average and standard deviation of $T_{a,k}$ computed each year independently, respectively.

In summary, the regression model proceeds as follows to estimate stream temperature in an ungauged basin: (a) it first computes the mean z-scored air temperature over Switzerland according to Eq. (25), based on the measurements of 14 meteorological stations, (b) it then uses \hat{T}_a to estimate the z-scored stream temperature in any catchment as per Eq. (24), and finally (c) it converts \hat{T} to the actual stream temperature using Eq. (23), where the scaling coefficients \bar{T}_i and σ_i are estimated for the catchment of interest using multi-linear regression models. These different steps will be illustrated into more detail in Sect. 5.4.

3 Selected catchments for model evaluation

In order to test the two stream temperature models, catchments are selected in Switzerland such that: (a) the natural regime of the river is as little affected by anthropogenic activities as possible, and (b) measurements of discharge and stream temperature are available for more than one year. This results in a set of 29 catchments, whose locations are depicted in Fig. 1 and physiographic properties are summarized in Table 3.

About half of the selected catchments is situated on the Swiss Plateau – a large area with little altitude variations between Lake Geneva in the south west and Lake Constance in the north east. The climate in this region is relatively mild, with precipitation mostly falling as rain in winter and mean daily maximum air temperature hardly exceeding 30°C in summer. The hydrological regimes of the catchments in the Plateau depend on the precipitation patterns and are therefore strongly variable from year to year (Aschwanden and Weingartner, 1985). Discharge does not vary by more than a factor two over the year; it usually reaches its maximum during winter, when

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evapotranspiration is the lowest. As catchments gain in altitude, the discharge control mechanism changes from evapotranspiration to snowmelt: higher-altitude catchments present a discharge peak during the melt season, in April–May.

Only two catchments are found in the Jura mountains, a relatively low-altitude (< 1700 m) mountainous range with rigorous winters. This region is characteristic for its karstic aquifers with preferential flow paths, generating fast and complex responses to precipitation events. Although more marked, the hydrological regimes of the Jura catchments are relatively similar to those of the watersheds in the Plateau. A clear peak in discharge is noticeable in April for the highest catchments (Aschwanden and Weingartner, 1985).

The Alpine region of Switzerland is typically subdivided into its north and south parts, based on their difference in climate. The Southern Alps are influenced by Mediterranean weather, implying warmer winters and more precipitation in autumn than in the Northern Alps. The hydrological regimes of the catchments in the Northern Alps are strongly related to altitude. The month in which the peak of discharge is observed ranges from May for low-altitude watersheds to July–August for catchments partially covered by glaciers. Moreover, the ratio of annual maximum to annual minimum discharge increases with altitude. Similar hydrological regimes are observed in the Southern Alps, except for a second discharge peak in autumn due to rainfall (Aschwanden and Weingartner, 1985). As seen in Fig. 1, only three unperturbed catchments could be found in the Northern Alps, while five are located in the Southern Alps.

All in all, 10 of the 16 hydrological regimes identified by Aschwanden and Weingartner (1985) in Switzerland are present among the 29 selected catchments (see Table 3). The surface area distribution is quite large, with catchments ranging from 3.31 km² (Rietholzbach at Mosnang) to 392 km² (Broye at Payerne). The mean altitudes of the watersheds are also spanning a wide range of values. Few catchments are partially covered by a glacier, with only two of them having a glacier cover fraction over 10%.

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4 Stream temperature data

The stream temperature data which is used in the present study was provided by the Swiss Federal Office for the Environment (FOEN). Advantage is taken of the present publication to describe this new data set, which is freely accessible for research purposes at the following address: <http://www.bafu.admin.ch/hydrologie/01832/01856/index.html?lang=en>. A map displaying the position of all available hydrological stations which measure stream temperature can also be found on the website of the FOEN (http://www.hydrodaten.admin.ch/en/index.html#temperatur_fliessgewaesser).

4.1 Data collection and validation

The FOEN is operating an automatic network of stream gauging stations, continuously measuring water level and discharge at more than 180 locations in Switzerland. Water level is recorded using an ultrasonic distance sensor, and converted into discharge values through a rating curve adapted each year. The water level values are validated against the measurements of a second instrument – a pressure probe – and rejected in case the difference between the two values is greater than 2 cm. A limited number of gauging stations has been equipped with a thermometer, the earliest starting in 1968. This number has increased greatly since 2002, with now more than 70 stations automatically probing water temperature every 10 min (Jakob, 2010). The measurement values are automatically uploaded and displayed in real time on the web page of the FOEN (same page as for the map displaying the positions of the stations).

Among the watersheds in which temperature is monitored, 25 have been identified in the present study as being little affected by anthropogenic activities. In order to complete this data set, the temperature and discharge measurements of four additional gauging stations were obtained from the Department for Construction, Transport and Environment of Canton Aargau (see Table 3). The period in which water temperature was measured by each station is also indicated in Table 3.

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The temperature data is usually not quality-proofed by the FOEN or Canton Aargau. As a validation procedure, we performed two different tests on the data at the hourly time step, on top of visual inspection:

- a. All temperature measurements lower than 0°C or greater than 30°C were removed, except for the values between -0.5 and 0°C which were set to 0°C, and the values between 30 and 30.5°C which were set to 30°C.
- b. The temperature variation between consecutive time steps was checked to remain within physical bounds. In particular, it was verified that temperature varied by more than 0.01°C over 5 h, but less than 3°C within one hour. Constant temperature values could result from a defect in the sensor, but also from the fact that the hourly values had been replaced with their daily mean in some cases. In order to distinguish between the two, the present quality control procedure was performed semi-manually.

After quality control, the hourly data were aggregated into monthly mean values.

4.2 Thermal regime classification

A preliminary study of the selected catchments was performed, with the aim of classifying the rivers according to their thermal behavior. This classification was intended to be used later in order to investigate whether the performance of the models was affected by the river thermal regime.

As a first attempt, we examined whether the catchments could be classified based on the shape of their stream temperature curve. To this end, we z-scored (i.e. standardized) the monthly mean stream temperature values in each watershed similarly to Garner et al. (2014). However, as observed by these authors, we could identify only one single thermal regime (Fig. 2a). Only two catchments among the 29 did not to present the same thermal regime as the others, namely those labeled as 5 and 14 in Table 3.

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As an alternative approach, we tested whether the characteristics of the stream–air temperature curve could be used to characterize the thermal regime of the catchments. For this purpose, monthly mean stream temperature was linearly regressed against monthly mean air temperature, excluding the points with negative air temperature values (e.g. Kelleher et al., 2012). Based on the values of the slope and intercept of this relationship, three groups of catchments could be clearly identified (Fig. 2b). The first group contains the watersheds in which a significant portion of discharge originates from deep aquifer infiltration (watersheds 9 and 14 in Table 3, labeled as “groundwater-fed streams” in Fig. 2b). This group is characterized by low slope and high intercept values, as reported by many studies (e.g. Caissie, 2006; Webb et al., 2008). The second group of watersheds corresponds to the high-altitude basins with more than 50% glacier cover. Both the slope and intercept of the stream–air temperature relationship are small for the members of this group, which is actually composed of only one catchment (watershed 5 in Table 3, denoted as “proglacial” in Fig. 2b). The vast majority of the watersheds do not fall into any of the two aforementioned groups. These catchments, denoted as “thermally climate-driven”, are characterized by relatively low intercept and high slope values, i.e. their stream temperature is strongly correlated to air temperature.

Because of the predominance of the “thermally climate-driven” streams, only the latter will be considered for the testing of the physically-based and regression models. The inclusion of the groundwater-dominated streams in the test set would require the amount of groundwater infiltrating into the stream to be estimated. We tested several methods, including the derivation of the baseflow index from discharge measurements (e.g. Eckhardt, 2005; van Dijk, 2010) or from the TOPMODEL topographic index (e.g. Ducharme, 2009). However, none of the investigated techniques succeeded in predicting a larger baseflow index for the catchments labeled as “groundwater-fed” as compared to the others (not shown). Similarly, the consideration of the proglacial streams would imply the glacier cover fraction to be included into the models. This addition of one calibration parameter was not considered justified given that this group

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contains only one catchment. In total, 26 catchments were used for the calibration and validation of the models, namely all those listed in Table 3 except watersheds 5, 9 and 14.

5 Model evaluation

In order to rigorously evaluate the performance of the two models described in the previous section, 5 of the 26 selected catchments were removed from the data set to create an independent validation set (watersheds 3, 6, 11, 13 and 27, displayed in orange in Fig. 1). Caution was given to single out basins with different size, mean elevation and geographic location. Among the four climatic regions of Switzerland, only the Jura could not be represented in the validation set, given that only one station (number 26) among the 26 available was located in this area.

The measurement time period is also split into a calibration (2007–2012) and a validation (all dates before and including 2006) period. Only the measurements performed by the calibration stations – whose drainage area is marked in green in Fig. 1 – during the period 2007–2012 are used to calibrate the models. Four different validation sets can be formed with the remaining station-months:

1. the data set containing the measurements of the validation stations during the calibration period. This set can be used to evaluate the ability of the models to make predictions in ungauged basins.
2. the data set containing the measurements of the calibration stations during the validation period. This set will be used to evaluate the precision of the models when predicting stream temperature in past or future years.
3. the data set formed by the measurements of the validation stations during the validation period. This set serves to evaluate the performance of the models when predicting stream temperature both in ungauged basins and in ungauged years.

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4. the data set corresponding to the union of all three previous validation sets, which may be used to obtain a synthetic evaluation of the precision of the models.

The complete data set is almost equally subdivided into its calibration and validation parts, with the former containing 1223 station-months and the validation sets 1–4 regrouping 360, 705, 204 and 1269 station-months, respectively.

As mentioned in Sect. 2.1, the value of the characteristic stream length L_c is expected to change over the course of the year. In order to ease capturing of this variability, the physically-based model is calibrated over each season separately. As such, the calibration and validation data sets are each subdivided into four groups, corresponding to winter (January–March), spring (April–June), summer (July–September) and autumn (October–December), respectively. Each one of these subgroups contains approximately one fourth of the station-months originally belonging to the parent group. The regression model is calibrated over all seasons at once, but evaluated in each season separately so as to investigate a potential effect of the period of the year on its precision.

Since the physically-based model expresses stream temperature as a linear function of air temperature, it cannot reproduce the asymptotic behavior of the former as the latter drops below 0°C. Consequently, data points associated with negative air temperature values are removed from the data set before calibration (Kelleher et al., 2012). When evaluating the model over the validation sets, all stream temperatures predicted to be negative are replaced with 0°C values.

In the following, the best seasonal formulations of the physically-based model are presented first. The precision of this model is then evaluated, and the influence of the stream network resolution on the model results investigated. Finally, comparison is made with the regression-based model. All the results presented in this section will be discussed and analyzed in Sect. 6.

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5.1 Model formulations

As mentioned in Sect. 2.1.2, the different possible formulations of the physically-based model are ranked in each season according to their respective AICc value. Following Burnham and Anderson (2002), AICc is preferred here over the classical definition of the Akaike information criterion (AIC) since it includes a correction term for finite-sized data sets. It should be mentioned that AICc is computed by calibrating the models not over the calibration set only, but rather over the entire data set (i.e. both the calibration set and validation set 4). Only in a second time is each model calibrated over just the calibration set, so as to evaluate its performances in terms of RMSE, R^2 and bias.

Table 4 presents the best model formulations selected in each season, ranked according to their respective Akaike weights w_i . The latter corresponds to the probability of each model to be a better descriptor of the observed data (according to information theory) as compared to the model with the minimum AICc value (Burnham and Anderson, 2002; Wagenmakers and Farrell, 2004). Considering models with $w_i \leq 0.1$ to be statistically insignificant, it can be observed that only a few formulations were identified in each season as being relevant for stream temperature prediction. The characteristic stream length L_c is found to be consistent among these formulations, with a value of 4 km in spring, summer and autumn, and 8 km in winter, regardless of the formulation.

The model selection reveals the radiation term $\gamma\phi_r$ to be preferentially expressed as a function of topographical shading f_s and riparian forest cover fraction f_t , or as a function of f_s alone. Among the tested buffer widths used to compute f_t , none of the three values 50, 100 or 200 m prevails significantly over the others. The order in which they appear in the ranked models varies depending on the season; for example in winter, forest cover computed over a 100 m wide buffer is expected to be a better predictor of $\gamma\phi_r$ than forest cover over a 50 m wide buffer, whereas the opposite is true in spring. Focusing on each season separately, the linear coefficient associated with any given term is observed to have a fairly constant value among the different

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measurements performed by the validation stations during the validation period. The only noticeable exception is in summer, where the model evaluation over set 3 provides satisfactory results ($RMSE = 1.13^{\circ}C$, $R^2 = 0.90$, bias = $-0.01^{\circ}C$).

5.3 Influence of the stream network resolution

5 The results reported above are based on the stream network geometries extracted from the land cover map at scale 1 :25 000 (see Sect. 2.1.2). These geometries directly affect the values of the distance-averaged predictor variables, since the operator $\langle \cdot \rangle_L$ averages over the entire stream network. As a consequence, modifying the network resolution is expected to impact the model performance.

10 To test this hypothesis, two additional stream networks with coarser resolution than the original one were investigated. These networks were obtained by removing stream segments with Strahler order 1, and those with Strahler order 1 and 2, respectively. Through this procedure, the mean drainage density of the 26 selected catchments decreased from 2.1 km km^{-2} for the original network to 0.5 km km^{-2} for the coarsest one, passing through 1.0 km km^{-2} for the intermediate resolution network. The different model formulations were evaluated over the two additional networks using the same procedure as described in the previous section. Although the results are not reported here, it was essentially observed that the network resolution had little influence on the ranking of the model formulations based on AICc in each season. Almost all selected models were associated with a characteristic stream length $L_c = 4$ or 8 km , as in the case of the original stream network. The parametrization of the net radiation heat flux $\gamma\phi_r$ was also similar to the one reported in Table 4. Topographical shading and riparian forest cover remained the two most statistically significant predictors for this term, except during winter, where stream orientation appeared as a relevant variable. The values of the coefficients a_w and b_w were noted to vary little among the selected model formulations in a given season. Finally, the parameter η was preferentially expressed as a constant term. Its value was identified as being zero in all seasons except summer

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in the case of the intermediate resolution stream network, whereas its parametrization was close to the one described in Table 4 in the case of the coarser network.

As a consequence of the little influence of the network resolution on the model parametrization, few variations in the model precision were observed between the three stream networks. As seen in Fig. 3, no clear tendency can be identified among the residuals. At most can a small increase in the model prediction error be detected for the coarsest network as compared to the first two, especially in autumn. The largest absolute residuals are also observed to be generated by this network. On the other hand, the strong bias previously noted in winter is present in the case of the intermediate resolution network, but less so in the case of the coarsest resolution one.

5.4 Comparison with the regression model

This section describes the characteristics of the calibrated regression model first, before presenting the results of its evaluation in a second step. Figure 4 pictures the observed monthly mean stream temperature, z-scored and averaged over the 21 calibration stations, as a function of \hat{T}_a over the period 2007–2012. As can be observed, the relationship between these two quantities displays a small hysteresis effect, which can be explained by stream cooling due to snow-melt in spring (Mohseni et al., 1998). The logistic equation introduced by Mohseni et al. (1998) is fitted to each one of the hysteresis branches separately,

$$\hat{T} = -1.87 + \frac{4.88}{1 + e^{-0.99 \cdot (\hat{T}_a - 0.66)}} \quad (\text{in January–June}), \quad (26)$$

$$\hat{T} = -1.86 + \frac{3.96}{1 + e^{-1.16 \cdot (\hat{T}_a - 0.06)}} \quad (\text{in July–December}). \quad (27)$$

It should be noted that the parameters corresponding to the lower and upper asymptotic values of the logistic curve are particularly sensitive to the data points located at both ends of the hysteresis. To limit inaccuracy errors, the temperatures measured



in January and July were used to fit both branches of the hysteresis, as they usually correspond to the annual extreme values. Equations (26)–(27) are those used in the model to determine the z-scored stream temperature \hat{T} at any location based on \hat{T}_a (see Sect. 2.2).

The multi-linear regression models which were selected to estimate the annual mean \bar{T}_i and the standard deviation σ_i of stream temperature in a given year are presented in Table 6. They correspond to the models associated with the lowest AICc values among the tested formulations (see Sect. 2.2). As observed in the table, the characteristic stream length used by the operator $\langle \cdot \rangle_{L_c}$ to average the predictor variables over the stream networks is significantly different in the two cases: $L_c = 4$ km for the \bar{T}_i model, whereas $L_c = 32$ km for the σ_i one.

Table 7 summarizes the prediction errors of the stream temperature regression model when evaluated over validation set 4 using the original stream network. Comparison with Table 5 reveals that its precision is greater than the one of the physically-based model. Its RMSE is about 0.2°C lower, its R^2 about 0.03 to 0.12 larger, and its absolute bias 0.05 to 0.20°C smaller depending on the season. However, its performance worsens when using the two stream networks with coarser resolution: its yearly average RMSE increases to 1.26°C in the case of the intermediate resolution network, and even 1.29°C for the coarsest network, which is close to the value obtained with the physically-based model.

6 Discussion

The formulations of the physically-based model selected by AICc ranking are consistent among the different seasons. In particular, topographical shading systematically appears to be the strongest predictor of the net radiation heat flux $\gamma\phi_r$. This observation is not particularly surprising in a mountainous country like Switzerland, where some valleys are steep enough for their bottom not to be illuminated by direct sun light for some period of the year. The basins referred to as numbers 14 and 24 in Table 3 are

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examples of such watersheds, both having a mean catchment slope larger than 35° . Riparian forest cover fraction corresponds to the second most important predictor for the net radiation heat flux term. It was rather unexpected to identify this parameter as relevant during autumn and winter, especially since more than half of the selected catchments are mainly covered with deciduous forests due to their relatively low mean elevation (< 1000 m). This result has to be balanced with the fact that a given fraction increase in riparian forest cover is predicted by the model to have an effect on $\gamma\phi_r$ about 4 to 6 times smaller in magnitude than the same fraction increase in topographical shading. It should also be reminded that the precision of the model is rather low in winter, hereby questioning the validity of its parametrization in this season. Certainly more unexpected is the absence of solar radiation among the predictors of $\gamma\phi_r$, which will be explained below. Regarding the parametrization of the discharge fraction due to lateral water inflow η , the model predicts the water in the stream channel to originate principally from surface and subsurface runoff during summer and autumn ($\eta = 1$). This partly matches our expectations, since the fraction of discharge originating from the sources is expected to decrease when moving downstream along a given network. The characteristic catchment size defining the transition from source-water-dominated to lateral-inflow-dominated discharge is controlled here by L_c , which is equal to 4 km in summer and autumn. This value is smaller than the main channel length in more than 90% of the selected watersheds (not shown), hereby strengthening our confidence in the parametrization of η during these two seasons. On the other hand, a value of 1 for η in all catchments may appear as a too simplified approach (see below). The questioning of the parametrization of η is all the more true in winter, where its value is predicted to be zero. Only in spring did the model ranking select the more physically-based formulation for η , expressed as a function of the area drained by each source. Concerning the parametrization of the source and lateral inflow temperatures, it should be mentioned that the linear expression as a function of air temperature was systematically preferred over the constant term. This certainly results from the large altitudinal range covered by the selected catchments, which does not allow for

a constant inflow temperature to reflect the diversity of encountered climatological conditions, and mainly air temperature.

As defined in Eq. (21), the physically-based model linearly relates air temperature to stream temperature through the proportionality coefficient ω_3 . The latter is compared in Fig. 5 with its actual observed value, namely the slope of the regression line between the monthly mean temperature measurements of the stream and air. As seen in the figure, the model systematically overestimates the value of ω_3 , particularly in winter and summer where the mean bias equals 0.2. Referring to Eq. (21), this implies that ω_1 and ω_2 are globally underestimated by the model, hereby indicating that the parametrization of the factor η could possibly be improved. As noted in Sect. 2.1.2, a more physically-based expression could be used to compute η , as long as a geomorphological analysis of the river watersheds can be performed. This approach was not investigated here for the reasons mentioned earlier.

The overestimation of ω_3 is probably at the origin of the fact that solar radiation is unexpectedly missing from the selected expressions for the net radiation heat flux $\gamma\phi_r$ (see Table 4). Contrary to the regression model, the physically-based model presents the advantage that the calibration range of each one of its parameters can be restricted based on physical considerations (see Table. 2). An attempt was made at removing these constraints, which resulted in incoming short-wave radiation being present in almost all models for $\gamma\phi_r$, but associated with a negative coefficient. It was concluded that the unconstrained model takes advantage of the fact that the annual cycles of air temperature and solar radiation have a similar shape to artificially reduce the value of air temperature by subtracting a fraction of solar radiation, hereby compensating for the too large value of ω_3 . This observation argues once more in favor of a better parametrization of the factor η .

As mentioned in Sect. 5, the characteristic stream length L_c is found to be of the order of 4–8 km regardless of the season or the stream network resolution in the case of the physically-based model. This range is in agreement with the findings of Isaak et al. (2010) and Macedo et al. (2013). Hrachowitz et al. (2010) and Chang and Psaris

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(2013) rather concluded that L_c was around 1 km, however they did not investigate values for L_c larger than 1 km. Contrary to our expectations, we do not observe a marked variation of L_c across seasons, probably due to the fact that we assumed a single value for all the catchments. The annual cycle of L_c may have been better captured by separately calibrating this parameter in each individual catchment, but this would have contradicted our aim to derive a regional model. It should be emphasized that the absence of observed annual cycle for L_c does not question the decision to calibrate the physically-based model on a seasonal basis, since the source temperature parametrization is observed to vary significantly over the year (see Table 4).

Our model is rather equivocal regarding the width of the riparian buffer which is relevant for the determination of stream temperature at a given point. As a matter of fact, none of the tested buffer widths appears to prevail over the other ones in the retained parametrizations of $\gamma\phi_r$. This ambiguity reflects the range of buffer widths used in the literature, which extends from 30 (e.g. Jones et al., 2006; Macedo et al., 2013) to 200 m (e.g. Scott et al., 2002; Segura et al., 2014).

The precision of the physically-based model was reported in the previous section to be rather low in January–March. This can be explained by the fact that the non-linearity of the stream–air temperature relationship at low air temperature values is not captured by the model. The latter rather simulates a sharp transition from the linear regime to a constant one, since the stream temperature values predicted to be negative are systematically replaced with 0°C . This implies a faster decrease towards 0°C , which is at the origin of the strong negative model bias in winter.

As noticeable in Table 5, the model RMSE is larger in spring as compared to the other seasons. This is attributable to the fact that many of the selected watersheds are impacted by snow melt in spring. Since the snow cover conditions are strongly variable both spatially and temporally, a large dispersion of the stream temperature values is typically observed in spring. The model performs nonetheless relatively well in this season, for its R^2 value is of the same magnitude in spring as during the rest of the year.

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Advantage can be taken of the physical basis of the model to investigate some aspects of the stream temperature dynamics. For example, Fig. 6 displays the respective values of the factors ω_1 , ω_2 and ω_3 appearing in Eq. (21) as a function of the season. These factors correspond to the weights associated with the mean source temperature \bar{T}_s , average lateral inflow temperature along the network $\langle T_e \rangle_L$ and average equilibrium temperature along the network $\langle T_e \rangle_{\mathcal{L}}$, respectively. As seen in the figure, ω_3 is the largest factor of the three in all seasons, with a value of about 0.6–0.8. This results from the fact that stream temperature is primarily impacted by the atmospheric conditions. The other two factors are nonetheless non-negligible, with ω_1 being of the order of 0.4 in winter and ω_2 being approximately equal to 0.2 from April to December. The value of ω_1 has to be put into perspective with respect to the fact that our confidence in the model parametrization is relatively low in winter. Moreover, following the above discussion about the computation of the factor η , the values reported here for ω_2 should be considered as a lower limit. It therefore appears that not only the net total heat flux at the air–water interface is important in determining stream temperature, but also the heat flux associated with the lateral inflow of water. This conclusion is in agreements with the findings of Bogan et al. (2004), who found that the precision of their stream temperature model was improved by including a term accounting for the lateral water inflow. Similarly, Herb and Stefan (2011) mention that the heat input associated with groundwater infiltration may be of the same order of magnitude as the heat flux due to atmospheric forcing in some cases. This effect seems to be largely underestimated in the literature, since the lateral inflow of water has often been neglected in previous stream temperature models (e.g. Edinger et al., 1968; Bogan et al., 2003; Caissie et al., 2005; Bustillo et al., 2014).

As opposed to the physically-based model, the parameter values of the regression model could not be constrained using physical considerations. As a result, the sign of some of the linear coefficients relating the predictor variables to \bar{T}_i and σ_i are in contradiction with our understanding of stream temperature dynamics (see Table 6). For example, the stream orientation θ , measured as the cosine of the angle

between north and the channel direction, is positively related to the annual mean stream temperature \bar{T}_i . It was rather expected that north-oriented catchments receive less radiation from the sun, hereby implying lower stream temperatures. The same observation is true for the riparian forest cover fraction, which is positively associated in the model with the annual standard deviation σ_i of stream temperature. However, experimental observations tend to conclude that riparian shading has a buffering effect on stream temperature, therefore dampening the amplitude of the variations of the latter (see e.g. Moore et al., 2005). Despite these inconsistencies, the regression model performs better than the physically-based one in terms of RMSE, R^2 and bias. This fact questions further the validity of the parametrization of the physically-based model, which could certainly be improved (see Sect. 7). On the other hand, the regression model appears to be much more sensitive to the stream network resolution as compared to its counterpart, possibly as a consequence of its lack of physical basis. This lack does also not allow for the investigation of the physics governing stream temperature, as can be done with the physically-based model (see Fig. 6).

7 Conclusions

This study aimed at presenting a new model for the prediction of monthly mean stream temperature in ungauged basins. The model corresponds to an analytical solution to the one dimensional heat advection equation, simplified using some approximations. Among the latter, the most important one assumes the ratio of stream width to discharge to remain spatially constant. As opposed to previous studies relying on the same approach, the heat advection equation is solved here over an entire stream network instead of a single stream reach. Moreover, the various terms of the equation are also not supposed to be spatially homogeneous, which leads to the apparition of a space averaging operator $\langle \cdot \rangle_L$ applied to most terms of the solution. This operator uses a weight which decreases exponentially with the distance to the catchment outlet, hereby giving more emphasis to the points located near the gauging station. The

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extent of the spatial area over which the operator acts is controlled by a parameter L_c , referred to as the stream characteristic length. This parameter is typically dynamic, which explains why the model needs to be calibrated separately in each season. Both the source and the lateral inflow terms – which are usually neglected – are retained in the final solution to the heat advection equation. This notably enables the model to be applied in small watersheds, where the influence of source temperature on the value of stream temperature measured at the catchment outlet cannot be discarded.

While most terms of the model expression could be evaluated based on meteorological observations or topographic maps, some required an additional modeling effort. In particular, the net radiation heat flux at the air–water interface was approximated as a linear combination of several predictor variables, e.g. topographical shading or riparian forest cover. Similarly, the source and lateral inflow temperatures were expressed as a linear function of air temperature measured at the source location and along the stream, respectively. Finally, the fraction η of discharge at the catchment outlet originating from lateral water inflow along the network was estimated based on the number of sources in the watershed. These parametrizations present the advantage that the information they require is readily available at the regional scale, namely: air temperature measurements, a land cover map and a digital elevation map. They differ from the physically-based parametrizations used in other studies (e.g. Bogan et al., 2004; Herb and Stefan, 2011), which require measurements of meteorological variables being hard to interpolate in mountainous terrain, such as wind speed or relative humidity.

The performance of the model is quite satisfactory, with a root-mean-square error of about 1.3°C and a coefficient of determination R^2 of 0.87 when used for stream temperature prediction in “thermally climate-driven” catchments. These catchments, which are by far the most abundant ones in Switzerland, correspond to those with a glacier cover lower than 50 % and whose stream is not impacted by groundwater infiltration from deep aquifer. Model precision is the lowest in winter, due to the inability of the model to reproduce the fact that stream temperature asymptotically tends

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towards 0°C for negative air temperature values. Closer investigation of the model error could attribute part of its imprecision to the parametrization of the factor η , which corresponds to the fraction of discharge originating from the lateral inflow of water (in opposition to the discharge fraction originating from the sources).

5 The precision of the model was also assessed by comparing it with a more simple regression model. The latter was observed to perform slightly better, with a RMSE about 0.2°C lower. However, its parameters could not be interpreted from a physical point of view, hereby hindering the restriction of their respective calibration ranges based on physical considerations. This led the regression model to simulate
10 some aspects of the stream temperature dynamics wrongly. For example, some physiographic variables known to have a cooling effect on water temperature were modeled as warming up the stream. The regression model was also observed to be much more sensitive than its physically-based counterpart with respect to the stream network resolution. When discarding all stream segments with a Strahler order equal
15 to one, the RMSE of the regression model increased from 1.12 to 1.26°C, whereas the one of the physically-based model remained constant up to 0.01°C.

Despite a few deficiencies, the physically-based model can be used to analyse some aspects of the physics governing stream temperature. As an example, the relative importance of each one of the stream heat sources could be determined from
20 the model. Climatic forcing was found to be the major driver of water temperature, as expected (e.g. Caissie, 2006). More interestingly, the lateral inflow of water was identified as a non-negligible secondary heat flux. This fact is confirmed by other studies (e.g. Bogan et al., 2004; Herb and Stefan, 2011), but nonetheless fails to be accounted for in many stream temperature models (e.g. Caissie et al., 2005; Bustillo
25 et al., 2014). We therefore wish at emphasizing the role of lateral water inflow on stream temperature, even in catchments – such as those used in this study – which are not impacted by groundwater infiltration originating from a deep aquifer.

Among the improvements that can be brought to the physically-based model, a more accurate parametrization of the discharge fraction originating from lateral

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water inflow η appears as a promising enhancement. In particular, η could be estimated from a geomorphological analysis of the catchments. This approach was not retained here due to the discrepancy between the stream networks predicted by the geomorphological analysis and the observed ones. In case it could be implemented, such a revision is expected to improve the predicted slope of the stream–air temperature curve. A geomorphological analysis could also positively influence the modeling of the source and lateral inflow temperatures. The parametrization of these two terms could be improved by including predictor variables accounting for e.g. the glacier cover fraction or the mean altitude of the area drained by each source (resp. stream reach). As a matter of fact, surface and subsurface runoffs originating from glacier-covered or high-altitude subcatchments are expected to have particularly low temperatures, especially during the snow- and ice-melt season. The model could also be substantially improved in case the characteristic stream length L_c could be computed instead of calibrated. Indeed, L_c does not only present a seasonal variation but also differs across the individual catchments, a fact which was neglected in the present work. The a priori computation of L_c would imply the ratio of discharge to channel width to be independently estimated in each catchment. Such an estimation would in turn require the stream rating curve to be known, hereby limiting the applicability of the model to gauged watersheds. Finally, one might expect the model precision to improve by using a more physically-based parametrization for the net radiation heat flux – instead of the multi-linear model used here. We actually tested an alternative expression based on an estimation of the incoming atmospheric radiation and a first-order approximation of the long-wave radiation emitted by the stream (not shown). Rather than an improvement, this parametrization led to a decrease of the model precision, as a result of its inability to compensate for the overestimation of another parametrized term (ω_3) in the model – contrary to the multi-linear expression.

We expect the physically-based model to be easily transferable to other regions of the globe. The parametrization of the net radiation heat flux at the air–water interface might need some adaptation in order to correctly reflect the dominant physiographic

controls on local stream climate. For example, topographic shading is certainly not a relevant predictor variable over flat regions. Similarly to the approach presented in this work, the most appropriate set of predictor variables for the net radiation heat flux over a particular region can be obtained through AICc ranking. Once set, the stream temperature model can be used to investigate e.g. the extent of the stream network which is thermally suitable for sensitive fish species at the regional scale (e.g. Isaak et al., 2010). This investigation can in turn serve as a basis for the introduction of regulation policies or protection measures.

Appendix: Solution to the energy-balance equation over a stream network

The analytical solution to Eqs. (5)–(6) is first derived for the case of a simple stream reach of length L (see Fig. 7a). Let the downstream distance be denoted as x , with x_0 and x_1 referring to the positions of the reach origin and end points, respectively. The discharge $Q(x_1)$ and stream temperature $T(x_1)$ can be easily computed by integrating Eqs. (5)–(6) between x_0 and x_1 ,

$$Q(x_1) = Q(x_0) + q_\ell L, \quad (\text{A1})$$

$$T(x_1) = \frac{Q(x_0)}{Q(x_1)} e^{-d(x_0)/L_c} T(x_0) + \frac{1}{Q(x_1)} \int_{x_0}^{x_1} e^{-d(x)/L_c} \psi(x) dx, \quad (\text{A2})$$

where

$$\psi(x) = q_\ell T_\ell(x) + Q(x) \left(\frac{\gamma \phi_r(x) + T_a(x)}{L_c} - \frac{g}{c_p} \frac{dz}{dx} \right). \quad (\text{A3})$$

In Eq. (A2), $d(x) = x_1 - x$ denotes the distance between any point x and the downstream end point x_1 (see Fig. 7a).

The above equations require the values of discharge and temperature at the upstream end of the reach to be known. By applying them iteratively to all the reaches of a network, starting from the most downstream one, the expressions for discharge Q_{out} and water temperature T_{out} at the network outlet can be expressed as a function of the discharges and temperatures of the sources. At the confluences, the discharges $Q_{u,1}$ and $Q_{u,2}$ and the temperatures $T_{u,1}$ and $T_{u,2}$ of the two upstream reaches can be related to the discharge Q_d and temperature T_d of the downstream reach using the mass and energy-balance equations (Westhoff et al., 2007),

$$Q_d = Q_{u,1} + Q_{u,2}, \quad (\text{A4})$$

$$T_d = \frac{Q_{u,1}}{Q_d} T_{u,1} + \frac{Q_{u,2}}{Q_d} T_{u,2}. \quad (\text{A5})$$

Based on Eqs. (A1)–(A5), the derivation of the expressions for Q_{out} and T_{out} is straightforward and leads to the following relations,

$$Q_{\text{out}} = \sum_{i=1}^{n_s} Q_{s,i} + q_\ell L_{\text{tot}} \quad (\text{A6})$$

$$T_{\text{out}} = \sum_{i=1}^{n_s} \frac{Q_{s,i}}{Q_{\text{out}}} e^{-d_{s,i}/L_c} T_{s,i} + \frac{1}{Q_{\text{out}}} \int_{\mathcal{L}} e^{-d(x)/L_c} \psi(x) dx. \quad (\text{A7})$$

In the above equations, n_s refers to the number of sources in the network, L_{tot} denotes the total length of the stream network, $d_{s,i}$ corresponds to the downstream distance of source point $x_{s,i}$ to the network outlet, $d(x)$ refers to the distance between any point x along the network and the network outlet, \mathcal{L} corresponds to the geometrical union of all reaches in the stream network, and $T_{s,i}$ and $Q_{s,i}$ denote the stream temperature and discharge at source point $x_{s,i}$, respectively. The reader is referred to Fig. 7b for a graphical illustration of some of the variables. The integral over \mathcal{L} is a short-hand notation for the sum of the respective integrals over all the reaches in the network.

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Equations (A6)–(A7) can be written in a more convenient form using space-averaging operators. Replacing ψ with its expression defined in Eq. (A3), the integral on the right-hand side of Eq. (A7) can be written as

$$\int_{\mathcal{L}} e^{-d(x)/L_c} \psi(x) dx = A_1 q_e \langle T_e \rangle_{\mathcal{L}} + \frac{A_2}{L_c} \langle \gamma \phi_r + T_a - L_c \frac{g}{c_p} \frac{dz}{dx} \rangle_{\mathcal{Q}}, \quad (\text{A8})$$

5 where the two averaging operators $\langle \cdot \rangle_{\mathcal{L}}$ and $\langle \cdot \rangle_{\mathcal{Q}}$ are defined as

$$\langle f \rangle_{\mathcal{L}} = \frac{1}{A_1} \int_{\mathcal{L}} e^{-d(x)/L_c} f(x) dx, \quad (\text{A9})$$

$$\langle f \rangle_{\mathcal{Q}} = \frac{1}{A_2} \int_{\mathcal{L}} e^{-d(x)/L_c} Q(x) f(x) dx, \quad (\text{A10})$$

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for any integrable function f defined on \mathcal{L} , with the normalizing factors A_1 and A_2 being defined as

$$\begin{aligned}
 A_1 &= \int_{\mathcal{L}} e^{-d(x)/L_c} dx, \\
 &= \sum_{k=1}^{n_r} \int_{x_{k,0}}^{x_{k,1}} e^{-d(x)/L_c} dx \\
 &= \sum_{k=1}^{n_r} L_c e^{-d_k/L_c} (1 - e^{-L_k/L_c}), \tag{A11}
 \end{aligned}$$

$$\begin{aligned}
 A_2 &= \int_{\mathcal{L}} e^{-d(x)/L_c} Q(x) dx \\
 &= \sum_{k=1}^{n_r} \int_{x_{k,0}}^{x_{k,1}} e^{-d(x)/L_c} Q_k(x) dx. \tag{A12}
 \end{aligned}$$

In the above equations, n_r denotes the number of reaches in the network; $x_{k,0}$, $x_{k,1}$ and L_k refer to the upstream point, downstream point and length of reach k respectively; d_k refers to the distance along the stream network between $x_{k,1}$ and the network outlet; and $Q_k(x)$ denotes the discharge along reach k (see Fig. 7b). Based on Eq. (A1), Q_k may be expressed as

$$Q_k(x) = Q(x_{k,0}) + q_e(x - x_{k,0}) = \sum_{j \in \Pi_k} Q_{s,j} + q_e \sum_{r \in \Gamma_k} L_r + q_e(x - x_{k,0}), \tag{A13}$$

where Π_k and Γ_k denote the set of source points and reaches draining into reach k , respectively, as illustrated in Fig. 7c. Inserting the above equation in Eq. (A12) and

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re-arranging the terms, A_2 may be written as

$$\begin{aligned}
 A_2 = & \sum_{i=1}^{n_s} Q_{s,i} \sum_{j \in \Omega_i} \int_{x_{j,0}}^{x_{j,1}} e^{-d(x)/L_c} dx \\
 & + q_\ell \sum_{k=1}^{n_r} L_k \sum_{r \in \Delta_k} \int_{x_{r,0}}^{x_{r,1}} e^{-d(x)/L_c} dx \\
 & + q_\ell \sum_{k=1}^{n_r} \int_{x_{k,0}}^{x_{k,1}} e^{-d(x)/L_c} x dx,
 \end{aligned} \tag{A14}$$

5 where Ω_i refers to the set of reaches linking the i th source point to the network outlet, and Δ_k denotes the set of reaches linking reach k to the network outlet, not including reach k itself (see Fig. 7c). Assuming that all source points have the same discharge Q_s , and replacing the integrals along the reaches with their respective values, Eq. (A14) can be written more simply as

$$\begin{aligned}
 10 \quad A_2 = & L_c Q_s \sum_{i=1}^{n_s} (1 - e^{-d_{s,i}/L_c}) \\
 & + q_\ell L_c \sum_{k=1}^{n_r} \left\{ L_k - L_c e^{-d_k/L_c} (1 - e^{-L_k/L_c}) \right\} \\
 = & L_c (Q_{\text{tot}} - q_\ell L_{\text{tot}}) (1 - \delta_s) + q_\ell L_c L_{\text{tot}} (1 - \delta_\ell),
 \end{aligned} \tag{A15}$$

where Eq. (A6) has been used in the second step to replace $n_s Q_s$ with $Q_{\text{tot}} - q_\ell L_{\text{tot}}$, and the factors δ_s and δ_ℓ are defined as

$$\delta_s = \frac{1}{n_s} \sum_{i=1}^{n_s} e^{-d_{s,i}/L_c}, \quad (\text{A16})$$

$$\delta_\ell = \frac{L_c}{L_{\text{tot}}} \sum_{k=1}^{n_r} e^{-d_k/L_c} (1 - e^{-L_k/L_c}) = \frac{A_1}{L_{\text{tot}}}. \quad (\text{A17})$$

5 Combining Eqs. (A7), (A8), (A11) and (A15), the expression for stream temperature at the network outlet can eventually be written in a more convenient form,

$$T_{\text{out}} = (1 - \eta) \delta_s \overline{T_s} + \eta \delta_\ell \langle T_\ell \rangle_L + [1 - (1 - \eta) \delta_s - \eta \delta_\ell] \left\langle \gamma \phi_r + T_a - L_c \frac{g}{c_p} \frac{dz}{dx} \right\rangle_L, \quad (\text{A18})$$

where the averaging operator $\langle \cdot \rangle_Q$ has been approximated by $\langle \cdot \rangle_L$, and $\overline{T_s}$ corresponds to the distance-weighted source temperature, averaged over all sources and weighted by a factor decreasing exponentially with the respective distance of each source to the network outlet,

$$\overline{T_s} = \frac{1}{n_s \delta_s} \sum_{i=1}^{n_s} e^{-d_{s,i}/L_c} T_{s,i}. \quad (\text{A19})$$

The factor η appearing in Eq. (A18) denotes the ratio between the discharge originating from lateral inflow and the total discharge at the network outlet,

$$\eta = \frac{q_\ell L_{\text{tot}}}{Q_{\text{tot}}}. \quad (\text{A20})$$

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Table 1. List of reviewed publications about statistical stream temperature prediction in ungauged basins.

Reference	Geographic Location	Model Type ^a	Number of Sites	Number of Years ^b	Temporal Scale	Model Precision ^{b,c}
Arcscott et al. (2001)	Italy	MLR	22	1	season	$R^2 = 0.37\text{--}0.8$
Bogan et al. (2003)	Eastern USA	AE	596	30	week	$R^2 = 0.80$, $\sigma_e = 3.1^\circ\text{C}$
Chang and Psaris (2013)	Western USA	MLR, GWR	74	n/a	week, year	$R^2 = 0.52\text{--}0.62$, $\sigma_e = 2.0\text{--}2.3^\circ\text{C}$
Daigle et al. (2010)	Western Canada	Various	16	0.5	month	$\sigma_e = 0.9\text{--}2.8^\circ\text{C}$
DeWeber and Wagner (2014)	Eastern USA	ANN	1080	31	day	$\sigma_e = 1.8\text{--}1.9^\circ\text{C}$
Ducharne (2008)	France	MLR	88	7	month	$R^2 = 0.88\text{--}0.96$, $\sigma_e = 1.4\text{--}1.9$
Gardner and Sullivan (2004)	Eastern USA	NKM	72	1	day	$\sigma_e = 1.4^\circ\text{C}$
Garner et al. (2014)	UK	CA	88	18	month	n/a
Hawkins et al. (1997)	Western USA	MLR	45	≥ 1	year	$R^2 = 0.45\text{--}0.64$
Hill et al. (2013)	Conterminous USA	RF	~ 1000	1/site	season, year	$\sigma_e = 1.1\text{--}2.0^\circ\text{C}$
Hrachowitz et al. (2010)	UK	MLR	25	1	month, year	$R^2 = 0.50\text{--}0.84$
Imholt et al. (2013)	UK	MLR	23	2	month	$R^2 = 0.63\text{--}0.87$
Isaak et al. (2010)	Western USA	MLR, NKM	518	14	month, year	$R^2 = 0.50\text{--}0.61$, $\sigma_e = 2.5\text{--}2.8^\circ\text{C}$
Isaak and Hubert (2001)	Western USA	PA	26	1/site	season	$R^2 = 0.82$
Johnson (1971)	New Zealand	ULR	6	1	month	n/a
Johnson et al. (2014)	UK	NLR	36	1.5	day	$R^2 = 0.67\text{--}0.90$, $\sigma_e = 1.0\text{--}2.4^\circ\text{C}$
Jones et al. (2006)	Eastern USA	MLR	28	3	year	$R^2 = 0.57\text{--}0.73$
Kelleher et al. (2012)	Eastern USA	MLR	47	2	day, week	n/a
Macedo et al. (2013)	Brazil	LMM	12	1.5	day	$R^2 = 0.86$

^a AE: Analytical Expression, ANN: Artificial Neural Network, CA: Cluster Analysis, CRT: Classification and Regression Trees, GWR: Geographically Weighted Regression, LMM: Linear Mixed Model, MLR: Multi-Linear Regression, NKM: Networked Kriging Model, NLR: Non-linear Regression, PA: Path Analysis, RF: Random Forest, ULR: Univariate Linear Regression.

^b n/a: not available.

^c σ_e : root-mean-square error, R^2 : coefficient of determination (sometimes referred to as Nash–Sutcliffe index).

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Table 1. (Continued).

Reference	Geographic Location	Model Type ^a	Number of Sites	Number of Years ^b	Temporal Scale	Model Precision ^{b,c}
Mayer (2012)	Western USA	MLR	104	≥ 2	week, month	$R^2 = 0.72$, $\sigma_e = 1.8^\circ\text{C}$
Miyake and Takeuchi (1951)	Japan	ULR	20	n/a	month	n/a
Moore et al. (2013)	Western Canada	MLR	418	1/site	year	$\sigma_e = 2.1^\circ\text{C}$
Nelitz et al. (2007)	Western Canada	CRT	104	1/site	year	n/a
Nelson and Palmer (2007)	Western USA	MLR	16	3	season	$R^2 = 0.36$ – 0.88
Ozaki et al. (2003)	Japan	ULR	5	8	day	n/a
Pratt and Chang (2012)	Western USA	MLR, GWR	51	1/site	season	$R^2 = 0.48$ – 0.78
Risley et al. (2003)	Western USA	ANN	148	0.25	hour, season	$\sigma_e = 1.6$ – 1.8°C
Rivers-Moore et al. (2012)	South Africa	MLR	90	1/site	month, year	$R^2 = 0.14$ – 0.50
Ruesch et al. (2012)	Western USA	NKM	165	15	year	$R^2 = 0.84$, $\sigma_e = 1.5^\circ\text{C}$
Segura et al. (2014)	Conterminous USA	MLR	171	≥ 1.5	week, month	$R^2 = 0.79$
Sponseller et al. (2001)	Eastern USA	MLR	9	1	year	$R^2 = 0.81$ – 0.93
Scott et al. (2002)	Eastern USA	MLR	36	1/site	season	$R^2 = 0.82$
Stefan and Preud'homme (1993)	Eastern USA	ULR	11	n/a	day, week	$\sigma_e = 2.1$ – 2.7°C
Tague et al. (2007)	Western USA	MLR	43	4	day	$R^2 = 0.49$ – 0.65
Wehrly et al. (2009)	Eastern USA	Various	1131	1/site	month	$\sigma_e = 2.0$ – 3.0°C
Westenbroek et al. (2010)	Eastern USA	ANN	254	1/site	day	$R^2 = 0.70$, $\sigma_e = 1.8^\circ\text{C}$
Young et al. (2005)	New Zealand	MLR	23	1	season	$R^2 = 0.75$ – 0.93

^a AE: Analytical Expression, ANN: Artificial Neural Network, CA: Cluster Analysis, CRT: Classification and Regression Trees, GWR: Geographically Weighted Regression, LMM: Linear Mixed Model, MLR: Multi-Linear Regression, NKM: Networked Kriging Model, NLR: Non-linear Regression, PA: Path Analysis, RF: Random Forest, ULR: Univariate Linear Regression.

^b n/a: not available.

^c σ_e : root-mean-square error, R^2 : coefficient of determination (sometimes referred to as Nash–Sutcliffe index).

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Table 3. Physiographic properties of the 29 selected hydrological catchments in Switzerland. The three watersheds indicated in bold are not used for the model evaluation.

Basin Number	Name	Basin Area [km ²]	Gauging Station Altitude [m]	Mean Basin Altitude [m]	Glacier Cover [%]	Hydrological Regime ^a	Temperature Measurement Period	Data Provider ^b
1	Broye at Payerne	392.0	441	710	0	pluvial inferior	1976–2012	FOEN
2	Sitter at Appenzell	74.2	769	1252	0.1	transition nival	2006–2012	FOEN
3	Murg at Wängi	78.0	466	650	0	pluvial inferior	2002–2012	FOEN
4	Gürbe at Belp, Mülimatt	117.0	522	849	0	transition pluvial	2007–2012	FOEN
5	Massa at Blatten, Naters	195.0	1446	2945	65.9	glacial	2003–2012	FOEN
6	Sense at Thörishaus, Sense matt	352.0	553	1068	0	pre-alpine nivo-pluvial	2004–2012	FOEN
7	Allenbach at Adelboden	28.8	1297	1856	0	alpine nival	2002–2012	FOEN
8	Rosegbach at Pontresina	66.5	1766	2716	30.1	glacial	2004–2012	FOEN
9	Grosstalbach at Isenthal	43.9	767	1820	9.3	alpine nival	2005–2012	FOEN
10	Goldach at Goldach, Bleiche	49.8	399	833	0	pluvial superior	2005–2012	FOEN
11	Dischmabach at Davos, Kriegsmatte	43.3	1668	2372	2.1	glacio-nival	2004–2012	FOEN
12	Langeten at Huttwil, Häberenbad	59.9	597	766	0	pluvial inferior	2002–2012	FOEN
13	Riale di Roggiasca at Roveredo	8.1	980	1710	0	meridional nivo-pluvial	2003–2012	FOEN
14	Riale di Calneggia at Caveragno, Pontit	24	890	1996	3.0	meridional nival	2002–2012	FOEN
15	Poschiavino at La Rôsa	14.1	1860	2283	0.4	meridional nival	2004–2012	FOEN
16	Mentue at Yvonand, La Mauguettaz	105.0	449	679	0	jurassian pluvial	2003–2012	FOEN
17	Necker at Mogelsberg, Aachsäge	88.2	606	959	0	pluvial superior	2007–2012	FOEN
18	Grossbach at Gross, Säge	9.1	940	1276	0	pre-alpine nivo-pluvial	2003–2012	FOEN
19	Rietholz bach at Mosnang, Rietholz	3.3	682	795	0	pluvial superior	2002–2012	FOEN
20	Gürbe at Burgstein, Pfandersmatt	53.7	569	1044	0	pre-alpine nivo-pluvial	2007–2008	FOEN
21	Biber at Biberbrugg	31.9	825	1009	0	pluvial superior	2003–2012	FOEN
22	Sellenbodenbach at Neuenkirch	10.5	515	615	0	pluvial superior	2003–2012	FOEN
23	Alp at Einsiedeln	46.4	840	1155	0	transition pluvial	2003–2012	FOEN
24	Riale di Pincascia at Lavertezzo	44.4	536	1708	0	meridional nivo-pluvial	2004–2012	FOEN
25	Rom at Müstair	129.7	1236	2187	0.1	meridional nival	2003–2012	FOEN
26	Sissle at Eiken	123.0	314	529	0	jurassian pluvial	2004–2012	Aargau
27	Bünz at Othmarsingen	110.6	390	526	0	pluvial inferior	2005–2012	Aargau
28	Wyna at Unterkulm	92.1	455	643	0	pluvial inferior	2005–2012	Aargau
29	Talbach at Schinz nach-Dorf	14.5	358	559	0	jurassian pluvial	2009–2012	Aargau

^a According to the classification by Ashwanden and Weingartner (1985).

^b FOEN: Swiss Federal Office for the Environment, Aargau: Department for Construction, Transport and Environment of Canton Aargau.

Table 4. Formulations of the physically-based model selected in each season based on their corresponding AICc value. The Akaike weights are denoted as w_i . Only the model formulations with $w_i \geq 0.1$ are presented here. The widths of the buffers used to compute the riparian vegetation cover are indicated as subscripts of the variable f_i (the indicated values correspond to the total buffer widths, i.e. accounting for both sides of the stream center line).

Season	w_i	L_c [km]	Formulation of $\gamma\phi_r$	Formulation of T_s and T_e	Formulation of η
Winter	1	8	$\gamma\phi_r = a_{\phi,s}f_s + a_{\phi,i}f_{i,100m} + b_{\phi}$, with $a_{\phi,s} = 18.2^\circ\text{C}$, $a_{\phi,i} = -2.9^\circ\text{C}$ and $b_{\phi} = -12.1^\circ\text{C}$	$T_s = a_w T_a + b_w$, with $a_w = 0.15$ and $b_w = 3.1^\circ\text{C}$	$\eta = 0$ (constant)
	0.25		$\gamma\phi_r = a_{\phi,s}f_s + b_{\phi}$, with $a_{\phi,s} = 19.4^\circ\text{C}$ and $b_{\phi} = -14.1^\circ\text{C}$		
	0.15		$\gamma\phi_r = a_{\phi,s}f_s + a_{\phi,i}f_{i,50m} + b_{\phi}$, with $a_{\phi,s} = 19.3^\circ\text{C}$, $a_{\phi,i} = -0.4^\circ\text{C}$ and $b_{\phi} = -13.9^\circ\text{C}$		
Spring	1	4	$\gamma\phi_r = a_{\phi,s}f_s + a_{\phi,i}f_{i,50m} + b_{\phi}$, with $a_{\phi,s} = 12.9^\circ\text{C}$, $a_{\phi,i} = -3.7^\circ\text{C}$ and $b_{\phi} = -11.3^\circ\text{C}$	$T_s = a_w T_a + b_w$, with $a_w = 0.27$ and $b_w = 5.3^\circ\text{C}$	$\eta = 1 - \eta_s (A_s/A_{\text{tot}})^\alpha$, with $A_s = 0.13 \text{ km}^2$ and $\alpha = 1$
	0.86		$\gamma\phi_r = a_{\phi,s}f_s + a_{\phi,i}f_{i,200m} + b_{\phi}$, with $a_{\phi,s} = 13.1^\circ\text{C}$, $a_{\phi,i} = -3.4^\circ\text{C}$ and $b_{\phi} = -11.6^\circ\text{C}$		
	0.53		$\gamma\phi_r = a_{\phi,s}f_s + b_{\phi}$, with $a_{\phi,s} = 13.1^\circ\text{C}$ and $b_{\phi} = -12.7^\circ\text{C}$		
	0.31		$\gamma\phi_r = a_{\phi,s}f_s + a_{\phi,i}f_{i,100m} + b_{\phi}$, with $a_{\phi,s} = 13.4^\circ\text{C}$, $a_{\phi,i} = -2.2^\circ\text{C}$ and $b_{\phi} = -12.3^\circ\text{C}$		
Summer	1	4	$\gamma\phi_r = a_{\phi,s}f_s + a_{\phi,i}f_{i,100m} + b_{\phi}$, with $a_{\phi,s} = 13.4^\circ\text{C}$, $a_{\phi,i} = -0.3^\circ\text{C}$ and $b_{\phi} = -13.0^\circ\text{C}$	$T_s = a_w T_a + b_w$, with $a_w = 0.33$ and $b_w = 6.6^\circ\text{C}$	$\eta = 1$ (constant)
	0.15		$\gamma\phi_r = a_{\phi,s}f_s + b_{\phi}$, with $a_{\phi,s} = 13.4^\circ\text{C}$ and $b_{\phi} = -13.1^\circ\text{C}$		
Autumn	1	4	$\gamma\phi_r = a_{\phi,s}f_s + b_{\phi}$, with $a_{\phi,s} = 10.4^\circ\text{C}$ and $b_{\phi} = -5.9^\circ\text{C}$	$T_s = a_w T_a + b_w$, with $a_w = 0.25$ and $b_w = 5.1^\circ\text{C}$	$\eta = 1$ (constant)
	0.54		$\gamma\phi_r = a_{\phi,s}f_s + a_{\phi,i}f_{i,100m} + b_{\phi}$, with $a_{\phi,s} = 10.0^\circ\text{C}$, $a_{\phi,i} = -2.8^\circ\text{C}$ and $b_{\phi} = -4.7^\circ\text{C}$		
	0.48		$\gamma\phi_r = a_{\phi,s}f_s + a_{\phi,i}f_{i,200m} + b_{\phi}$, with $a_{\phi,s} = 10.1^\circ\text{C}$, $a_{\phi,i} = -2.9^\circ\text{C}$ and $b_{\phi} = -4.7^\circ\text{C}$		
	0.4		$\gamma\phi_r = a_{\phi,s}f_s + a_{\phi,i}f_{i,50m} + b_{\phi}$, with $a_{\phi,s} = 10.2^\circ\text{C}$, $a_{\phi,i} = -2.2^\circ\text{C}$ and $b_{\phi} = -5.1^\circ\text{C}$		

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Table 6. Best multi-linear regression models for the prediction of annual mean \bar{T}_i and standard deviation σ_i of the monthly mean stream temperature in a given year. All predictor variables are averaged over the stream networks using the operator $\langle \cdot \rangle_L$.

Predictand	Predictors* (with coefficients)	L_c [km]
\bar{T}_i [$^{\circ}\text{C}$]	$f_{f,25\text{m}}$ (-1.86°C), θ (0.60°C), A_{tot} ($1.6 \times 10^{-3}^{\circ}\text{C km}^{-2}$), Δf_s (-4.90°C), $\bar{T}_{a,i}$ ($0.75^{\circ}\text{C }^{\circ}\text{C}^{-1}$), intercept (3.88°C)	4
σ_i [$^{\circ}\text{C}$]	$ dz/dx $ (6.03°C), $f_{f,25\text{m}}$ (6.70°C), θ (0.93°C), n_s ($1.6 \times 10^{-3}^{\circ}\text{C}$), Δf_s (-12.8°C), $\sigma_{a,i}$ ($0.39^{\circ}\text{C }^{\circ}\text{C}^{-1}$), intercept (0.34°C)	32

* Δf_s denotes the difference in topographical shading between summer and winter, $\bar{T}_{a,i}$ and $\sigma_{a,i}$ refer to the annual mean value and standard deviation of air temperature in the year of interest, respectively, A_{tot} denotes the watershed area and $|dz/dx|$ the channel slope. The other variables have been defined in the text.

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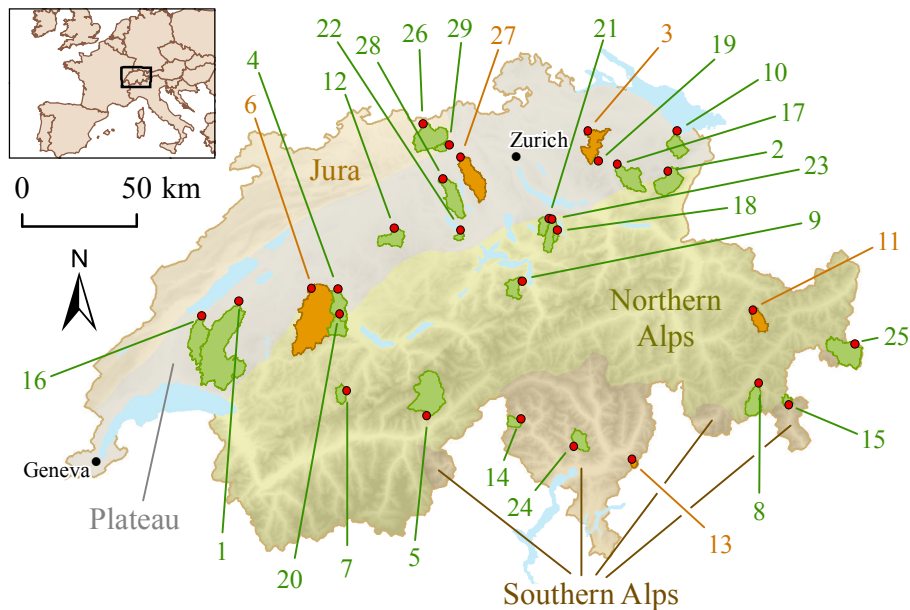


Figure 1. Locations of the gauging stations selected for the evaluation of the physically-based and regression models. The stations are displayed as red points and their associated catchments as green or orange areas, depending on whether they are used to calibrate or validate the model. The four main climatic regions of Switzerland – Jura mountains, Plateau, Northern Alps and Southern Alps – are displayed in different colors. The numbering corresponds to Table 3.

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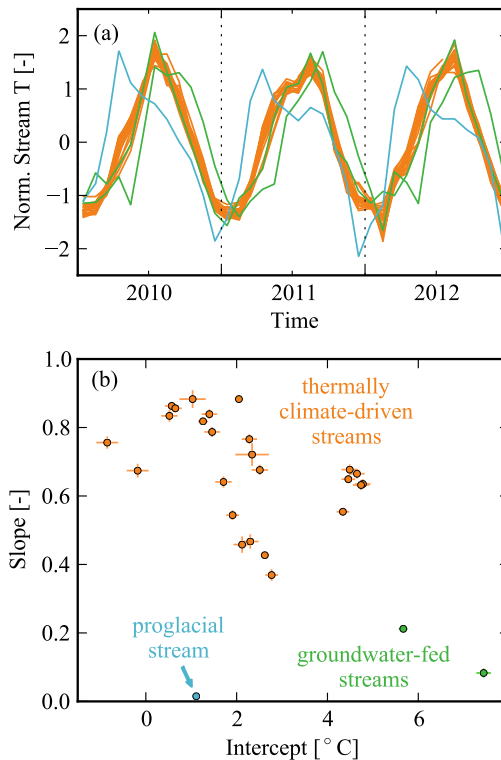


Figure 2. Classification of the thermal regimes of the selected catchments. Streams impacted by groundwater infiltration are shown in green, the proglacial stream in blue and the thermally climate-driven streams in orange. **(a)** Normalized monthly mean stream temperature curves over 3 consecutive years (2010–2012); all curves are z-scored independently each year. **(b)** Slopes and intercepts of the regression lines fitted to the stream–air temperature points of the respective catchments. All points with negative air temperature values have been discarded prior to fitting. The bars indicate the standard error estimates.

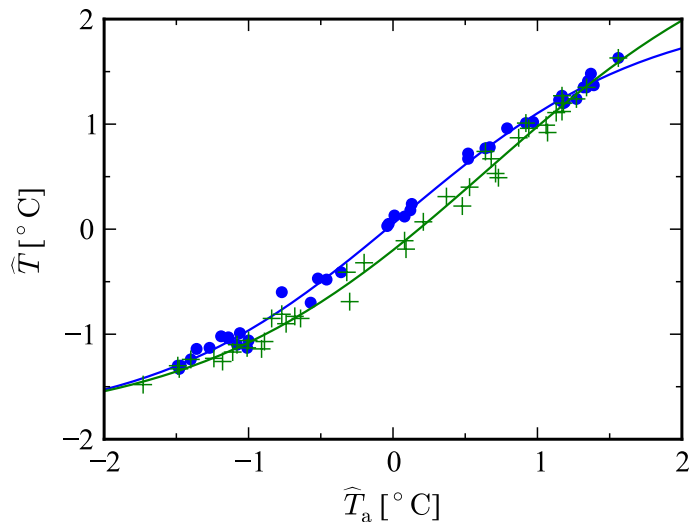


Figure 4. Non-linear relationship between the z-scored stream temperature \hat{T} and the z-scored air temperature \hat{T}_a averaged over 14 reference meteorological stations. The values of \hat{T} are obtained by averaging in each month the z-scored stream temperatures measured at the 21 calibration stations. Each point corresponds to a single month of the calibration period 2007–2012. Months from January to July are displayed as green crosses, and those from July to December as blue dots. The two solid lines correspond to the respective fits of the data points in the two year halves (see Eqs. 26–27).

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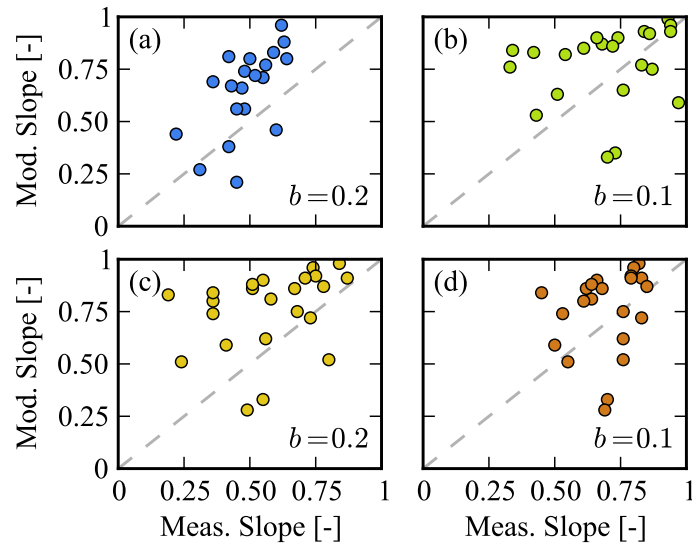


Figure 5. Comparison of modeled against measured slopes of the regression line between stream and air temperatures. The panels correspond to the different seasons: **(a)** January–March, **(b)** April–June, **(c)** July–September, and **(d)** October–December. The bias b corresponds to the average, in each season, of the difference between the modeled and measured regression slopes over all the selected stations and years (i.e. belonging to both the calibration set and validation set 4). The 1 : 1 line is indicated as a dashed grey curve.

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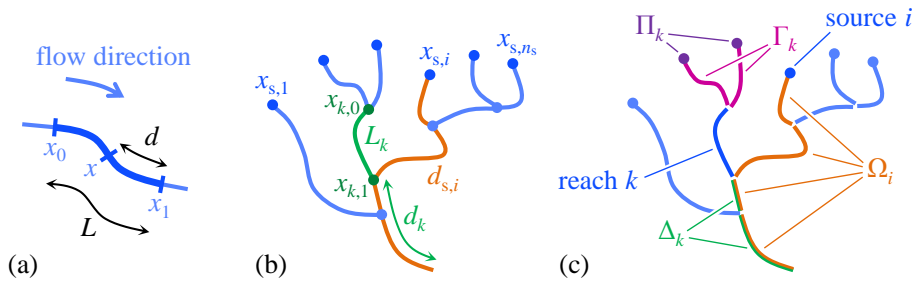


Figure 7. Schematic representations of (a) a stream reach, and (b)–(c) a stream network, illustrating the notation used in Appendix to derive the analytical solution to the stream energy-balance.

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