A Global Approach to Assess the Potential Impact of Climate Change on Stream Water Temperatures and Related In-Stream First-Order Decay Rates

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ABSTRACT
Stream water temperature is an important factor used in water quality modeling. To estimate monthly stream temperatures on a global scale, a simple nonlinear regression model was developed. It was applied to stream temperatures recorded over a 36-yr period (1965–2001) at 1659 globally distributed gauging stations. Representative monthly air temperatures were obtained from the nearest grid cell included in the new global meteorological forcing dataset—the Water and Global Change (WATCH) Forcing Data. The regression model reproduced monthly stream temperatures with an efficiency of fit of 0.87. In addition, the regression model was applied for different climate zones (polar, snow, warm temperate arid, and equatorial climates) based on the Köppen–Geiger climate classification. For snow, warm temperate, and arid climates the efficiency of fit was larger than 0.82 including more than 1504 stations (90% of all records used). Analyses of heat-storage effects (seasonal hysteresis) did not show noticeable differences between the warming/cooling and global regression curves, respectively. The maximum difference between both limbs of the hysteresis curves was 1.6°C and thus neglected in the further analysis of the study. For validation purposes time series of stream temperatures for five individual river basins were computed applying the global regression equation. The accuracy of the global regression equation could be confirmed. About 77% of the predicted values differed by 3°C or less from measured stream temperatures. To examine the impact of climate change on stream water temperatures, gridded global monthly stream temperatures for the climate normal period (1961–90) were calculated as well as stream temperatures for the A2 and B1 climate change emission scenarios for the 2050s (2041–70). On average, there will be an increase of 1–4°C in monthly stream temperature under the two climate scenarios. It was also found that in the months December, January, and February a noticeable warming predominantly occurs along the equatorial zone, while during the months June, July, and August large-scale or large increases can be observed in the northern and southern temperate zones. Consequently, projections of decay rates show a similar seasonal and spatial pattern as the corresponding stream temperatures. A regional increase up to ~25% could be observed. Thus, to ensure sufficient water quality for human purposes, but also for freshwater ecosystems, sustainable management strategies are required.

1. Introduction
Temperature is a significant stream water quality parameter. Most physical properties of water and most chemical and biological processes in water are a function of temperature. The temperature of a stream directly affects the entire aquatic ecosystem including fish survival, growth, and reproduction (Sinokrot and Stefan 1993; Eaton and Scheller 1996). Many freshwater organisms are bounded on typical thermal ranges. Extreme changes of water temperature can have adverse impacts on their fertility, growth, life cycle, or distribution, and finally could lead to a loss of biodiversity (Thomann and Mueller 1987; Moog and Wimmer 1994; Golladay et al.)
2004; Millennium Ecosystem Assessment 2005). As well, ecological zones on Earth depend on temperature changes; each 1°C will move the boundaries by some 160 km (or 160 m in altitude) (Thuiller 2007).

Indeed, it is likely that global warming will cause a shift in temperature of freshwater systems and therefore an assessment of the potential impacts of global change on the state of surface water resources is required.

Impacts of climate change on freshwater biota can already be observed today. Effects on community structure, food web dynamics, and life cycle of different freshwater organisms have been found (Schindler 1997; Poff et al. 2002; Wrona et al. 2006). Durance and Ormerod (2007) published a decline in macroinvertebrate abundance at a small catchment in Wales with increasing stream temperatures over a 25-yr period. Decline in freshwater biodiversity has been linked, with climate-induced changes in water temperature and hydrological regimes ranking amongst the most influential factors (Lake et al. 2000; Xenopoulos et al. 2005).

Future water temperature is of particular importance in climate change projection on freshwater systems (Mohseni et al. 1999) because of its role as a water quality indicator. Furthermore, various water quality parameters that are related to water temperature, like nitrogen concentration level, biological oxygen demand (BOD), and total coliform bacteria numbers, (Thomann and Mueller 1987; Ducharme 2008), also have an influence on the ecological health and the level of eutrophication in freshwater systems. Increased water temperatures affect chemical reaction kinetics and, thus, the level of these water quality parameters. Therefore, water temperature modeling is an important tool for present and future water quality assessment (Benyahya et al. 2008).

In the past, various models of different complexity have been developed to calculate stream temperatures. Two broad categories are usually identified (Guillemette et al. 2008): (i) deterministic or physical models (e.g., Gu and Li 2002; St-Hilaire et al. 2003; Caissie et al. 2007) and (ii) statistical/stochastic models (e.g., Caissie et al. 1998; Mohseni et al. 1998; Ahmadi-Nedushan et al. 2007).

The first model category is often used to calculate energy budget equations or to predict water temperatures as well. These deterministic models rely on a conceptual method based on thermal budget calculations, which requires demanding data inputs like air temperature, solar radiation, and evaporation. On the one hand, deterministic models are quite flexible in terms of input parameter modification, but on the other hand they are more complex in model development and data requirements than statistical/stochastic models (Benyahya et al. 2008; Guillemette et al. 2008). Models of this second category are based on a computational relationship between water temperature and individual parameters like air temperature and discharge. They are mainly used for prediction of stream temperatures on different time scales (e.g., daily, weekly, or monthly) (Mohseni and Stefan 1999; Erickson and Stefan 2000; Morrill et al. 2005).

To estimate the effect of climate change on stream temperatures, a relationship with easily obtainable climate variables is often preferred. A simple approach to estimate water temperatures is a nonlinear regression model introduced by Mohseni et al. (1998). This method, based on the strong relationship between stream water temperature and the surrounding air temperature, only needs one input variable: air temperature. Regression models of stream temperature versus air temperature are very attractive for climate change effect studies. Not only because general circulation models (GCMs) simulate this variable better than they simulate other climate parameters (Lau et al. 1996), but also for their satisfactory application to investigate longer time scales.

This study investigates the impact of the expected global warming on temperatures of global–continental freshwater resources for different climatic zones. Thus, the paper aims at providing a deeper insight with respect to the influence of water temperature to biogeochemical water quality in the context of climate change on a global scale using a simple numerical framework. This approach is part of the development of the WorldQual model (F. Voß et al. 2009; A. Voß et al. 2012) to estimate the changes in the status of water quality on a continental-scale model, including key water quality indicators like BOD and total coliform bacteria numbers. BOD is used as an indicator of the level of organic pollution and its oxygen-depleting potential as well as for the overall health of aquatic ecosystems. Organic pollution is amongst the dominating sources, endangering biodiversity as well as human water security (Vörösmarty et al. 2010). BOD decay rates are strongly temperature dependent and the impacts of global warming will be discussed here.

2. Methods and material

a. Nonlinear regression model

A number of studies have successfully sought to assess stream temperatures with air temperatures using regression models (Webb and Nobilis 1997; Mohseni et al. 1998, 1999; Caissie et al. 1998, 2001; van Vliet et al. 2011). Researchers have often used linear regression models, but at the highest and lowest air temperatures the air–water temperature relationship does not usually remain linear. When air temperature drops down below 0°C, the decrease in water temperature slows down and converges to a lower limit near 0°C. At higher air
temperatures, above ~25°C, stream temperature approximates toward an upper limit as consequence of increasing evaporative heat loss (Webb et al. 2008). A piecewise linear regression may seem an appropriate approach to explain the nonlinear relationship between water and air temperature. Taking this nonlinearity into account, the monthly water–air temperature relationship resembles an s-shaped function (Mohseni et al. 1998; Morrill et al. 2005; Ducharne 2008). In this study a logistic function with three degrees of freedom was tested according to Ratkowsky (1983) and Mohseni et al. (1998). The mathematical formulation for the nonlinear regression model is given in Eq. (1):

\[ T_{\text{water}} = \frac{C_0}{1 + e^{(C_1T_{\text{air}}+C_2)}} \]  

where

\( T_{\text{water}} \) = water temperature (°C),  
\( T_{\text{air}} \) = air temperature (°C),  
\( C_0 \) = upper bound water temperature (°C),  
\( C_1 \) = steepest slope of the function (°C\(^{-1}\)), and  
\( C_2 \) = measure for inflexion point of the function (°C) (inflexion point = \(-C_2/C_1\)).

The coefficients of an s-shaped function have physical properties relating to the water–air temperature relationship.

b. Data and data processing

1) DATA

To determine the coefficients \( C_0, C_1, \) and \( C_2 \) of Eq. (1), pairs of measured monthly stream temperatures and the respective gridded monthly air temperatures were used as data input. Water temperature data were compiled from 935 U.S. Geological Survey (USGS) water gauging stations, 570 stations of United Nations Environmental Programme (UNEP) Global Environment Monitoring System (GEMS), and 154 additional gauging stations situated at various European main streams (Table 1). The measured water temperatures are monthly means of single values available for the period 1965–2001. For gridded monthly air temperatures, the new global meteorological forcing dataset named the Water and Global Change (WATCH) Forcing Data (WFD; WATCH is a European Union–funded research project—for details on WFD see Weedon et al. 2010) was used. The data were derived from the 40-yr European Centre for Medium-Range Weather Forecasts (ECMWF) Re-Analysis (ERA-40) product as described by Uppala et al. (2005) via sequential interpolation to 0.5° resolution, elevation correction, and monthly-scale adjustments (corrected temperature, diurnal temperature range) based on the Climatic Research Unit (CRU) TS2.1 time series data product (University of East Anglia, United Kingdom; New et al. 1999, 2000; Mitchell and Jones 2005). Each measured water temperature was linked to a corresponding air temperature grid cell. If there were several measurement points located in a grid cell, the mean of all stations was taken to get a single water temperature value for each grid cell. Finally, a dataset of 97 964 water–air temperature pairs was used at 1659 gauging stations in total.

2) PROCEDURES

The aim in this study was to achieve one overall global regression model to calculate water temperature.
in a representative way. To estimate the parameters $C_0$, $C_1$, and $C_2$ of Eq. (1), a numerical method such as Newton’s method has to be implemented. The criterion was to minimize the sum of squared errors between measured and fitted water temperatures.

Here we introduce a stepwise approach to gain one single regression equation for use in impact analysis of climate change on stream water temperatures and related in-stream first-order decay rates:

(i) calculation of a global standard regression model,
(ii) testing of various formulations for different climate zones,
(iii) testing of seasonal hysteresis effects on a global scale, and
(iv) validation with individual rivers in different climate zones.

(i) Global standard regression model

The nonlinear regression model [Eq. (1)] was applied to the available pairs of air–water temperature (60 837) of the period from 1965 to 1994 to support the formulation of one representative global regression model. First tests have shown that coefficient $C_0$, representing the upper bound of water temperature, converges to an upper limit of 32°C. With respect to application in different climate zones, as described in the following section, $C_0$ was kept constant at a value of 32°C. The coefficients $C_1$ and $C_2$, which both describe the nonlinear properties in the regression model, were calculated with the Newton method iteratively.

(ii) Regression models derived in Köppen–Geiger climate zones

It is well known that regional climate plays a major role for thermal regime of freshwater systems. Therefore, the dataset was subdivided according to main regional climate zones. The division into climate zones hereby followed the updated Köppen–Geiger climates as presented by Kottek et al. (2006). It is a quantitative classification of world climates based on vegetation, temperature, and precipitation. Five major climate zones are differentiated: equatorial zone (A), the arid zone (B), the warm temperate zone (C), the snow zone (D), and the polar zone (E). In Fig. 1, the regional distribution of these climate zones is shown.

Most of the water temperature records (60%), collected at 55% of the water measurement stations, were
located in the warm temperate climate zone (see Table 2). For the polar region only 164 water temperature measurements (0.2%, from 3 gauging stations) were available. The range between the maximum and minimum water temperature was 32.3\(^\circ\)C–35.1\(^\circ\)C for all climate zones except for the polar one, where the spread was just 15.3\(^\circ\)C.

Highest mean temperatures occurred at equatorial climates (27.1\(^\circ\)C) and the lowest one could be found in the polar region (4.3\(^\circ\)C; see Table 2).

For each of the five climate zones, fitting coefficients were calculated separately (see Table 3).

(iii) Seasonal hysteresis effects on a global scale

Previous studies noticed the occurrence of heat-storage effects in some streams (Webb and Nobilis 1997; Mohseni et al. 1999; van Vliet et al. 2011) influencing the regression model. To test the meaning of seasonal hysteresis on a global scale, separate functions were fitted to the rising and falling limbs. The maximum of monthly mean air temperature was set as the start of the falling limb, whereas the minimum of monthly mean air temperatures was used to set the start of the rising limb.

To take the shift of seasons of the Northern and Southern Hemispheres into account, the rising and falling limb for each hemisphere was determined separately. Then the temperature data were combined for each hemisphere respectively to calculate a single, global hysteresis regression equation. Highest maximum temperatures for the Northern Hemisphere were observed in July and the lowest ones in January; therefore, the falling limb is represented by the months July–December, while the period from January to June is set as the rising limb as shown in Fig. 2. For the Southern Hemisphere, the falling limb is defined from February to June and the rising limb represents data from July to January. Hysteresis should be taken into account if the mean NSC for the rising and the falling limb is higher than for the single fitted regression model (Mantua et al. 2010).

(iv) Validation

In contrast to most of the approaches described in recent literature, the global standard regression model was used to simulate time series of stream water temperatures of individual rivers in different climate zones. To perform a validity test, the regression equation fitted for the period 1965–94 was adopted to the time period 1995–2001. To verify the accuracy of the global regression function, the equation was applied to five representative streams in the form of time series representation. The

\[ \text{TABLE 2. Statistical overview of measured water temperatures according to their respective Köppen–Geiger climate zone.} \]

<table>
<thead>
<tr>
<th>Region</th>
<th>Mean</th>
<th>Min</th>
<th>Max</th>
<th>Median</th>
<th>Standard deviation</th>
<th>Number of stations</th>
<th>Number of water temperature records</th>
</tr>
</thead>
<tbody>
<tr>
<td>Equatorial</td>
<td>27.1</td>
<td>2.0</td>
<td>34.8</td>
<td>27.5</td>
<td>3.1</td>
<td>165</td>
<td>13 054</td>
</tr>
<tr>
<td>Arid</td>
<td>17.2</td>
<td>-0.1</td>
<td>34.2</td>
<td>18</td>
<td>8.2</td>
<td>132</td>
<td>6577</td>
</tr>
<tr>
<td>Warm temperate</td>
<td>13.4</td>
<td>-0.5</td>
<td>34.6</td>
<td>12.8</td>
<td>6.7</td>
<td>930</td>
<td>63 238</td>
</tr>
<tr>
<td>Snow</td>
<td>9.4</td>
<td>-2.3</td>
<td>30.0</td>
<td>8.4</td>
<td>7.5</td>
<td>429</td>
<td>21 965</td>
</tr>
<tr>
<td>Polar</td>
<td>4.3</td>
<td>-0.3</td>
<td>15</td>
<td>3.9</td>
<td>3.4</td>
<td>3</td>
<td>170</td>
</tr>
<tr>
<td>Global</td>
<td>14.3</td>
<td>-2.3</td>
<td>34.8</td>
<td>14.0</td>
<td>5.72</td>
<td>1659</td>
<td>105 004</td>
</tr>
</tbody>
</table>

\[ \text{TABLE 3. Results of curve fitting showing the three fitting coefficients and respective efficiencies: quality of fit for calibrated (calib) and validated (valid) datasets. Values in bold distinguish a higher performance for validation compared to the training dataset.} \]

<table>
<thead>
<tr>
<th>Region</th>
<th>( C_0 )</th>
<th>( C_1 )</th>
<th>( C_2 )</th>
<th>NSC Calib</th>
<th>NSC Valid</th>
<th>RMSE Calib</th>
<th>RMSE Valid</th>
</tr>
</thead>
<tbody>
<tr>
<td>Warm temperate</td>
<td>32</td>
<td>-0.13</td>
<td>1.94</td>
<td>0.82</td>
<td>0.83</td>
<td>2.9</td>
<td>2.6</td>
</tr>
<tr>
<td>Snow</td>
<td>32</td>
<td>-0.14</td>
<td>2.08</td>
<td>0.84</td>
<td>0.88</td>
<td>3.1</td>
<td>2.4</td>
</tr>
<tr>
<td>Arid</td>
<td>32</td>
<td>-0.12</td>
<td>1.82</td>
<td>0.81</td>
<td>0.88</td>
<td>3.6</td>
<td>2.7</td>
</tr>
<tr>
<td>Equatorial</td>
<td>32</td>
<td>-0.18</td>
<td>3.02</td>
<td>0.22</td>
<td>0.20</td>
<td>3.3</td>
<td>2.9</td>
</tr>
<tr>
<td>Polar</td>
<td>32</td>
<td>-0.11</td>
<td>2.15</td>
<td>0.66</td>
<td>0.56</td>
<td>1.8</td>
<td>2.0</td>
</tr>
<tr>
<td>Global</td>
<td>32</td>
<td>-0.13</td>
<td>1.94</td>
<td>0.88</td>
<td>0.88</td>
<td>3.0</td>
<td>2.6</td>
</tr>
<tr>
<td>Global—rising limb</td>
<td>32</td>
<td>-0.13</td>
<td>2.15</td>
<td>0.85</td>
<td>0.85</td>
<td>3.3</td>
<td>2.6</td>
</tr>
<tr>
<td>Global—falling limb</td>
<td>32</td>
<td>-0.12</td>
<td>1.80</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\[ \text{FIG. 2. Heat-storage effects: thermal history of monthly mean air and water temperatures of the Northern Hemisphere. The vertical bar marks the border of the rising and the falling limb.} \]
assortment includes the following river basins: Yangtze River (China), Delaware River (United States), Medina River (United States), Rhine (Germany), and Ob River (Russia). For better comparability, time series of the global regression function were calculated for both periods: 1965–94 (calibration) and 1995–2001 (validation).

To compare simulated with recorded water temperatures Nash–Sutcliffe coefficient (NSC; Nash and Sutcliffe 1970) and root-mean-square error (RMSE) were calculated for the different regression models and for the different streams listed above. NSC and RMSE are common parameters to determine the quality of the fits, often used in water temperature studies (Caissie et al. 1998; Mohseni et al. 1998; St-Hilaire et al. 2003; Benyahya et al. 2008).

The NSC, also known as efficiency of fit, is defined as

\[
\text{NSC} = 1 - \frac{\sum_{i=1}^{n} (T_{\text{sim}} - T_{\text{meas}})^2}{\sum_{i=1}^{n} (T_{\text{meas}} - \bar{T}_{\text{meas}})^2}, \quad \text{NSC} \leq 1, \quad (2)
\]

where

- \(T_{\text{sim}}\) = monthly simulated stream temperatures (°C),
- \(T_{\text{meas}}\) = monthly measured stream temperatures (°C), and
- \(\bar{T}_{\text{meas}}\) = mean monthly measured stream temperatures (°C).

Using RMSE assumes that the smallest error between estimated and measured temperature would represent the best agreement. There exists a multiplicity of equations to calculate the RMSE that do not significantly differ in their results. In this study it was estimated, according to Mohseni et al. (1998),

\[
\text{RMSE} = \sqrt{\frac{\sum_{i=1}^{n} (T_{\text{sim}} - T_{\text{meas}})^2}{n - 3}}, \quad (3)
\]

where

- \(T_{\text{sim}}\) = monthly simulated stream temperatures (°C),
- \(T_{\text{meas}}\) = monthly measured stream temperatures (°C), and
- \(n\) = number of data points.

c. The global water quality model WorldQual and the projection of climate change on water temperatures and first-order decay rates

To assess the future state of aquatic ecosystems and to determine the suitability of surface water supply for different water users, a new continental-scale model of water quality (WorldQual; F. Voß et al. 2009; A. Voß et al. 2012) has been developed. The aim of the WorldQual model is to determine chemical fluxes in different pathways that will allow a combination of water quantity with water quality analyses. In particular, effects of changed climate and anthropogenic conditions can be analyzed.

The effect of climate change on transport and transformations of substances can be manifold; for example, changes in precipitation and air temperature can affect the hydrological cycle, or changed runoff conditions can affect transport processes like diffuse pollution from agriculture and loading from sealed areas, and finally several transformation processes, like degradation, are temperature dependent. The impacts of global warming within this study will be discussed by selecting one key water quality indicator, BOD, as an example. BOD serves as a metric for the overall health of aquatic ecosystems. BOD measures the rate of oxygen uptake by micro-organisms in a sample of water and can be defined as the definite test for organic pollution of rivers. Decay rates for BOD are temperature dependent \([\text{dec}(T_{\text{water}})]\) and can be expressed with the following equation (Benham et al. 2006; Bowie et al. 1985):

\[
\text{dec}(T_{\text{water}}) = \text{dec}(20) T_{\text{water}}^{-20}, \quad (4)
\]

where

- \(\text{dec}(T_{\text{water}})\) = decay rate at water temperature (month\(^{-1}\)),
- \(T_{\text{water}}\) = water temperature (°C),
- \(\text{dec}(20)\) = decay rate at 20°C (month\(^{-1}\)), and
- \(\Theta\) = temperature correction coefficient.

In this study we defined \(\text{dec}(20)\) at a constant rate of 6.9 month\(^{-1}\) and \(\Theta\) at 1.07 (Paliwal et al. 2007; Chapra 1997).

Climate change was described using two 30-yr simulations performed with the coupled atmosphere–ocean GCM ECHAM5/Max Planck Institute Ocean Model (MPI-OM) (Roeckner et al. 2003; Jungclaus et al. 2006). The simulations corresponded to the time period 2041–70 and were driven by the Intergovernmental Panel on Climate Change (IPCC) Special Report on Emissions Scenarios (SRES) A2 and B1 (Meehl et al. 2007). Data for climate projections was made available through WATCH. Temperature data was bias corrected (Uppala et al. 2005; Weedon et al. 2011; New et al. 1999) and could be directly used within this study (for details see Piani et al. 2010 and Hagemann et al. 2011). The time frame of the climate normal refers to the years 1961–90, making use of the WFD dataset described above.

The projection of future climate changes based on A2 indicates more extreme shifts in mean air temperatures and precipitation than those of B1, which is a more moderate scenario. By the end of this century, A2 predicts a rise
in mean air temperature by 3.5°–4.6°C and an increase in precipitation of some 5.7%, while B1 forecasts weaker changes with values of 1.7°–2.6°C and 3.8% in air temperature and precipitation, respectively (Meehl et al. 2007).

3. Results and discussion

a. Nonlinear regression model on a global scale and for different climate zones

Regression models for the global dataset, as well as for snow climates, warm temperate climates, and arid climates, show good accordance with measured data expressed in terms of NSC (0.81) and moderate if expressed in terms of RMSE (3.6°C; see Table 3). The NSC of all 1659 gauging stations was 0.88, whereas RMSE was 3.0°C for the period 1965–94.

A t test on the coefficients confirmed a high water–air temperature relationship (p = 0.0001). Ninety-five percent confidence intervals on global regressions parameters were −0.131 and −0.130 and 1.93 and 1.95 for C1 and C2, respectively.

Regression parameters do not differ very much between these four datasets (see Table 3) and respective regression curves overlap just as well, which is illustrated in Fig. 3. In arid zones, results derived from the regression model may deviate slightly in upper temperature ranges (between 20° and 40°C). This means, in three out of five climate zones, representing ~92% of all gauging stations used in this study, NSC is larger than 0.81.

The parameters of fit for the validation set likewise indicate a good performance of the regression model: in all four climate regions, both NSC and RMSE show improved values.

The polar regression model fits with an efficiency of 0.66 and an RMSE of 1.8°C but there is a loss in measures of fit for the validation period (0.56; 2.0°C). At air temperatures below 5°C, the curve matches well to the global standard model (Fig. 3). But at higher temperatures, deviation from global regression model becomes more distinct. Monthly air temperatures (WFD) of that climate zone naturally occur at a range of −27° to 13°C. Overall, the polar regression was based on a weak dataset of 34 air–water temperature pairs for the calibration set and 130 pairs for the validation set derived from three water gauging stations (see Table 2). Perhaps an extensive data record would lead to a more precise prediction of water temperatures in this region.

In contrast to the polar zone, the equatorial regression model differs most in lower temperature ranges. Here the weak NSCs of 0.22 and 0.20 and the high RMSE of 3.3°C and 2.9°C suggest that the model has to be improved for the equatorial zone.

Especially in areas with highly variable weather, there is an uncertainty in estimation of water temperature (Mohseni et al. 1998). However, on a global scale it is difficult to take these additional factors into account because for many regions they are not available.

Global distribution of NSC for the validation dataset is shown as mean for each 0.5°C grid cell where a gauging station is located (Fig. 1). Overall, the global regression model indicates good performance (NSC > 0.8) in many parts of the eastern United States, central Europe, central Asia, and Australia (for the latter, the training data achieved an NSC > 0.8; for the validation period, no data were available), while poorer NSC values (<0.6) were found for Central America, western Africa, India, the Mekong basin, and a few stations in central Europe and the western part of North America.

Analysis of maximum likelihood did not meet the criterion of normal distribution because of heteroskedasticity. However, the test on quasi maximum likelihood using heteroskedasticity consistent standard errors (Hansen et al. 2006) showed high significance (p = 0.0001).

Intension of heteroskedasticity was weak but it reveals some uncertainty of model performance. Heteroskedasticity could be caused by other sources (industrial cooling systems, snowmelt, etc.) than air temperature influencing water temperature.

Results from previous studies support our findings. Van Vliet et al. (2011) provided a nonlinear regression model applied to 157 stations worldwide using daily temperature data and in addition considering discharge.
The NSC distribution pattern they published is quite similar to that presented in Fig. 1. Even the NSC values are within the range of our global model.

Mohseni et al. (1998) determined in his study of weekly air–water temperatures for 584 U.S. gauging stations in total an NSC value greater than 0.8 for 96% of all stations with an RMSE of 1.64°C. Another investigation of weekly air–water temperatures for 43 streams worldwide (Europe: 24, North America: 18, and Japan: 1) found that the nonlinear regression model fits with an efficiency of fit greater than 0.8 for 20 sites (46% of all stations; Morrill et al. 2005). The RMSE in this study was 2.37°C and hence higher than obtained in Mohseni et al. (1998), but similar to our study.

Further on, analysis of relative frequency in the absolute difference of measured and simulated water temperatures based on the regression equation of the global dataset was performed. In summary, 77% of the total simulated values \(n = 97,964\) differ less than 3°C from the observed water temperatures and only 6.8% have a difference of more than 5°C (Fig. 4).

b. Seasonal hysteresis effects on a global scale

The analysis of heat-storage effects did not show noticeable differences between both limbs on a global scale under application of the global regression model (see Fig. 5). Maximum difference between both limbs, the rising and the falling one, are 1.6°C.

For both limbs a mean NSC of 0.85 was calculated, which is weaker than the NSC of the global regression (0.88; see Table 3). So obviously hysteresis only has marginal effects on the global approach and will thus be neglected in this study.

Mohseni et al. (1998) noticed the occurrence of seasonal hysteresis effects at 250 (43% of 584 stations investigated) North American streams, which was attributed to heat-storage effects (Webb and Nobilis 1997). But Morrill et al. (2005) could not find statistically significant differences between models considering hysteresis and those that do not for most of the 22 investigated streams.

c. Application to time series of selected river basins

Time series of air temperature (WFD) and measured and simulated water temperature for a subset of five gauging stations are plotted in Fig. 6 for training (right column) and validation (left column) datasets, respectively. In general, curves for the test sites of the Rhine, Yangtze River, Delaware River, and Ob River show a good accordance with NSC greater than 0.82. Additionally, at these four stations an improvement in terms of fit for the validation dataset could be seen.

Although air temperatures vary in the range of −29.5°C up to 31.5°C, simulated water temperatures match not only in the high temperature ranges but also for the lower ones.

At Medina River, the training data has a fit of 0.80 and 1.0°C for NSC and RMSE, respectively, and the fit becomes weaker for the validation (0.75; 1.4°C). There is also a considerable lack of agreement between observed and fitted water temperatures at air temperatures between 10°C and 15°C. Here the simulated water temperatures obviously follow the air temperature curve.

At Ob River near Salelhard, van Vliet et al. (2011) published an NSC of 0.75 and an RMSE of 3.1°C produced by their daily temperature regression model including discharge, while our global regression fitted an NSC of 0.84 and an RMSE of 2.0 at this site.
FIG. 6. Time series comparing recorded and simulated stream temperatures of exclusive gauging stations. They are presented for (right) the training data (1965–94) and (left) the validation data (1995–2001). Temperature values are projected as monthly means. Climate regions are warm temperate (C) and snow (D).
d. Projections of climate change scenarios on stream temperatures and corresponding decay rates

In assessing how stream and river temperature may change in the future, direct impacts of changing climate needs to be taken into account. Therefore, the global regression model is adapted to global change scenarios (see Fig. 7). For each 0.5° grid cell, the regression model was applied to long-term mean monthly values of the WFD climate normal (1961–90) as well as to the gridded long-term mean monthly temperatures of the bias-corrected (Uppala et al. 2005; Weedon et al. 2011; New et al. 1999, 2000) A2 and B1 scenarios (2041–70). Results are shown for the winter season (Figs. 7a,c,e) including the months December, January, and February while the months June, July, and August are combined to form the summer season (Figs. 7b,d,f) according to seasons of the Northern Hemisphere. The plots of the climate normal (Figs. 7a,b) illustrate potential spatial water temperature distribution while the scenario plots (Figs. 7a–d) indicate the difference to the climate normal.

In the winter season, a temperature gradient from north to south can be observed for the climate normal (Fig. 7a). In the Northern Hemisphere, mean water temperatures are predominantly between 1°C and 5°C. Along 30° latitude, temperatures up to 20°C are simulated, and at the equatorial zone and most areas of Southern Hemisphere they can reach even more than 25°C, except for central Africa. Here, in many areas, temperature is below 25°C. In the summer period the gradient looks different. Along
the equatorial zone temperatures vary in the range between 25° and 32.3°C and become cooler, converging to the poles, gradually.

In general, the scenarios predict an increase in water temperature; especially for the A2 scenario, some areas show a higher warming than B1. This particularly can be observed during the summer period in central and southern Europe, central Asia, and central Australia, where A2 predicts 1°–2°C higher temperatures than B1. In the winter season in the Northern Hemisphere, but also in northern parts of Australia and South America, temperature increase compared to the climate normal is up to 1°C for both scenarios (Figs. 7c,e). Highest increments in water temperature can be observed at the equatorial zone where increases of about 2°–4°C can be observed.

The projected changes in water temperature are in line with earlier findings as reported—for example, by EEA (2008), where it is stated that increases in surface water temperature are often 50%–70% of the projected increases in air temperature. It is to be noted, however, that the projected changes by WorldQual due to climate change are of the same magnitude as the model uncertainty (see section 3a). This needs to be taken into account when interpreting the results.

The distribution of RMSE (Fig. 1b) can be used to assess the accuracy of the predictions in different regions. Mohseni et al. (1999) demonstrated in their scenario analysis from projections of doubled CO₂ concentrations [temperature data were derived from the Canadian Centre for Climate Modelling and Analysis (CCCma) GCM] that mean annual stream temperatures will rise by 2°–5°C across the United States. Maximum changes in weekly stream temperature were predicted in spring and fall, while projected changes in winter and summer were low.

In the winter period the projection (Figs. 7c,e) also showed a weak change in water temperature. But in opposition to Mohseni et al. (1999), the maximum increase in stream temperatures was observed in summer (Figs. 7d,f) and was lower in spring and autumn (results not shown). Thus, seasonal and spatial temperature dispersals are obviously dependent on the choice of GCM.

As an indicator of how climate change may influence future water quality variables, we calculated stream-temperature-dependent BOD decay rates. BOD decay rates have been calculated for both the climate normal and the A2 and B1 scenarios (Fig. 8). In general, decay rates are linked directly to temperature, so their spatial patterns look very similar to that of the temperature distribution (Fig. 7). Because of application of Eq. (2), rates above 20°C in water temperature [here dec(20) is equal to 6.9 month⁻¹] will have a steeper increase than the decline for rates below 20°C. This means that a shift to higher water temperatures will also have a significant impact on the spatial patterns in related BOD decay rates.

Projections of decay rates are shown for the summer season because maximum change in surface water temperatures was observed then, as mentioned above. Hence, most observable change in the decay rate will be expected during this season.

Calculated decay rates for the climate normal cover a spread from 2.9 to 11.3 month⁻¹. Highest rates can be observed at equatorial climates and neighboring areas like North Africa, Central America, and India, predominately with values larger than 8.4 month⁻¹. Decay rates become lower in cooler climates (e.g., South Africa and Canada) and higher altitudes (e.g., the Andes and the Himalayas), gradually.

For the 2050s scenarios, decay rates are shown as percentage change to the climate normal. In general, for
most areas worldwide, an increase up to 10% is projected. Primarily in regions with high decay rates like North Africa or Central America, the rise is equal to or lower than 5%. Here, increments of decay rates up to 20% compared to the climate normal are predicted, for instance, in central Europe, South Africa, northern Australia, central Asia, and some areas in the North American Midwest. Increases in decay rates predicted for the B1 scenario overlap with areas of increase for the A2 scenario. However, the spatial extent is lower, which is in accordance with the spatial distribution of stream temperatures.

4. Conclusions

This work was motivated by the need to find an easy approach for estimation of monthly stream water temperatures to gauge the potential impacts of climate change on stream temperatures and related stream water quality indicators on a global scale for use in the WorldQual model. Therefore, a nonlinear regression model, named the global standard regression equation, was tested to assess monthly stream temperature as a function of air temperature.

The global standard regression equation fulfilled the requirements in a reliable way. Only one input parameter—air temperature—is needed. The fitting results show a high accordance between the global equation and three of the five main climate zones, according to the Köppen–Geiger climate classification, representing 90% of total records. Nash–Sutcliffe coefficients in these are higher than 0.82.

To improve the performance of the regression model for the equatorial and the polar region, a more detailed assessment is still necessary. Here, an extension of the dataset is required.

Analyses of seasonal heat-storage effects (hysteresis) did not show relevant distinctions between the rising and the falling limb and the global standard regression model. Time series of five individual river basins confirm the efficiency of the method (NSC > 0.75).

Seventy-seven percent of the simulated water temperature values differ from measured temperatures equal or less than 3°C. Exogenous influences of different other variables such as heavy rainfall or evaporation will have a significant impact on water temperature (Bogan et al. 2003). Especially in areas with a highly variable weather situation, the model would require further development.

Furthermore, in developed countries, water temperature is also influenced by point sources like warm water discharges from power plants, reservoir releases, and other industrial facilities (Vörosmarty et al. 2010; Nolan et al. 1998, 2003). These impacts will affect the air–water temperature relationship and the predictions can become imprecise. Therefore, the accuracy of estimation could be improved by implementation of additional parameters such as discharge or evaporation. Air temperature, on the other hand, is easily available nearly worldwide.

Projections of future changes in stream temperature indicates for the ECHAM5 A2 and B1 scenarios an increase by 1°–5°C and, hence, are within the range of previous studies.

The projected changes of stream temperature by WorldQual due to climate change scenarios are of the same magnitude as the model uncertainty (see section 3a). This has to be taken into account when interpreting the results.

The choice of GCM also will influence temperature dispersal on temporal as well as on a spatial scale. Consequently, projections of decay rates show a similar seasonal and spatial pattern as the corresponding stream temperatures. A regional increase up to ~25% could be observed, but in general increases for most parts of the world are up to 10%. Higher decay rates would lead to a drop of in-stream organic loadings within particular thresholds. This has to be taken into account for subsequent investigations on water quality status.

Intended research of continental human water security and aquatic ecosystems will use water temperature data output of the global standard regression model to assess the impact on additional water quality indicators like total nitrogen, total phosphate, and total coliform numbers.

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