Comparison of non-parametric and parametric water temperature models on the Nivelle River, France

LOUBNA BENYAHYA[1,2], ANDRÉ ST-HILAIRE[1], TAHA B. M. J. OUARDA[1], BERNARD BOBÉE[1] & JACQUES DUMAS[3]

1 *Chair in Statistical Hydrology, INRS-ETE, Université du Québec, 490 de la Couronne Street, Québec City, Quebec G1K 9A9, Canada*

2 *Department of Civil Engineering, Dalhousie University, Halifax, Nova Scotia B3J 2X4, Canada*
loubna_benyahya@hotmail.com

3 *INRA, Institut National de la Recherche Agronomique, UMR ECOBIOP, Pôle d'Hydrobiologie, Quartier Ibarron, F-64310 St Pée sur Nivelle, France*

Abstract Water temperature is an important abiotic variable in aquatic habitat studies and may be one of the factors limiting the potential fish habitat (e.g. salmonids) in a stream. Stream water temperatures are modelled using statistical approaches with air temperature and streamflow as exogenous variables in the Nivelle River, southern France. Two different models are used to model mean weekly maximum temperature data: a non-parametric approach, the *k*-nearest neighbours method (*k*-NN) and a parametric approach, the periodic autoregressive model with exogenous variables (PARX). The *k*-NN is a data-driven method, which consists of finding, at each point of interest, a small number of neighbours nearest to this value, and the prediction is estimated based on these neighbours. The PARX model is an extension of commonly-used autoregressive models in which parameters are estimated for each period within the years. Different variants of air temperature and flow are used in the model development. In order to test the performance of these models, a jack-knife technique is used, whereby model goodness of fit is assessed separately for each year. The results indicate that both models give good performances, but the PARX model should be preferred, because of its good estimation of the individual weekly temperatures and its ability to explicitly predict water temperature using exogenous variables.

Key words stream water temperature; non-parametric *vs* parametric models; PARX, *k*-nearest neighbours

Comparaison de modèles paramétriques et non-paramétriques de température de l'eau de la Rivière Nivelle, France

Résumé La température de l'eau est une variable très importante pour les études d'habitat aquatique. Elle peut être un facteur limitant pour plusieurs espèces de poisson, telles que les salmonidés. Cet article présente une modélisation statistique de la température de l'eau en utilisant la température de l'air et le débit comme variables explicatives. Les données utilisées dans la modélisation numérique sont les températures hebdomadaires de la rivière Nivelle (France). Deux modèles de température de l'eau sont alors proposés et comparés, soit la méthode non-paramétrique des *k* plus proches voisins (VPP) et le modèle périodique autorégressif avec variables exogènes (PARX). La méthode des VPP consiste à chercher dans tout l'historique, les *k* plus proches voisins qui serviront à estimer la température actuelle. Le modèle PARX est un modèle autorégressif dont les paramètres de chaque variable explicative sont estimés indépendamment pour chaque période de l'année. Plusieurs attributs de température de l'eau et du débit sont considérés. La performance des modèles a été évaluée pour chaque année en utilisant une technique de validation croisée de type "jack-knife". Les résultats préliminaires ont montré que le modèle PARX et le modèle VPP présentent une performance similaire dans la simulation des températures hebdomadaires. Toutefois, le modèle PARX demeure le plus approprié, car il préserve la persistance des séries périodiques et il offre une équation explicitant la relation entre la température de l'eau et les variables explicatives.

Mots clefs température de l'eau en rivière, modèles non-paramétrique *vs* paramétrique; PARX, *k* plus proches voisins

INTRODUCTION

Water temperature is recognized as an important water quality parameter. It plays a major role in many chemical and biological processes present in streams and, hence, influences the health and the distribution of aquatic ecosystems. Water temperature extremes can have adverse impacts on aquatic habitats, especially when they are outside the optimal thermal range (Coutant, 1977). For example, warm waters have been observed to affect the mortality of trout (Lee & Rinne, 1980; Bjornn & Reiser, 1991). In addition, Lund *et al.* (2002) have shown that high water temperatures can have an impact on the development of juvenile salmonids. They showed that high summer water temperatures can cause significant protein damage and induce a heat-shock response. Water

Open for discussion until 1 December 2008

temperature is a variable for which changes are governed by the interaction of natural environmental processes (e.g. air temperature, solar radiation, topography, riparian shading, humidity, wind velocity, etc.) and by human activities such as thermal pollution and deforestation (Brown & Krygier, 1970; Holtby, 1988). Therefore, water temperature modelling is a fundamental tool for the planning and management of water resources.

Existing water temperature models can be categorized in three groups: (a) deterministic models; (b) regression models; and (c) stochastic models (Caissie, 2006). Deterministic conceptual models are generally based on thermal budget calculations, which require numerous inputs (e.g. physiographic, hydrological and meteorological parameters). Examples of deterministic models include the US Fish and Wildlife SNTEMP model (Bartholow, 1989), the SSTEMP model (Bartholow, 1999) and the CEQUEAU hydrological and water temperature model (Morin & Couillard, 1990; St-Hilaire *et al*., 2003). Other references of simpler deterministic water temperature models include those of Gu *et al*. (1998) and Caissie *et al*. (2005), who used an equilibrium temperature concept.

An alternative approach to deterministic models in predicting water temperature is the use of statistical models (e.g. regression). In contrast to the deterministic models, the main advantage of the statistical models is their relative simplicity and minimal data requirement. Several regression approaches have been tested in the past. Water–air temperature regression models have been developed successfully for different time periods, including 2-hourly, daily, weekly, monthly and annual means (e.g. Stephan & Preud'homme, 1993; Webb & Walling, 1993; Webb & Nobilis, 1997; Pilgrim *et al*., 1998; Erickson & Stefan, 2000). Nonlinear regressions are recommended for small time steps (e.g. Mohseni & Stefan, 1999). In streams with important subsurface flow contributions, groundwater discharge can reduce the daily maximum water temperature, which gives the stream a nonlinear behaviour (Caissie, 2006). Other models have also been developed to assess relationships between water temperature and air temperature. For example, the so-called stochastic models are generally applied for relatively small time steps (e.g. daily or sub-daily). In this approach, the seasonal component of water temperatures is first removed and time series models are then fitted to water temperature residuals. Early developments of this approach include those of Kothandaraman (1971) and Cluis (1972). More recently, Caissie *et al*. (1998, 2001) adapted the approach of Cluis (1972) to a relatively small system (Catamaran Brook, Canada, with a drainage basin of 50 km^2).

Stochastic and regression models have the advantage of being computationally simple, and applicable to locations where air temperature data are available. However, such approaches do not guarantee that the seasonality of the data is completely removed to achieve stationary residuals, because the correlation structure of the series may be dependent on the period. This level of predictive capability calls for periodic models that are able to model periodicity in autocorrelations. Periodic autoregressive (PAR) and periodic autoregressive moving average (PARMA) models are variants of ARMA models (Box & Jenkins, 1976) that use periodic parameters. Periodic models have been widely and successfully used in econometrics applications (Osborn & Smith, 1989; Novales & de Frutto, 1997), as well as in the field of hydrology (Vecchia, 1985; Bartolini *et al*., 1988; Ula & Smadi, 1997; Benyahya *et al*., 2007). Most applications are purely autoregressive and do not include exogenous variables. To our knowledge, PAR models with exogenous variables (PARX) have never been used to model water temperature.

Another approach, seldom used in water temperature modelling, consists of developing non-parametric models. The models are labelled non-parametric because they are based on calculating a certain attribute without using a parameterised statistical model. One such approach is the *k*-nearest neighbours (*k*-NN) method (Yakowitz & Karlsson, 1987). The method consists of searching among past observations for the *k* events which are most similar to the present situation. A prediction is then built from the water temperatures which are associated with these *k* events. The technique has been used to analyse rainfall–runoff processes and has been advantageously compared with autoregressive moving average models with exogenous inputs (ARMAX) (Karlsson & Yakowitz, 1987; Yakowitz & Karlsson, 1987). Galeati (1990) evaluated and compared the performances of the *k*-NN method and autoregressive model with exogenous inputs (ARX) to predict daily mean discharge and found the performances of the two methods substantially equal.

Although most statistical models only incorporate air temperature as an exogenous variable, the influence of discharge on water temperature has also been recognized (e.g. Webb *et al*., 2003; Neumann *et al*., 2003). Both the PARX model and the *k*-NN approaches can include discharge as an input. Therefore, the specific objectives of the present study are: (1) to evaluate the possibility of employing the *k*-nearest neighbours method (*k*-NN), and (2) to compare its performance with that of a PARX model with air temperature and streamflow as exogenous inputs. These two approaches were implemented using weekly maximum temperature data from a French river with an important salmon population: the Nivelle River in France.

METHODS

Study area

Time series of water temperature were obtained from the Nivelle River, located in southwestern France (Fig. 1). It is a relatively small river with a drainage area of 238 km^2 and length of 39 km from its source in Spain to the Bay of Biscay at Saint-Jean-de-Luz. The catchment is well known for its population of Atlantic salmon (*Salmo salar*) (Dumas & Prouzet, 2003). The oceanic climate is mild and wet (1700 mm/year average rainfall at St-Pée-sur-Nivelle) and provides a mean annual discharge of 5.4 m^3/s downstream from the confluence of the main tributary, the Lurgorrieta.

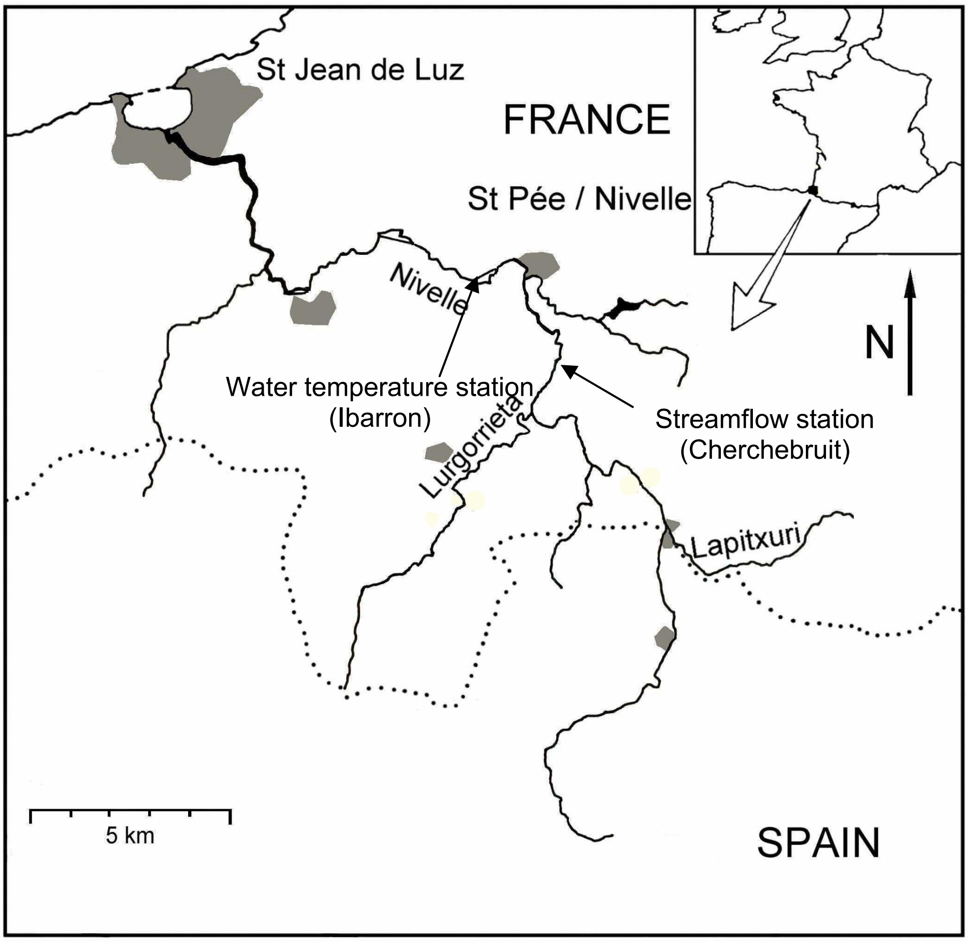

Fig. 1 Nivelle River catchment area indicating the water temperature and streamflow stations.

Water temperatures were measured daily at one stream location (Ibarron; Fig. 1) by the National Institute of the Agronomic Research (INRA) using Tidbit, Minilog Vemco and Jules Richard temperature data loggers (accuracy ±0.2°C, ±0.3°C and ±0.4°C, respectively). Water temperature data were available from 1984 to 2004. There were some missing values between 18 July and 31 August 1994, which were interpolated using an interannual mean. Daily air temperatures were obtained from the Biarritz Airport weather station, which is located 13 km north of the water temperature station. Streamflow for the same period was measured at the Nivelle streamflow station (Fig. 1), which is located in the downstream portion of the drainage area. Mean weekly maximum temperatures (MWMT) were calculated from daily maximum temperatures (mean of seven consecutive calendar days). Weekly values were selected for this study based on their potential use in fisheries management. To assess changes in fish habitat and growth conditions, the weekly time scale is sometimes deemed more appropriate (Eaton & Scheller, 1996; Oliver & Fidler, 2001). Moreover, previous research showed that weekly and monthly averages of stream temperature and air temperature are more correlated than daily values (Pilgrim *et al.*, 1998; Erickson & Stefan, 2000).

The present study focuses on the period within every year spanning from 1 May to 31 November (30 weeks). Outside these periods (i.e. December–April), the water temperature variations on the Nivelle River were typically less than 5°C (Fig. 2(b1)). It was therefore decided to study the period during which the largest temperature variations occurred (magnitude between

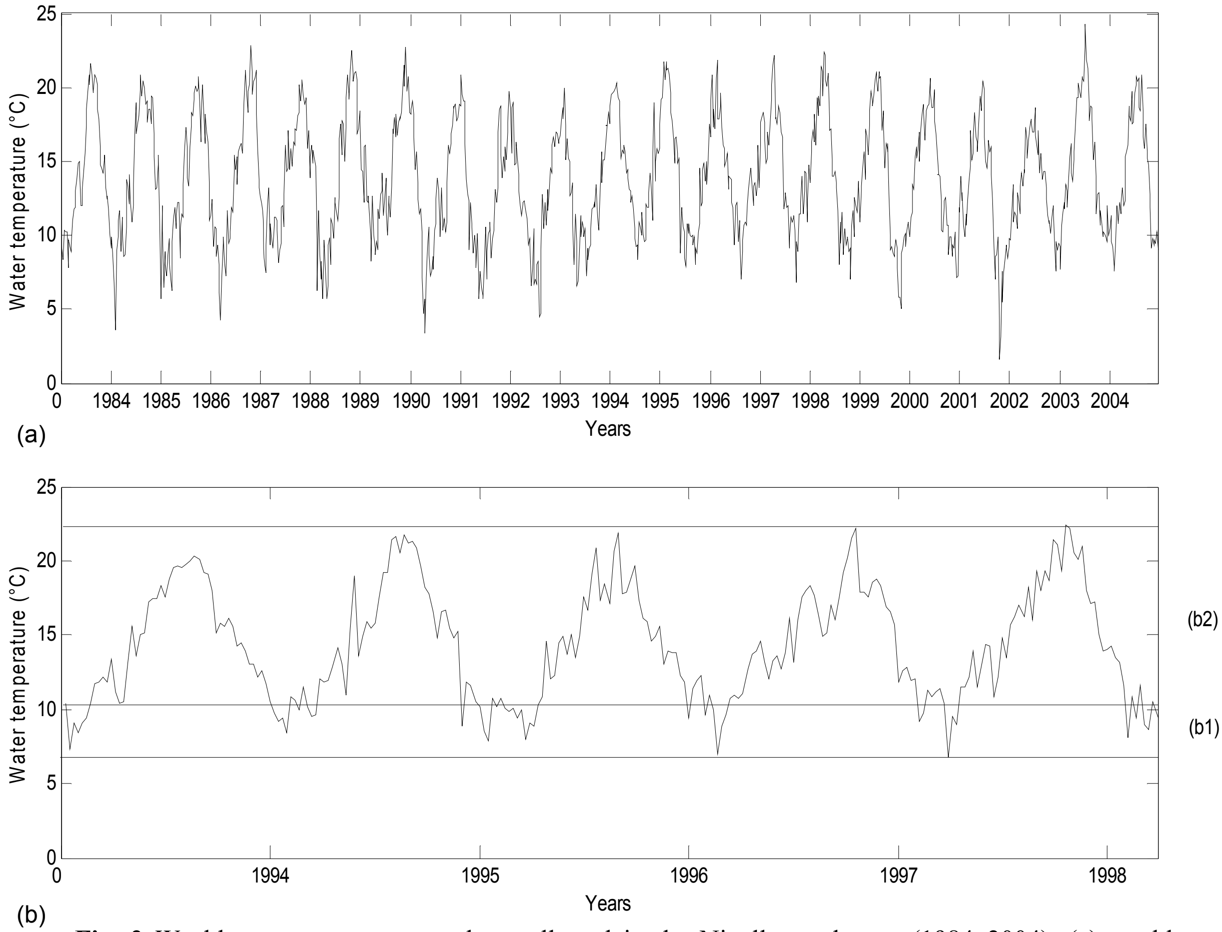

Fig. 2 Weekly water temperature data collected in the Nivelle catchment (1984–2004): (a) weekly water temperature data including the December–April periods; and (b) example of detailed view of weekly water temperature data (1994–1998). (b1) and (b2) represent the amplitude of the water temperature variation from December to April and from May to November, respectively.

10 and 12°C during the warmer period of May–November; Fig. 2(b2)). One of the reasons for this selection was the fact that salmonids are much more likely to experience thermal stress during the warmer period, when maximum water temperature may exceed a certain tolerable limit. Indeed, Hodgson & Quinn (2002) demonstrated that, during the spawning season, some species of pacific salmon will suspend their spawning activity when the water temperature exceeds 19°C. Moreover, Crozier & Zabel (2006) showed that juvenile Chinook salmon survival is negatively correlated with summer temperature.

k-Nearest neighbours (k-NN)

The key steps in the *k*-NN algorithm are as follows:

(a) *Compile a feature vector*. The feature vector ***X*** consists of values of the selected input attributes for which the *k*-nearest neighbours were to be found (usually <4). In the present study, a total of 11 candidate independent variables were initially considered. All are derived from three observed variables: water temperature (Tw), air temperature (Ta) and streamflow (*Q*) (Table 1). The potential inputs include autoregressive terms of water temperature, weekly degree-days, lagged air temperature, lagged streamflow and relative flow change. Relative flow change was used as opposed to direct flow measurements because it was shown by Ahmadi-Nedushan *et al.* (2007) to yield better results for daily water temperature models. Weekly degree-days were defined here as the cumulative sum of the weekly air temperature over the period of analysis.

(b) *Find the weighted sum of the attributes*. Since the scales of water and air temperature units differ from that of streamflow, the weighted attributes were generalized as a weighted standardized norm (*N*):

$$N = \sum_{i=1}^{n_1} w_i X_i \tag{1}$$

where n_1 is number of attributes, w_i and X_i are, respectively, the optimized weights and the vectors of standardized (i.e. subtract mean value and divide by the standard deviation) values of the selected attributes. In this study, weights were varied between 1 and 1000, and all possible combinations tested by increments of 100.

(c) *Calculate the Euclidean distance between the norm of the period of interest and the norm of all other available data*. The period of interest is the week for which the forecast or simulation is required. For two norms (N_{j1}, N_{j2}) calculated using vectors $\boldsymbol{X}_{j1}$ for the period of interest and $\boldsymbol{X}_{j2}$ (j_2 = 1, …, j_1 − 1, j_1 + 1, …, m) for the m other periods in the database, the Euclidean distance (δ) was defined as:

$$\delta\left(N_{j1}, N_{j2}\right) = \left|N_{j1} - N_{j2}\right| = \sum_{i=1}^{n_1} w_i \left|X_{i,j1} - X_{i,j2}\right| \tag{2}$$

(d) *Sort the distances (δ) in ascending order, and retain only the first k nearest neighbours*. In this study, *k* was limited to a maximum value of 3. The strategy for choosing the optimal *k* was to try several successive values of *k* (e.g. 2, 3 and 4) and to select the combination for which the model gave the best prediction.

(e) *Assign a weight* (k_i) *to each of the k neighbours*. Thus the predicted value of the final output was a weighted sum of the values of neighbours ($\sum_{i=1}^{k} k_i T_i$, where T_i are the neighbours).

(f) Repeat steps (a)–(e) for each of the time steps.

Obviously, this approach can be computationally intensive. However, applications indicate that a solution can be obtained in a relatively short time (less than a day, depending on computing power).

Table 1 List of attributes included in the preliminary analysis of *k*-NN method.

Attributes	Description	Formula
Tw0	Water temperature of the present week (t)	Tw(t)
Tw1	Water temperature of the week (t – 1)	Tw(t – 1)
Tw2	Water temperature of the week (t – 2)	Tw(t – 2)
Tw3	Mean of water temperature of the two past weeks	mean[Tw(t – 1), Tw(t – 2)]
Ta1	Air temperature of the week (t – 1)	Ta(t – 1)
Ta2	Air temperature of the week (t – 2)	Ta(t – 2)
Ta3	Mean of air temperature of the two past weeks	mean[Ta(t – 1)), Ta(t – 2)]
Ta4	Weekly degree-days	Cumulative sum of air temperature
Q1	flow of the week (t – 1)	Q(t – 1)
Q2	flow of the week (t – 2)	Q(t – 2)
Q3	Mean of flow of the two past weeks	mean[Q(t – 1)), Q(t – 2)]
Q4	Relative flow change	[Q(t) – Q(t – 1)]/Q(t)

Periodic autoregressive model with exogenous variables (PARX)

Once calibrated, parametric models can predict values without using past historical record. The key steps in the PARX model are as follows:

(a) *Define the independent variables*. Consider $\mathrm{Tw}_{v,z}$, $\mathrm{Ta}_{v,z}$ and $Q_{v,z}$, the time series of water temperature, air temperature and streamflow, respectively. The subscripts v and τ denote the year and the period (e.g. week), respectively, where $\tau = 1, \ldots, \omega$, with ω being the number of periods in the year.

(b) *Test the normality of the data*. Parametric time series models generally require that the underlying series follows a normal distribution (Salas, 1993). Otherwise, the original series should be transformed to a Gaussian shape via log, square root or Box-Cox transformations. The predicted values from the model were then back-transformed into the original space. In the present study, the Shapiro-Wilk test (Shapiro & Wilk, 1965) was used to test the normality of the data. This test is appropriate when the sample size is lower than 50.

(c) *Estimate the parameters of the model*. Following the earlier work of Salas (1993), a PARX model representing the water temperature series may be written in the following form:

$$\mathrm{Tw}_{v,\tau} = \sum_{i_1=1}^{p_1} \varphi 1_{i_1,\tau} \mathrm{Tw}_{v,\tau-i_1} + \sum_{i_2=1}^{p_2} \varphi 2_{i_2,\tau} \mathrm{Ta}_{v,\tau-i_2} + \sum_{i_3=1}^{p_3} \varphi 3_{i_3,\tau} Q_{v,\tau-i_3} + \varepsilon_{v,\tau} \quad (3)$$

where $\tau > i_1, i_2, i_3$; $\varphi 1_{i_1,\tau}$, $\varphi 1_{i_2,\tau}$ and $\varphi 1_{i_3,\tau}$ are periodic parameters; p_1, p_2 and p_3 are the lags of water temperature, air temperature and streamflow, respectively; and $\varepsilon_{v,\tau}$ is the error term, which was excluded from the comparative study. In the present study, the time series of each of the variables were first standardized. Subsequently, to obtain the final estimated value of water temperature, a back transformation was applied. Parameters may be estimated for each time step (period) from the data by a number of techniques such as the method of moments, the least squares method, or the method of maximum likelihood (Salas, 1993). In this study, the least squares method was used. Generally, estimates obtained by this method are consistent, unbiased and efficient (Hsia, 1977).

Model evaluation and validation

To compare the predicted (P) and the observed (O) water temperatures, the root mean square error (RMSE, equation (4)), the bias (Bias, equation (5)) and the Nash-Sutcliffe coefficient of efficiency (NSC, equation (6)) were used (Nash & Sutcliffe, 1970; Janssen & Heuberger, 1995). The RMSE is defined as:

$$\mathrm{RMSE} = \sqrt{\frac{1}{n_2} \sum_{i=1}^{n_2} \left(P_i - O_i\right)^2} \quad (4)$$

where n_2 is the number of water temperature observations. The RMSE, being the square root of the sum of the variance and the square of the bias, was calculated to inform on the average magnitude of the water temperature errors. This criterion is often used in water temperature modelling studies (e.g. Caissie *et al.*, 1998, 2001; St-Hilaire *et al.*, 2003; Ahmadi-Nedushan *et al.*, 2007).

The Bias error was computed simply as the sum of the differences between predicted and observed values divided by n_2:

$$\text{Bias} = \frac{1}{n_2}\sum_{i=1}^{n_2}\left(P_i - O_i\right) \tag{5}$$

Efficiency of fit for both the *k*-NN method and the PARX model was determined as:

$$\text{NSC} = 1 - \frac{\sum_{i=1}^{n_2}\left(P_i - O_i\right)^2}{\sum_{i=1}^{n_2}\left(\overline{O} - O_i\right)^2} \tag{6}$$

where $\overline{O}$ is the mean weekly water temperatures for the period τ. The NSC compares model performances with the sample mean. It ranges from minus infinity (poor model: model does not perform better than using the sample mean) to 1 (perfect model).

To test the performance of the above models, the leave-one-out (jackknife) validation technique (Quenouille, 1949) was used. This method consists of removing one year from the data and estimating the model using the rest of the data set. The performance was judged by using the model to estimate the left out data. Thereafter, the performance criteria (equations (4)–(6)) were calculated by year and an average value of all years was also calculated. All models and performance estimation were done using Matlab 6.5.

RESULTS

Time series of water temperature, air temperature and flow used in this study are plotted in Fig. 3. Water temperature data in the Nivelle River showed a good correlation with air temperatures and streamflow ($r = 0.93$ and –0.48, respectively). This result indicated the relevance of including air temperature and streamflow as exogenous variables in the water temperature modelling. The results are organized as follows: first, *k*-NN results are shown and are thereafter compared to that of the PARX model, with air temperature and flow as exogenous predictor variables.

k-NN model

In order to select the best set of the explanatory variables presented in the Table 1, the simplest approach consisted of performing a correlation analysis between Tw0 and each attributes independently for each year. Figure 4 shows the correlation box plots. Box boundaries represent the interquartile range and the whiskers represent the 10th and 90th percentile, whereas the median is indicated by the black centre line. The extreme values are shown as individual points. As expected, among the selected attributes, Tw1, Tw2, Ta1, Ta4 and Q1 have the highest correlation coefficients with the present water temperature (Tw0; see Fig. 4). Indeed, median correlation coefficient values are 0.86, 0.73, 0.83, –0.55 and –0.38 for Tw1, Tw2, Ta1, Ta4, and Q1, respectively. Therefore, these five attributes were considered in the analysis. Result of the analysis showed that there was a negative relationship between water temperature (Tw0) and flow of the past week (Q1), which can be explained by the effect of thermal inertia of the river (i.e. a time lag between flow and water temperature variations caused by the ability of a river to conduct heat).

In order to build the best *k*-NN model, single attributes were first tested independently. Then, the so-called best subset approach was used, i.e. all possible combinations of attributes were considered and the subset yielding the best results was selected as the final model. The *k*-NN models

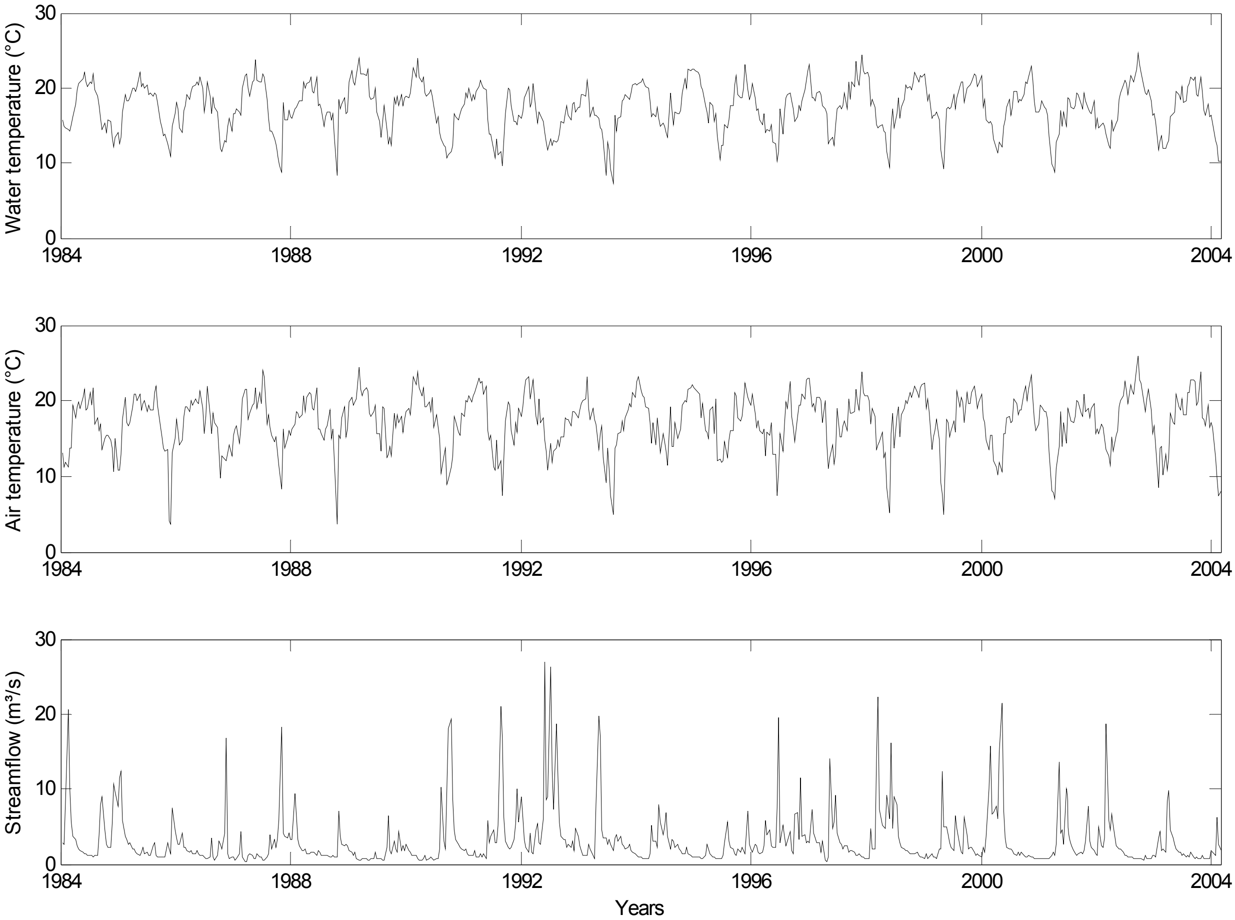

Fig. 3 Water and air temperature and streamflow data, excluding the periods December–April, collected in the Nivelle catchment from 1984 to 2004.

which included one, two, three, four and five attributes were denoted *k*-NN1, *k*-NN2, *k*-NN3, *k*-NN4 and *k*-NN5. In order to compare the performance of these models, we used the three different criteria described previously, i.e. the RMSE, Bias and NSC. Results are presented in Table 2. These results indicated that the performance associated with one attribute models (*k*-NN1) was modest. The mean values of RMSE ranged from 2.52 to 4.02°C. All attributes slightly underestimated the water temperatures, with annual mean bias values between –0.59 and –0.53°C. The interannual average NSC ranged from –0.83 to 0.27.

The performance of subsets *k*-NN2, *k*-NN3, *k*-NN4 and *k*-NN5 was also compared (Table 2). These results indicated that these models outperformed the *k*-NN1. The interannual mean values of RMSE varied between 1.20 and 2.14°C. Also, the NSC values calculated for all models were higher (>0.49) than the value reported for *k*-NN1. It can be seen from results presented in Table 2 that interannual RMSE values were similar for *k*-NN3, *k*-NN4 and *k*-NN5 (between 1.20 and 1.34°C) among which the model *k*-NN4 provided the lowest RMSE value (1.20°C). Small interannual mean bias values were observed for these models (–0.02°C < Bias < 0.01°C) and NSC values were above 0.80. The results indicated that the *k*-NN method performed well for the prediction of weekly water temperatures of the Nivelle River. The *k*-NN4 model had the best performance among the models based on the lowest RMSE and bias and the maximum NSC values. This model achieved this level of performance with Tw1, Tw2, Ta1 and Q1 as exogenous variables. These results also indicated that streamflow (Q1) can be included in the model as an independent variable, and that considering streamflow in *k*-NN models improved performance; however, the improvement was relatively weak (decrease in RMSE < 0.12°C).

Table 2 Performance measures (RMSE, Bias, NSC) of best-subset k-NN and PARX models.

Model description	Variables	RMSE (°C)		Bias (°C)		NSC	
		Mean	Range	Mean	Range	Mean	Range
k-NN1	Tw1	2.52	[2.14, 2.94]	–0.54	[–0.79, –0.24]	0.27	[–0.47, 0.60]
	Tw2	3.15	[2.67, 3.57]	–0.53	[–0.74, –0.13]	–0.12	[–0.86, 0.27]
	Ta1	2.76	[1.75, 3.81]	–0.57	[–1.10, 0.12]	0.14	[–0.71, 0.59]
	Ta4	2.85	[1.99, 3.78]	–0.56	[–0.97,–0.17]	0.08	[–0.43, 0.67]
	Q1	4.02	[2.86, 4.98]	–0.59	[–1.14, –0.17]	–0.83	[–2.48, –0.05]
Best subset of *k*-NN2	Tw1, Ta1	2.14	[1.76, 2.61]	–0.44	[–0.67, –0.16]	0.49	[0.05, 0.70]
Best subset of *k*-NN3	Tw1, Tw2, Ta1	1.31	[0.78, 1.60]	0.01	[–0.09, 0.24]	0.81	[0.64, 0.89]
Best subset of *k*-NN4	Tw1, Tw2, Ta1, Q1	1.20	[0.80, 1.50]	–0.01	[–0.19, 0.19]	0.84	[0.67, 0.90]
k-NN5	Tw1, Tw2, Ta1, Ta4, Q1	1.34	[0.94, 1.67]	–0.02	[–0.19, 0.17]	0.80	[0. 64, 0.90]
Best subset of PARX2	Tw1, Ta4	1.59	[1.19, 2.44]	–0.01	[–1.28, 1.79]	0.70	[0.04, 0.85]
Best subset of PARX3	Tw1, Tw2, Ta4	1.58	[1.19, 2.37]	–0.01	[–0.99, 1.50]	0.70	[0.12, 0.86]
Subset of PARX4	Tw1, Tw2, Ta4, Q1	1.68	[1.16, 2.76]	0.00	[–1.00, 1.38]	0.66	[–0.18, 0.88]
PARX5	Tw1, Tw2, Ta1, Ta4, Q1	1.74	[1.08, 2.98]	0.01	[–0.80, 1.39]	0.62	[–0.38, 0.90]

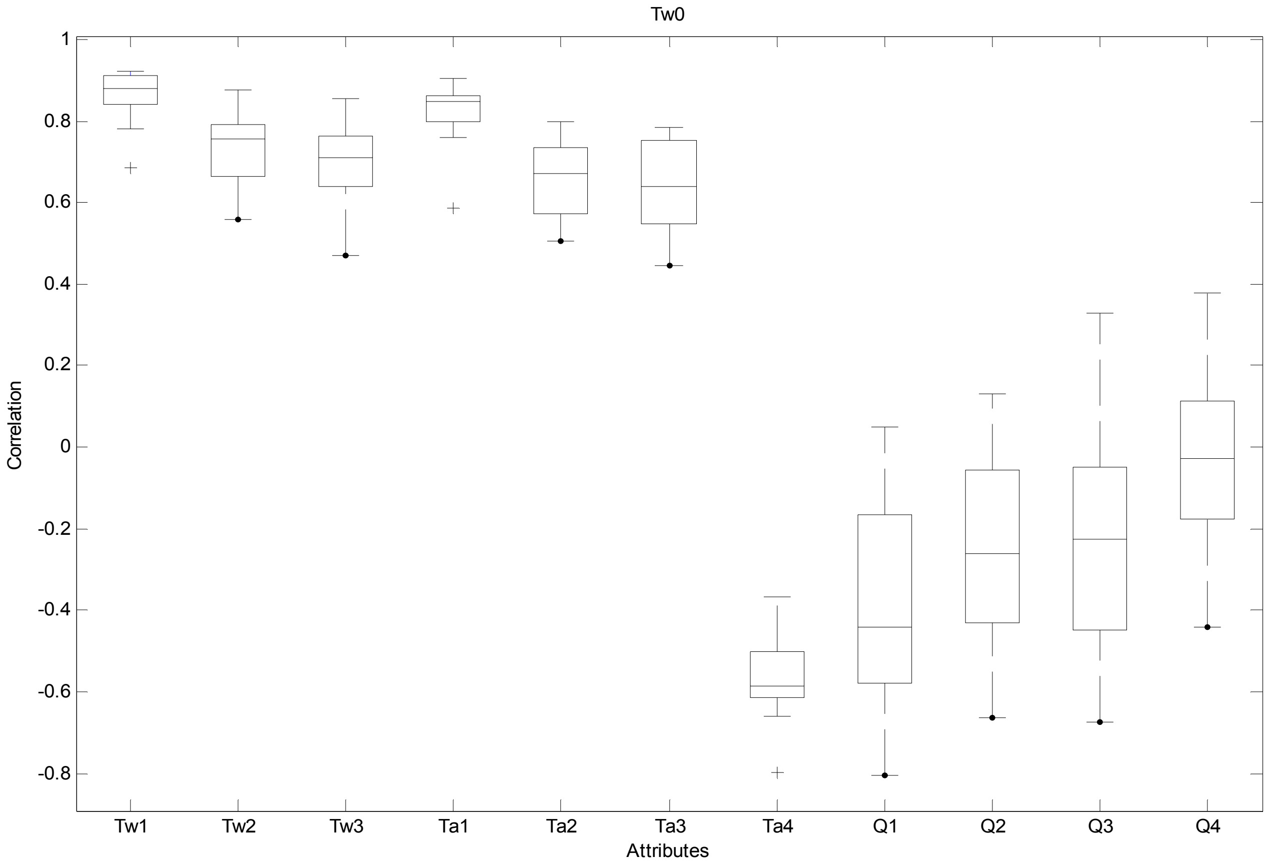

Fig. 4 Box plots showing the correlation between Tw0 and each attribute.

PARX model

The models developed in the first part of the study have excellent descriptive ability; however, they did not take into account the significant periodic autocorrelation of water temperatures. A plot of the original data, excluding December–April periods, shows the cyclic behaviour of the weekly air and water temperatures (Fig. 3). The nonstationarity of water temperatures was apparent since the mean, standard deviation and autocorrelation functions vary from week to week (Fig. 5). Therefore, considering a periodical model was deemed appropriate. Hence, in the second part of the study, the *k*-NN method was compared to the PARX model.

Before applying the PARX model, it was necessary to ensure that the original data were normally distributed. Results of the Shapiro-Wilk test with a 5% significance level revealed that the normality assumption was accepted for each period ($0.08 < p < 0.99$). Therefore, these data were not transformed.

The second part of the study was devoted to the testing and the development of PARX models that included air temperature and flow. Over 15 different variants of water temperature, air temperature flow were initially tested in the model development. However, only the subset of the most important variables (in terms of the performance obtained by the models) are shown in Table 1 and used in the final analysis to identify the best PARX models which had good descriptive ability. As in the *k*-NN method, the PARX models, which included two, three, four and five variables were denoted, respectively, PARX2, PARX3, PARX4 and PARX5. The MWMT series were broken down into 30 periods with $\tau = 1$ corresponding to the first week of May and $\tau = 30$ corresponding to the last week of November.

Results for the performance evaluation are presented in Table 2. This table indicates that all models performed well, with RMSE values between 1.58 and 1.74°C, among which the PARX3 provided the lowest value (1.58°C). All models had very similar interannual NSC means (0.62 < NSC < 0.70). The PARX models were found to have small relative mean bias (centred on 0°C). The range of annual biases were also similar for all PARX models (Table 2), among which

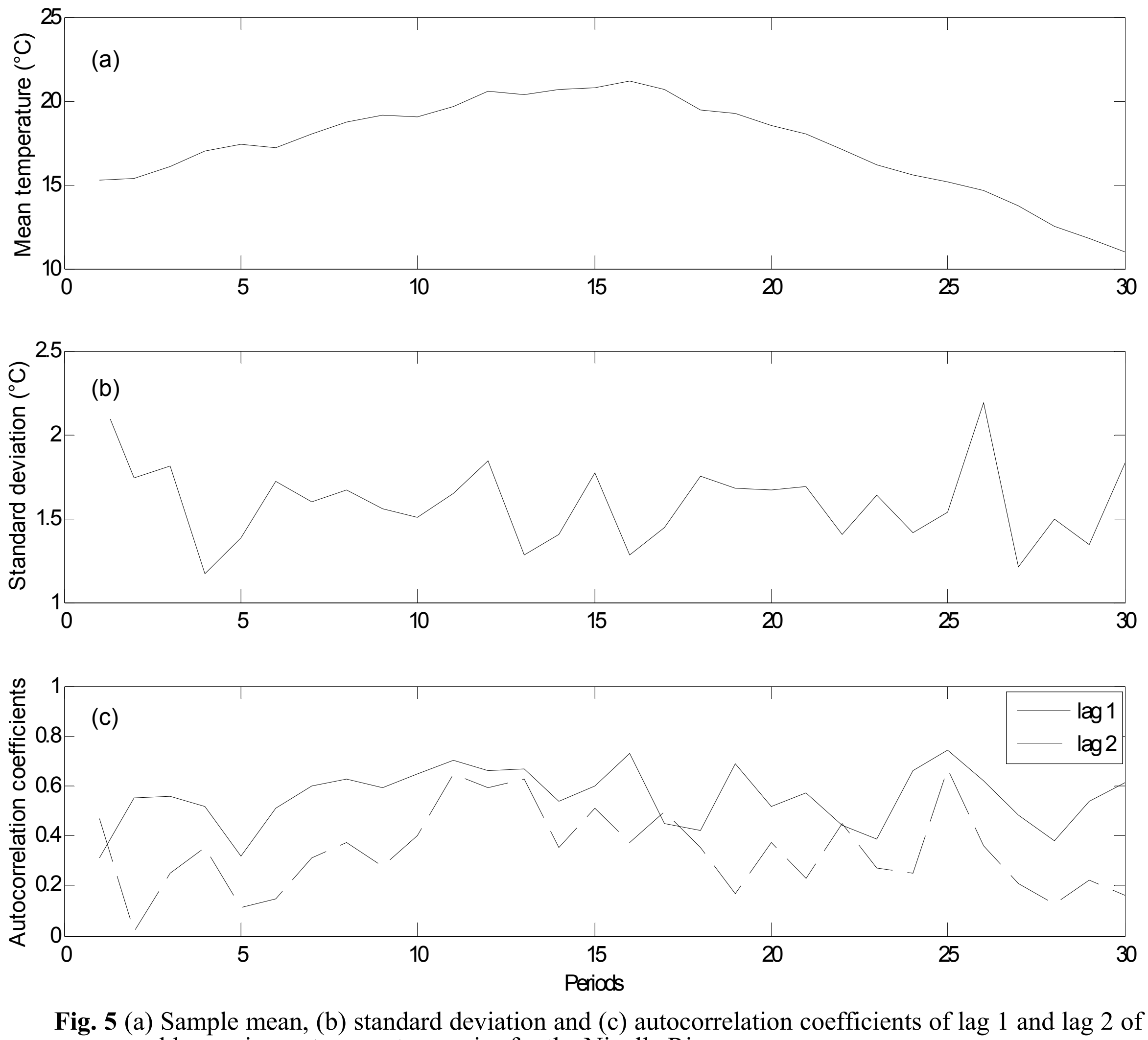

Fig. 5 (a) Sample mean, (b) standard deviation and (c) autocorrelation coefficients of lag 1 and lag 2 of mean weekly maximum temperature series for the Nivelle River.

the annual bias values of PARX3 ranged from –0.99 to 1.50°C. While the models performed comparably and the differences were minimal (≤0.16°C), the PARX3 model was selected as the best model based on minimum RMSE and maximum NSC coefficient. This level of performance was achieved with two autoregressive terms (Tw1, Tw2) and one exogenous independent variable: weekly degree days (Ta4). The PARX3 model was defined as follows:

$$\mathrm{Tw}_{\nu,\tau} = \varphi 1_{1,\tau}\,\mathrm{Tw}_{\nu,\tau-1} + \varphi 1_{2,\tau}\,\mathrm{Tw}_{\nu,\tau-2} + \varphi 2_{1,\tau}\,\mathrm{Ta4}_{\nu,\tau-1} \qquad (7)$$

and $\tau > 2$.

It should be noted that the inclusion of streamflow did not bring improvement (PARX4). As an example, parameter estimates for the validated year 2004 are displayed in Table 3. In order to illustrate the general quality of those results, Fig. 6 shows the time series of predicted values by the *k*-NN4 and PARX3 models *versus* observed water temperatures for some validation years, which had the lowest values of RMSE. It can be seen that both models were suitable to capture the seasonal variation of water temperature and provided relatively good estimates of measured values.

Table 3 Model parameters estimates for PARX3 of mean weekly maximum temperatures of the validated year 2004.

Parameters	Period (τ): 1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
$\varphi 1_{1,\tau}$	1.04	–0.34	–1.19	–0.11	0.5	–0.37	–0.04	0.17	–0.16	0.24	0.31	0.02	0.25	0.04	0.21
$\varphi 1_{2,\tau}$	–0.27	–0.21	–0.24	–0.2	0.33	0.22	–0.11	–0.16	–0.29	–0.13	–0.35	–0.1	–0.59	–0.22	–0.27
$\varphi 2_{1,\tau}$	–0.86	0.26	–0.18	–0.39	0.39	0.21	0.05	0.60	0.12	0.36	–0.13	0.17	–0.16	0.08	–0.20
	Period (τ): 16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
$\varphi 1_{1,\tau}$	0.27	–0.08	0.05	0.89	0.3	0.82	0.46	0.3	0.04	–0.3	0.28	0.21	–0.5	–0.28	0.16
$\varphi 1_{2,\tau}$	–0.37	0.1	–0.4	–0.55	–0.29	0.12	0.04	–0.05	0.23	0.04	–0.01	–0.67	–0.21	–0.12	–0.15
$\varphi 2_{1,\tau}$	–0.24	0.38	0.27	0.19	–0.27	–0.49	–0.24	–0.44	–0.37	–0.59	–0.33	0.36	–0.21	–0.19	–0.33

DISCUSSION AND CONCLUSION

This work was motivated by the need to develop a robust model to predict mean weekly maximum temperature with air temperature and streamflow as exogenous inputs. To this end, two statistical approaches were used to relate water temperature to air temperature and streamflow in the Nivelle River, in southwestern France. The first model was a non-parametric *k*-NN method which was compared to the parametric model PARX. Because of its non-parametric nature (data driven method), the *k*-NN method does not make any assumption about the underlying statistical distributions. This approach does not take into account the periodic autocorrelation in the weekly water temperature series, which is significant. Moreover, the *k*-NN method cannot be easily extrapolated outside of the temperature range encountered in the data set used to calibrate it. The PARX model can thus be seen as more appropriate. The most striking feature of the PARX model, widely used in practice, is that it preserves the periodic correlation structure in the seasonal data. However, the disadvantage of this model is the assumption that the distributions are normal; therefore, the PARX model should be applied only after a normalizing transformation of data for which density functions exhibit departures from Gaussian distributions. However, a transformation is not necessary when considering temperature time series, which seldom depart from normality.

Different variants of water temperature, air temperature and streamflow were used in model development. Box plots of correlation coefficients showed that the best attributes included lagged water temperature (lags 1 and 2 weeks) and lagged air temperature (lag 1 and weekly degree days) and streamflow (lag 1). The results (Table 2) indicated that the best models (PARX3 and *k*-NN4) require, respectively, one air temperature input (weekly degree days of air temperature) and both lagged air temperature (lag 1) and streamflow (lag 1). However, the improvement in *k*-NN performance by including the streamflow variable was modest.

A major conclusion of this first comparison, although with only one study site and relatively short time series (21 years), is that the *k*-NN method, which is a data-driven method, may provide good results in terms of RMSE, NSC and bias error. These goodness-of-fit indicators are focused on comparing observed and simulated values and do not necessarily take into account uncertainty associated with measurements. The fact that the RMSE was significantly larger than sensor accuracy implies that the uncertainty can be mostly attributed to model shortcomings and intrinsic natural uncertainty, rather than measurement errors.

It should be remembered that, for all multi-attribute *k*-NN models, the weight of the neighbours was also optimised. The result showed a substantial equivalence of the two methods, which is in agreement with the conclusion reported by Galeati (1990). However, the PARX model may be preferred, due to its good estimation of the individual weekly temperatures and its ability to capture the periodic autocorrelation of the weekly water temperature series. Once the PARX model (equation (7)) is developed for a site, it can be used to estimate future water temperatures using weekly degree days of air temperature and lagged water temperature. In so doing, it might have a greater practical interest, such as using predicted water temperatures to anticipate the health of an aquatic habitat.

Comparison of models results with those reported in other studies is limited. The comparison between a periodic autoregressive model and a so-called stochastic model (i.e. seasonal component is estimated deterministically and residuals are modelled with AR methods) had already been performed in a previous study completed on the Deschutes River (Oregon, USA) by Benyahya *et al*. (2007). This comparison was not repeated in the present study. It was shown that PAR model performance is similar to that of the stochastic approach with an average error (RMSE) less than 1°C. Recently, Koutsoyiannis *et al*. (2008) compared a parametric (periodic autoregressive) model and a non-parametric (*k*-NN and artificial neural network) model for the Nile flow prediction. They found good performance of the non-parametric model, and even better performance of the parametric model.

Each study tends to be unique in terms of model application, and there are several confounding factors, such as climate, physiographic and geomorphologic characteristics, that prevent a straightforward comparison. Nonetheless, some results found in the literature are listed here in order to provide a qualitative, first comparison of model performances.

For instance, the use of the deterministic CEQUEAU model on Catamaran Brook, Canada, yielded a RMSE of 1.8°C for a time series of daily temperatures measured between 1990 and 1995 (St-Hilaire *et al*., 2000). Most deterministic model performance values found in the literature were calculated for short simulation periods; which makes comparison even more difficult. For instance, a commonly used deterministic model, QUAL2E, was calibrated and validated on the Yakima River (Washington, USA) on a very limited data set (10 measurements). RMSE values were less than 0.5°C (Carroll & Joy, 2001). Another deterministic model, BASINTEMP (Allen *et al*., 2007) yielded RMSE values smaller than 0.5°C when used to simulate maximum weekly temperature on the South Fork Eel River (North Carolina, USA) for a period of two years. Tung *et al*. (2007) designed a deterministic model that includes a shading algorithm. They obtained RMSE values ranging between 0.33 and 0.93°C. However, their model was used at an hourly time step.

The use of the equilibrium temperature model (Caissie *et al*., 2005) on Catamaran Brook yielded an overall RMSE of 1.2°C for 8-year time series of daily temperatures. Ahmadi-Nedushan *et al*. (2007) compared air–water regression, multiple regression using air and flow as exogenous variables and the so-called stochastic approaches to simulate daily water temperature on the Moisie River for a period of six years. They obtained RMSE varying between 0.5 and 1.7°C. The Moisie River is a larger, more damped system than the Nivelle River, which may explain the somewhat better performance of some of the regression-based approaches in this case. Morill *et al*. (2005) had higher RMSE (>2.65°C) when they used the nonlinear model of Mohseni *et al*. (1998)

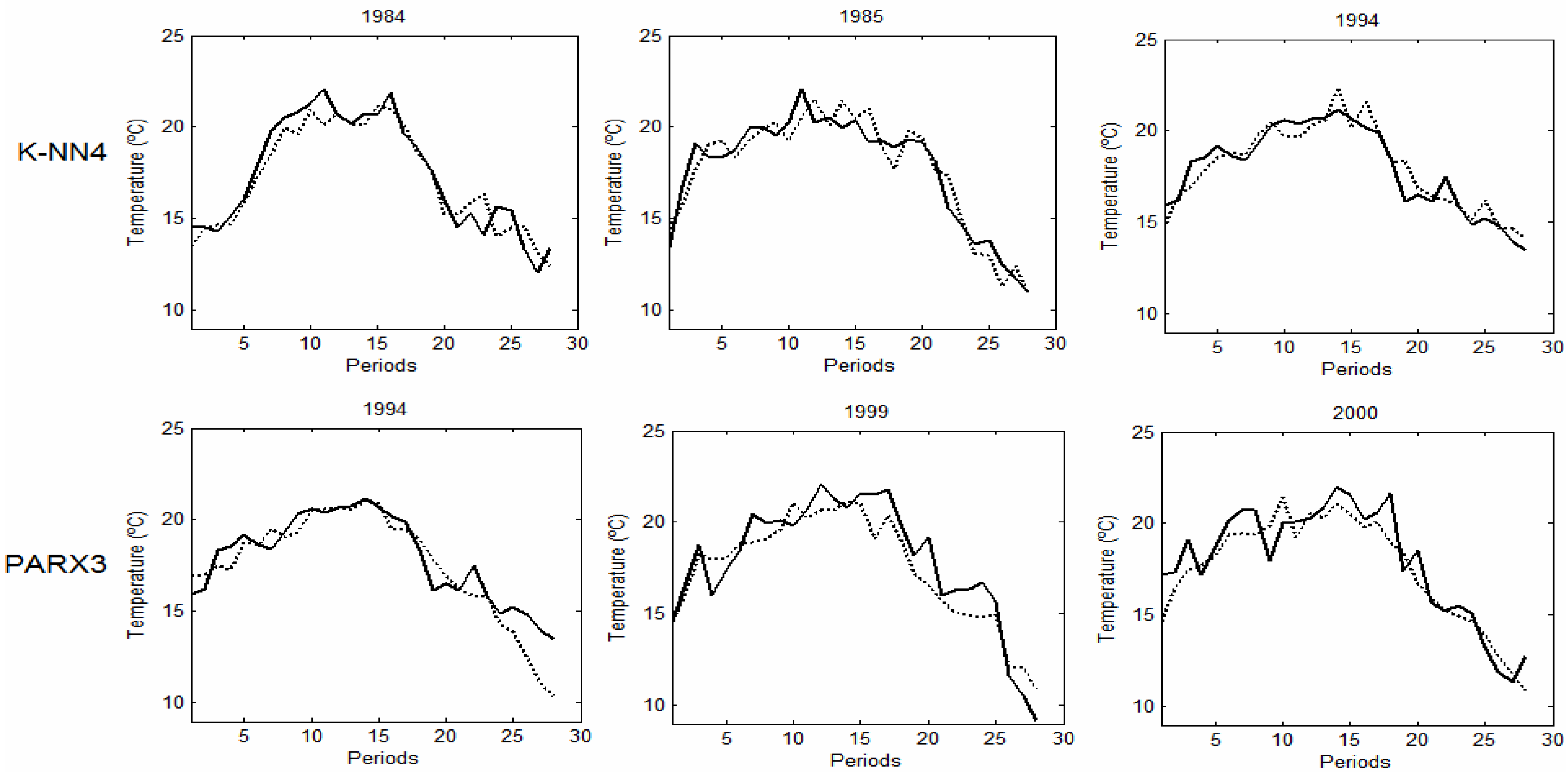

Fig. 6 Time series of observed and predicted water temperatures obtained by *k*-NN4 and PARX3 for some validation years, the solid lines represent the observations.

on different rivers and streams from different countries. It can therefore be seen that, generally, the RMSE obtained for the two models used in the present study are of the same order of magnitude as other models, when they are used to simulate the available length of time series (i.e. > 5 years).

The importance of model differences to predictions must be analysed within the scope of their potential impact on aquatic habitat management. Temperature forecasting can be of great use to identify events that may lead to thermal stress for fish and other aquatic species. Hence, the ability of the proposed models to accurately reproduce MWMT is of specific interest. No systematic bias in the estimation of MWMT by the *k*-NN or the PARX models was observed in this study (Fig. 6). This is crucial for operational use of these approaches, as a systematic underestimation of the MWMT could jeopardize managerial decision-making during periods of potential thermal stress.

Another important feature of models that use exogenous variables as inputs is the ability to include flow as predictor. This is of great importance for habitat management in regulated rivers. Models such as *k*-NN4, which include flow, can be used to test the impact of various flow management scenarios on the thermal regime. Such a feature will likely become essential for river water quality and habitat management. Flow and water temperature monitoring is becoming increasingly easier to implement with technological improvements and the decreasing cost of the monitoring equipment. Hence, multiple monitoring sites can be envisaged for a number of river systems. Managerial decisions on the allowed fishing effort, effluent regulation and water consumption can all benefit from the generation of scenarios that could be performed using these models.

In this study we used parametric and non-parametric approaches to model water temperature. There are still many methods which have been used successfully in many forecasting applications in engineering and science; however, they have not yet been fully explored in water temperature modelling. Examples include parametric approaches, such as the logistic regression for threshold exceedance (St-Hilaire *et al.*, 2006), and geostatistical models (Gardner *et al.*, 2003). Non-parametric models include artificial neural networks (Bélanger *et al.*, 2005) and regression trees (Dzeroski *et al.*, 2000). The validation presented in this study was limited to one site. To fully validate the preliminary conclusions of the present study, applications to other sites with longer time series would be useful.

Acknowledgements This paper is part of a PhD thesis completed at the National Institute of Scientific Research (INRS, University of Quebec). The research was supported by the National Sciences and Engineering Research Council of Canada (NSERC) and Hydro-Quebec.

REFERENCES

Ahmadi-Nedushan, B., St-Hilaire, A., Ouarda, T. B. M. J., Bilodeau, L., Robichaud, É., Thiémonge, N. & Bobée, B. (2007) Predicting river water temperatures using stochastic models: case study of the Moisie River (Québec, Canada). *Hydrol. Processes* **21**(1), 21–34.

Allen, D., Dietrich, W., Baker, P., Ligon, F. & Orr, B. (2007) Development of a mechanistically based, basin-scale stream temperature model: applications to cumulative effects modeling. USDA Forest Service Gen. Tech. Rep. PSW-GTR-194.

Bartholow, J. M. (1989) Stream temperature Investigations: field and analytic methods. Instream flow information. US Fish and Wildlife Service Paper no. 13.

Bartholow, J. M. (1999) SSTEMP for Windows: The Stream Segment Temperature Model (Version 1.1.3). US Geological Survey computer model and help file.

Bartolini, P., Salas, J. D. & Obeysekera, J. T. B. (1988) Multivariate periodic ARMA(1,1) processes. *Water Resour. Res.* **24**(8), 1237–1246.

Bélanger, M., El-Jabi, N., Caissie, D., Ashkar, F. & Ribi, J.-M. (2005) Estimation de la température de l'eau en rivière en utilisatn les réseaux de neuronnes et la régression linéraire multiple. *Rev. Sci. Eau* **18**(3), 403–421.

Benyahya, L., St-Hilaire, A., Ouarda, T. B. M. J., Bobée, B. & Nedushan, B. (2007) Modeling of water temperatures based on stochastic approaches: case study of Deschutes River (Oregon, USA). *J. Environ. Engng Sci*. **6**, 437–448.

Bjornn, J. R. & Reiser, G. W. (1991) Habitat requirements of salmonids in streams. Influences of forest and rangeland management in salmonid fishes and their habitats. In: Special Publication 15, 73–158. American Fisheries Society, Bethesda, Maryland, USA.

Box, G. E. P. & Jenkins, G. M. (1976) Time series analysis: forecasting and control (second revised edn). Holden-Day, San Francisco, USA.

Brown, G. W. & Krygier, J. T. (1970) Effects of clear-cutting on stream temperature. *Water Resour. Res.* **6**(4), 1133–1139.

Caissie, D. (2006) The thermal regime of rivers: a review. *Freshwater Biol*. **51**(8), 1389–1406.

Caissie, D., El-Jabi, N. & St-Hilaire, A. (1998) Stochastic modelling of water temperatures in a small stream using air to water relations. *Can. J. Civil Engng* **25**, 250–260.

Caissie, D., El-Jabi, N. & Satish, M. (2001) Modeling of maximum daily water temperatures in a small stream using air temperatures. *J. Hydrol*. **251**, 14–28.

Caissie, D., Satish M. G. & El-Jabi, N. (2005) Predicting river water temperatures using equilibrium temperature concept with application on Miramichi River catchments (New Brunswick, Canada). *Hydrol. Processes* **19**, 2137–2159.

Carroll, J. & Joy, J. (2001) USBR Columbia River pump exchange project. Potential water quality impacts on the Yakima River. Washington State Department of Ecology Publ. no. 01–03-000.

Cluis, D. (1972) Relationship between stream water temperature and ambient air temperature—a simple autoregressive model for mean daily stream water temperature fluctuations. *Nordic Hydrol*. **3**(2), 65–71.

Coutant, C. C. (1977) Compilation of temperature preference data. *J. Fish. Res. Board Can*. **34**, 739–747.

Crozier, L. & Zabel, R. W. (2006) Climate impacts at multiple scales: evidence for differential population responses in juvenile Chinook salmon. *J. Anim. Ecol*. **75**(5), 1100–1109.

Dumas, J. & Prouzet, P. (2003) Variability of demographic parameters and population dynamics of Atlantic salmon (*Salmo salar* L.) in a southwest French river. *ICES J. Mar. Sci*. **60**(2), 356–370.

Dzeroski, S., Demsar, D. & Grbovic, J. (2000) Predicting Chemical parameters of river water quality from bioindicator data. *Applied Intelligence* **13**, 7–17.

Eaton, J. G. & Sheller, R. M. (1996) Effects of climate warming on fish thermal habitat in streams of the United States. *Limnol. & Oceanogr*. **41**(5), 1109–1115.

Erickson, T. R. & Stefan, H. G. (2000) Linear air/water temperature correlations for streams during open water periods. *J. Hydrol. Engng ASCE* **5**(3), 317–321.

Galeati, G. (1990) A comparison of parametric and non-parametric methods for runoff forecasting. *Hydrol. Sci. J*. **35**(1), 79–94.

Gardner B., Sullivan P. J. & Lembo, A. J., Jr (2003) Predicting stream temperatures: geostatistical model comparison using alternative distance metrics. *Can. J. Fish. Aquat. Sci*. **60**(3), 344–351.

Gu, R., Montgomery, S. & Austin, T. (1998) Quantifying the effects of stream discharge of summer river temperature. *Hydrol. Sci. J*. **43**(6), 885–894.

Hodgson, S. & Quinn, T. P. (2002) The timing of adult sockeye salmon migration into fresh water: adaptations by populations to prevailing thermal regimes. *Can. J. Zool.* **80**(3), 542–555.

Holtby, L. B. (1988) Effects of logging on stream temperatures in Carnation Creek, British Columbia, and associated impacts on the coho salmon (*Oncorhynchus kisutch*). *Can. J. Fish. Aquat. Sci*. **45**, 502–515.

Hsia, T. J. (1977) *System Identification.* Lexington Books, Massachusetts, USA.

Janssen, P. H. M. & Heuberger, P. S. C. (1995) Calibration of process-oriented models. *Ecol. Modelling*. **83**, 55–66.

Karlsson, M. & Yakowitz, S. (1987) Nearest-neighbor methods for non-parametric rainfall–runoff forecasting. *Water Resour. Res*. **23**(7), 1300–1308.

Kothandaraman, V. (1971) Analysis of water temperature variations in large river. *J. Sanit. Engng Div. ASCE* **97**(SA1), 19–31.

Koutsoyiannis, D., Yao, H. & Georgakakos, A. (2008). Medium-range flow prediction for the Nile: a comparison of stochastic and deterministic methods. *Hydrol. Sci. J.* **53**(1), 142–164.

Lee, R. M. & Rinne, J. N. (1980) Critical thermal maxima of five trout streams in the southwestern United States. *Trans. Am. Fish. Soc*. **109**(6), 632–635.

Lund, S. G., Caissie, D., Cunjak, R. A., Vijayan, M. M. & Tufts, B. L. (2002) The effects of environmental heat stress on heat-shock mRNA and protein expression in Miramichi Atlantic salmon (*Salmo salar*) parr. *Can. J. Fish. Aquat. Sci.* **59**, 1553–1562.

Mohseni, O., Stefan, H. G. & Erickson, T. R. (1998) A nonlinear regression model for weekly stream temperatures. *Water Resour. Res*. **34**(10), 2685–2692.

Mohseni, O. & Stefan, H. G. (1999) Stream temperature/air temperature relationship: a physical interpretation. *J. Hydrol*. **218**, 128–141.

Morill, J. C., Bales, R. C. & Conklin, M. (2005) Estimating stream temperature from air temperature: implications for future water quality. *J. Environ. Engng ASCE* **131**(1), 139–146.

Morin, G., & Couillard, D. (1990) Predicting river temperatures with a hydrological model. In: *Encyclopaedia of Fluid Mechanics*, 10. Gulf Publishing Company, Hudson, Texas, USA.

Nash, J. E. & Sutcliffe, J. V. (1970) River flow forecasting through conceptual models. Part A. Discussion of principles. *J. Hydrol*. **10**, 282–290.

Neumann, D. W., Zagona, E. A. & Rajagopalan, B. (2003) A regression model for daily maximum stream temperature. *J. Environ. Engng* **129**(7), 667–674.

Novales, A. & de Frutto, R. F. (1997) Forecasting with periodic models: a comparison with time invariant coefficient models. *Int. J. Forecasting* **13**(3), 393–405.

Oliver, G. & Fidler, L. (2001) Towards a water quality guideline for temperature in the province of British Columbia. Ministry of Environment, Lands and Parks, Victoria, BC, Canada.

Osborn, D. & Smith, J. (1989) The performance of periodic autoregressive models in forecasting seasonal UK consumption. *J. Bus. Econom. Statist*. **7**(1), 117–127.

Pilgrim, J. M., Fang, X. & Stefan, H. G. (1998) Stream temperature correlations with air temperatures in Minnesota: implications for climate warming. *J. Am. Water Resour. Assoc*. **34**(5), 1109–1121.

Quenouille, M. (1949) Approximate tests of correlation in time series. *J. Roy. Statist. Soc.* B **11**, 18–84.

Salas, J. D. (1993) Analysis and modeling of hydrologic time series. Chapter 19, in: *Handbook of Hydrology* (ed. by D. R. Maidment). McGraw-Hill, New York, USA.

Shapiro, S. S. & Wilk, M. B. (1965) An analysis of variance test for normality (complete samples). *Biometrika*. **52**(3-4), 591–611.

St-Hilaire, A., Morin, G., El-Jabi, N. & Caissie, D. (2000) Water temperature modelling in a small forested stream: implication of forest canopy and soil temperature. *Can. J. Civil Engng* **27**(6), 1095–1108.

St-Hilaire, A., Morin, G., El-Jabi, N. & Caissie, D. (2003) Sensitivity analysis of a deterministic water temperature model to forest canopy and soil temperature in Catamaran Brook (New Brunswick, Canada). *Hydrol. Processes* **17**(10), 2033–2047.

St-Hilaire, A., Courtenay, S.C., Diaz-Delgado, C., Pavey, B., Ouarda, T. B. M J., Boghen, A. & Bobée, B. (2006) Suspended sediment concentrations downstream of a harvested peat bog : analysis and preliminary modelling of exceedances using logistic regression. *Can. J. Water Resour.* **31**(3), 139–156.

Stefan, H. G. & Preud'homme, E. B. (1993) Stream temperature estimation from air temperature. *Water Resour. Bull.* **29**, 27–45.

Tung, C. P., Yang, Y-C. E. & Li, M. H. (2007) Modification of a stream temperature model with Beer's law and application to Gaoshan Creek in Taiwan. *Ecol. Mod*. **200**(1-2), 217–224.

Ula, T. A. & Smadi, A. A. (1997) Periodic stationarity conditions for periodic autoregressive moving average processes as eigenvalue problems. *Water Resour. Res*. **33**(8), 1929–1934.

Vecchia, A. V. (1985) Periodic autoregressive-moving average (PARMA) modeling with applications to water resources. *Water Resour. Bull.* **21**(5), 721–730.

Webb, B. W. & Walling, D. E. (1993) Temporal variability in the impact of river regulation on thermal regime and some biological implications. *Freshwater Biol*. **29**(1), 167–182.

Webb, B. W. & Nobilis, F. (1997) A long-term perspective on the nature of the air–water temperature relationship: a case study. *Hydrol. Processes* **11**(2), 137–147.

Webb, B. W., Clack, P. D. & Walling, D. E. (2003) Water-air temperature relationships in a Devon river system and the role of flow. *Hydrol. Processes* **17**(15), 3069–3084.

Yakowitz, S., & Karlsson, M. (1987) Nearest-neighbor methods with application to rainfall/runoff prediction. In: *Stochastic Hydrology* (ed. by J. B. MacNeil & G. J. Humphries), 149–160. D. Reidel, Norwell, Massachusetts, USA.

Received 8 February 2007; accepted 18 February 2008