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IDENTIFYING DOMINANT VARIABLES FOR WATER TEMPERATURE USING A TIME SERIES MODEL

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ABSTRACT: *To estimate water temperature, models of varying complexity have been developed in terms of input data needed. All models require calibration to optimize parameters to enhance model performance. However, the paucity of measured data beyond air temperature for parameter calibration makes complicated model applications impractical. A watershed hydrological response could be determined by a dominant hydrological process. Identifying the dominant variable(s) in the hydrological process could assist in selecting an efficient model to estimate water temperature. In this study, using time-series model analysis, mean air temperature was identified as the dominant variable for water temperature. In addition, streamflow significantly influenced water temperature at higher stream orders. Due to the number of variables, the results suggest that there is not one model that can reliably estimate water temperature for all rivers, even those within the same watershed. Identifying the dominant variable(s) can direct the priority of variables collected for modeling water temperature.*

Keywords: *water temperature, ARIME time series model, dominant variable*

INTRODUCTION

River water temperature is one of the most important physical characteristics regulating water quality and the health of aquatic ecosystems (Webb et al. 2008, Caissie 2006, Coutant 1999). Increasing water temperature may decrease dissolved oxygen and increase the release of sediment-attached nutrients and chemical reactions (Hou et al. 2013). Changes in water temperature influence the distribution, abundance and growth rate of aquatic organisms because most aquatic organisms have distinct tolerable water temperate ranges (FWPCA 1967). Accurate water temperature data is critical for water resources management, particularly in the context of water quality and aquatic ecosystem sustainability.

Measured water temperature data is sparse especially in ungauged watersheds, thus modeling water temperature is necessary for the management of water resources (Risley, Roehl, and Conrads 2003). To estimate water temperature, a range of models of varying complexity have been developed. Model complexity is represented by the number of variables composing numerical equations in a model. When there are more variables involved in the model, the model is more complicated (Chien and Mackay 2014). An important question in this study is, "How many variables are needed to estimate water temperature in a given river?". Water temperature can be estimated through linear or nonlinear regression models based on air temperature for different time scales (Stefan and Preud'homme 1993, Mohseni, Stefan, and Erickson 1998, Mohseni and Stefan 1999, Webb, Clack, and Walling 2003, Webb et al. 2008). Additionally, more complicated models determining river water temperature are based on heat transfer at the air-water surface and at the streambed-water interface (Caissie, Satish, and El-Jabi 2005, Hannah et al. 2008) by incorporating watershed hydrologic data such as streamflow, surface runoff, snowmelt, and groundwater inflow (van Vliet et al. 2011, Blaen et al. 2013, Ficklin et al. 2012, Garner et al. 2014, Lowney 2000, Webb, Clack, and Walling 2003, Webb and Walling 1997). With most models, calibration is necessary to match the measurements and predictions as closely as possible by adjusting the parameters. In practice, measured watershed hydrological data support is limited. Many of the required physical properties are unobservable at the watershed scale, and these models cannot be adequately calibrated. A number of studies have focused on modeling water temperature (Ficklin et al. 2012, Brown 1969, van Vliet et al. 2011, Bogan, Stefan, and Mohseni 2004, Caissie, Satish, and El-Jabi 2005). Few of these studies have assessed whether variables embedded in these water temperature models are appropriate for predicting water temperature.

Previous studies have shown that a hydrological response can be controlled by a major or dominant (dominant afterwards) hydrological process. Instead of modeling all hydrological processes, it is more important to identify the dominant processes that control hydrological response (Woods 2002, Sivakumar 2004, Grayson and Blöschl 2000, Sivapalan et al. 2003, Sivakumar 2008). Identifying the dominant variables for water temperature can simplify water temperature models while maintaining model performance. The specific objectives of this research are: 1) to measure water temperature at two different stream orders, 2) to assess the relative importance of environmental variables controlling water temperature at different stream orders, and 3) to compare the model performance with and without the dominant variables.

METHODS

Study site

The study site is located in the upper Esopus Creek Watershed, NY and its sub-watershed, the Stony Clove Creek watershed (Figure 1). Using ArcGIS Hydrology in Figure 1, Esopus Creek (EC) and Stony Clove Creek (SCC) were classified as third- and second-order streams. The upper Esopus Creek is the main stream flowing into the Ashokan Reservoir, which provides 40% of the water supply to New York City. The confluence of SCC and EC is located at Phoenicia, NY. The Geology of the upper Esopus Creek Watershed is composed of sedimentary bedrock including sandstones, shales and conglomerate. The broken sedimentary rock is the source of stream sediment, which was deposited by glaciers during the most recent glacial advance of 12,000 – 25,000 years ago (CCEUC 2007). The main land use/land cover is forest covering over 95% of the watershed. Development associated residences, businesses, and town centers are concentrated along Route 28 and roads along the tributaries.

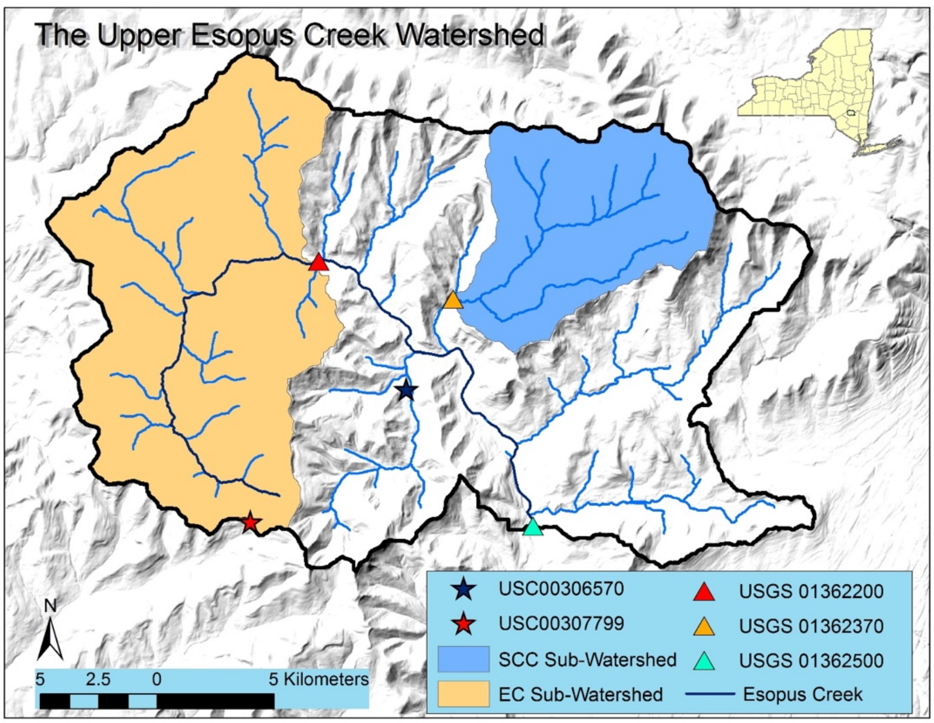

Figure 1: Map of the study area indicating the locations of the weather stations (USC00306570 and USC00307799) and USGS gauge stations. USGS 01362200 and 01362370 is located at Esopus Creek, Allaben, NY, and Stony Clove Creek, Chichester, NY, respectively. USGS 01362500 is the outlet of the upper Esopus Creek Watershed at Coldbrook, NY.

Water temperature data and environmental variables

Temperature data loggers were deployed to measure stream temperature at USGS gauge station #01362370 at SCC at Chichester, NY and #01362200 EC at Allaben, NY, with drainage areas of 80.03 km^2 and 164.98 km^2, respectively (Figure 1). Water temperatures were recorded at 15-minute intervals using HOBO temperature data loggers (±0.2 °C accuracy, Model U22-001, Onset Computer Inc., Bourne, MA, USA) from June 20, 2015 to September 30, 2016. The 15-minute interval water temperatures were aggregated into daily mean water temperatures, on which the time series analysis was based. Air temperature data loggers were placed near the two USGS gauge stations to collect maximum, minimum, and mean daily air temperatures in 15-minute intervals. Daily precipitations were download from NOAA weather stations (https://www.ncdc.noaa.gov/cdo-web/ Station ID #USC00306570 at Phoenicia, NY and #USC00307799 at Slide Mountain, NY). Daily streamflow data were available from two USGS gauge stations (Figure 1). Daily solar radiation around Phoenicia, NY from 6/20/2015 to 12/31/2015 were downloaded from National Renewable Energy Laboratory (https://maps.nrel.gov/nsrdb-viewer/). Daily solar radiation from 1/1/2016 to 9/30/2016 were not available and substituted using daily mean solar radiation averages for corresponding dates from 2011 to 2015. For validation, estimates of solar radiation from 1/1/2016 to 9/30/2016 were compared with data of the same time period of each year from 2011 to 2015 using the coefficient of determination (R^2). The R^2 were ranged from 0.60 to 0.71. Cooling degree days base 15°C (CDD_{15}) and Heating degree days base 15°C (HDD_{15}) were calculated as follows:

$$CDD_{15} = \frac{(T_{max} - T_{\min})}{2} - 15 \tag{1}$$

$$HDD_{15} = 15 - \frac{(T_{max} - T_{\min})}{2} \tag{2}$$

where T_{max} and T_{min} represent maximum and minimum air temperature, respectively. All environmental variables were presented in time series from 6/20/2015 to 9/30/2016. Additionally, all environmental variables were squared to test for nonlinear effects (Table1).

Table 1: Statistics of environmental variables from 6/20/2015 to 9/30/2016.

Daily Environmental Variables	units	Maximum	Minimum	Mean	Standard Deviation
Water temperature (T_{water}) at SCC	°C	23.28	0.01	11.96	6.89
Water temperature (T_{water}) at EC	°C	21.39	0	11.53	6.13
Maximum Air Temperature (T_{max})	°C	32.2	-12.78	17.82	9.17
Minimum Air Temperature (T_{min})	°C	23.3	-24.44	5.57	8.12
Mean Air Temperature (T_{ave})	°C	27.5	-18.33	11.7	8.4
Precipitation (P)	mm	98.81	0	3.64	10.67
Streamflow (Q) at SCC	cms	26.93	0.14	1.66	2.14
Streamflow (Q) at EC	cms	31.71	0.28	2.71	2.98
Cooling Degree Days 15 (CDD_{15})	Degree days	9.5	0	0.74	1.56
Heating Degree Days 15 (HDD_{15})	Degree days	36.33	0	7.04	7.6
Solar Radiation (SR)	Watt m^{-2}	17,220.00	618	8,452.28	3,802.28
T_{max} x T_{max}	°C^2	1036.84	0	401.53	283.54
T_{min} x T_{min}	°C^2	597.53	0	97.03	100.45
$T_{ave\ x\ Tave}$	°C^2	756.25	0	207.33	170.89
P x P	mm^2	9762.63	0	126.98	741.04
Q x Q at SCC	cms^2	725.19	0.02	7.35	37.21
Q x Q at EC	cms^2	1005.83	0.08	16.24	56.63
CDD_{15} x CDD_{15}	Degree $days^2$	90.25	0	2.97	8.78
HDD_{15} x HDD_{15}	Degree $days^2$	1320.11	0	107.31	174.41
SR x SR	(Watts $m^{-2})^2$	2.97E+08	3.82E+05	8.59E+07	6.45E+07

Analysis method for identifying dominant variables

Time series analysis methodology and techniques have been applied in water resources management for analysis and prediction of watershed hydrological responses including water quantity and quality. For example, time series analysis was used to investigate the trends and predict nitrate concentration (Worrall and Burt 1999, Worrall, Swank, and Burt 2003, Howden 2008), to forecast flow discharge (Wong et al. 2007, Wen 2009), to investigate the seasonal and long-term trends in water quality (Lehmann and Rode 2001, Bouza-Deaño, Ternero-Rodríguez, and Fernández-Espinosa 2008, Renwick et al. 2008, Bhangu and Whitfield 1997), to infer the controls on suspended sediment transfer (Hodgkins 1999). Time series analysis can articulate the importance of the predictors that have a statistically significant relationship with the dependent time series (IBMSPSS 2016). Previous researchers have employed time series analysis to identify the dominant variables for streamflow, sediment, and phosphorus (Rodriguez-Iturbe and Nordin 1968, Chien and Mackay 2014).

In this research a statistical time series model, autoregressive integrated moving average (ARIMA), was used to identify the dominant environmental variables controlling water temperature at SCC and EC. An ARIMA time series model could be expressed as ARIMA (p,d,q), which represents the order of autoregressive (p), integrated (d), and moving average (q). Differencing is needed to keep the time series stationary and the order of integrated (d) could be estimated. The orders of autoregressive (p) and moving average (q) could be identified using the autocorrelation plot (ACF) and partial autocorrelation plot (PACF), which are built in many statistical software packages like SPSS. In ARIMA a linear model is used to predict the current observations value using the previous observations (AR) and errors (MA). Water temperature and other environmental variables (Table 1) were available from 6/20/2015 to 9/30/2016. Data from 6/20/2015 to 6/19/2016 were used for ARIMA time series model development. Data from 6/20/2016 to 9/30/2016 were used for validating developed models. Our basic ARIMA model was first developed for water temperature at SCC and EC during the period 6/20/2015 - 6/19/2016. When several possible ARIMA models were available for water temperature data, the optimal ARIMA model was selected based on the root mean square error (RMSE) and Bayesian information criterion (BIC) (Fabozzi et al. 2014, Janssen and Heuberger 1995). RMSE was calculated as:

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}(P_i - O_i)^2}{n}} \tag{3}$$

where P_i is prediction, O_i is observation, and n is the number of observations in the time series. For a sample size of n observations, BIC was calculated as:

$$BIC = -2ln(\hat{\theta}) + rln(n) \tag{4}$$

where $\hat{\theta}$ is the maximum likelihood estimate of the residual variance θ; r is the number of parameters estimated in the model. The optimal ARIMA models with smaller RMSE and BIC were preferred, which suggests the model is a better fit with less parameters (Bisgaard and Murat 2011).

After the optimal ARIMA model (Model 1 in Table 2) was selected for water temperature time series, the dominant environmental variables (Table 1) for water temperature time series were selected using a stepwise regression. To select the first dominant variable, the environmental variables (Table 1) were added into the optimal ARIMA Model (Model 1) one by one. The final first dominant variable was selected with the lowest RMSE and BIC. To select the second dominant variables, the environmental variables (Table 1) were added into the optimal ARIMA mode with the first dominant variable (Model 2 in Table 2) one by one. The final second dominant variable was selected when the lower RMSE and BIC were found. The procedure was repeated to look for the third dominant variable. If the third variable was included in Model 2 and the RMSE and BIC were not lower than the those from Model 2, the third variable was not selected and there were one two dominant variables significant for water temperature time series (Chien and Mackay 2014, Trawinski and Mackay 2008).

The developed ARIMA models were validated by comparing the predictions and observations during the period 6/20/2016 to 9/30/2016. During model validation, goodness-of-fit of the models' predictive capability was assessed using RMSE and index of agreement (*d*) (Willmott,1981). *d* was calculated as:

$$d = 1 - \frac{\sum_{i=1}^{n}(P_i - O_i)^2}{\sum_{i=1}^{n}(|P_i - \bar{O}| + |O_i - \bar{O}|)^2} \tag{5}$$

where $\bar{O}$ is the mean of observations. Higher *d* suggests better fit between predictions and observations. When *d* is 1, predictions and observations are identical. All time series analyses were performed using IBM SPSS, version 23.

Table 2: ARIMA models and dominant variables for daily water temperature time series at Stony Clove Creek and Esopus Creek for time period 6/20/2015- 6/19/2016.

	Stony Clove Creek	Esopus Creek
	Daily Water Mean	Daily Water Mean
	ARIMA (2,1,0)	ARIMA (2,1,0)
Non-seasonal Lags	AR1	AR1
	AR2	AR2
	Difference 1	Difference 1
Regression Coefficients	Mean Temperature at lag 0	Mean Temperature at lag 0
		Flow lag0

RESULTS

Statistics of environmental variables

Table 1 shows the summary of statistics of water temperature and streamflow at SCC and EC and environmental variables from 6/20/2015 to 9/30/2016. The maximum, minimum, and mean water temperatures were 23.28°C, 0.01°C, and 11.96°C, respectively, at SCC and 21.39°C, 0.00°C, and 11.53°C, respectively, at EC. The daily maximum, minimum, and mean air temperatures were 17.82°C, 5.57°C, and 11.70°C, respectively. Figure 2 shows the time series of daily mean water temperature and mean air temperature and temperature range. Generally, water temperature had similar trends with air temperature (Figure 2). Both water temperature and air temperature data showed seasonality. In both SCC and EC, the average high water temperature in summer (June, July, and August) was 18.78°C. The average air temperature in summer was a little higher than water temperature at 19.77°C and the highest monthly air temperature was measured 20.21°C on July 2016. Water temperature and air temperature were colder in winter (December, January, and February) in comparison to other seasons (Figure 2). The average water temperature in winter was 2.97°C at both SCC and EC. The average air temperature was relatively lower as 0.54°C in winter and the lowest monthly air temperature was observed for January at -2.91°C (Figure 2).

The daily mean streamflow was 1.66 cms at SCC and 2.71 cms at EC. The mean of precipitation, cooling degree days, heating degree days, and solar radiation were 3.64 mm, 0.74 (degree days), 7.04 (degree days), 8452 (Watts m^{-2}). The analysis of the daily solar radiation from 06/20 to 09/30 between 2015 and 2016 showed that the mean, maximum, and minimum of 2015 (2016) were 11046 (10723), 17220 (16189), and 2838 (5291), respectively.

The dominant variables for daily water temperature

The basic ARIMA model for daily water temperature from 06/20/2015 to 06/19/2016 at both SCC and EC were (2, 1, 0), which had 2 autoregressive and 1 difference, both in non-seasonal lags (Table 2). The common dominant variables for daily water temperature at SCC and at EC were mean air temperature at lag 0 (Tave_lag0) during the calibration period. Additionally, Streamflow at lag 0 (Flow_lag0) was the second dominant variable for daily water temperature time series at ECC (Table 2). The RMSE and BIC of the basic ARIMA water temperature time series model at SCC were 0.96 and 0.06, respectively. With predictor, Tave_lag0, added in the ARIMA time series model, the RMSE and BIC were improved to 0.84 and -3.11, respectively (Table 3). With Tave_lag0 added into basic ARIMA model for water temperature time series at EC, the RMSE and BIC were improved to 0.77 and -0.48 from 0.92 and -0.14, respectively. The RMSE and BIC were further improved to 0.76 and -0.49 when the environmental variable, flow_lag0, was added in the ARIMA model (Table 3).

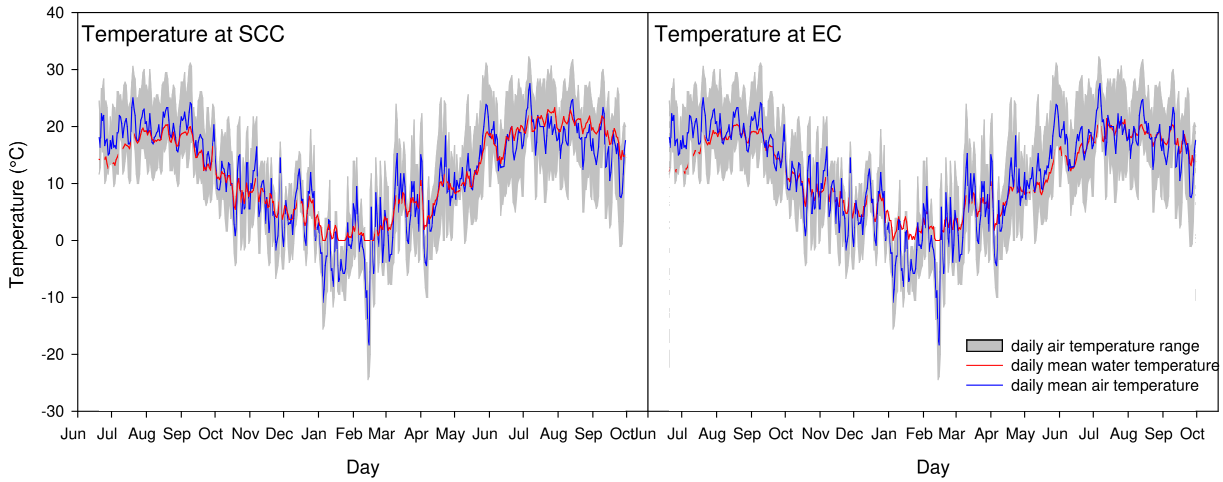

Figure 2: The time series of daily mean water temperature (blue line), daily mean air temperature (red line), and daily temperature range (grey area, daily maximum temperature – daily minimum temperature) from 6/20/2015 to 9/30/2016.

Table 3: Daily mean water temperature ARIMA time series diagnostics from 6/20/2015 to 06/19/2016 at SCC (a) and EC (b).

		June 20, 2015-June 19, 2016	
	Predictor added	RMSE	BIC
Daily mean water temperature at SCC			
Model 1	No	0.96	0.06
Model 2	Tave_lag0	0.84	-3.11
Daily mean water temperature at EC			
Model 1	No	0.92	-0.14
Model 2	Tave_lag0	0.77	-0.48
Model 3	Tave_lag0, flow_lag0	0.76	-0.49

SCC, Stony Clove Creek; EC, Esopus Creek.

Prediction with dominant variables

Figure 3 shows the forecasting validation of daily mean water temperature at SCC and EC from 6/20/2016 to 9/30/2016. Generally, the ARIMA time series model developed during the calibration period without a predictor can accurately represent the observed daily mean water temperature at both SCC and EC, but the predictions average a one-day lag. With the predictors added in the developed ARIMA time series model, the delay problem was improved. For example, predicted water temperatures using ARIMA time series models with predictors better match the observations during September and August at SCC and EC, respectively. Figure 3 shows the measured and predicted water temperature time series from 6/20/2016 to 9/30/2016 and the goodness-of -fit measures using *d* and RMSE. With predictors added to daily mean water temperature ARIMA time series at SCC and EC, the predicted water temperature time series can better catch the fluctuations of observations (Figure 3). The improvement was reflected in the *d* and RMSE, which was increased to 0.96 (from 0.95) and reduced to 0.70 (from 0.81) at SCC. The *d* (RMSE) was improved to 0.95 (0.74) from 0.93 (0.92) after the predictors were included in the developed ARIMA mode for water temperature time series at EC.

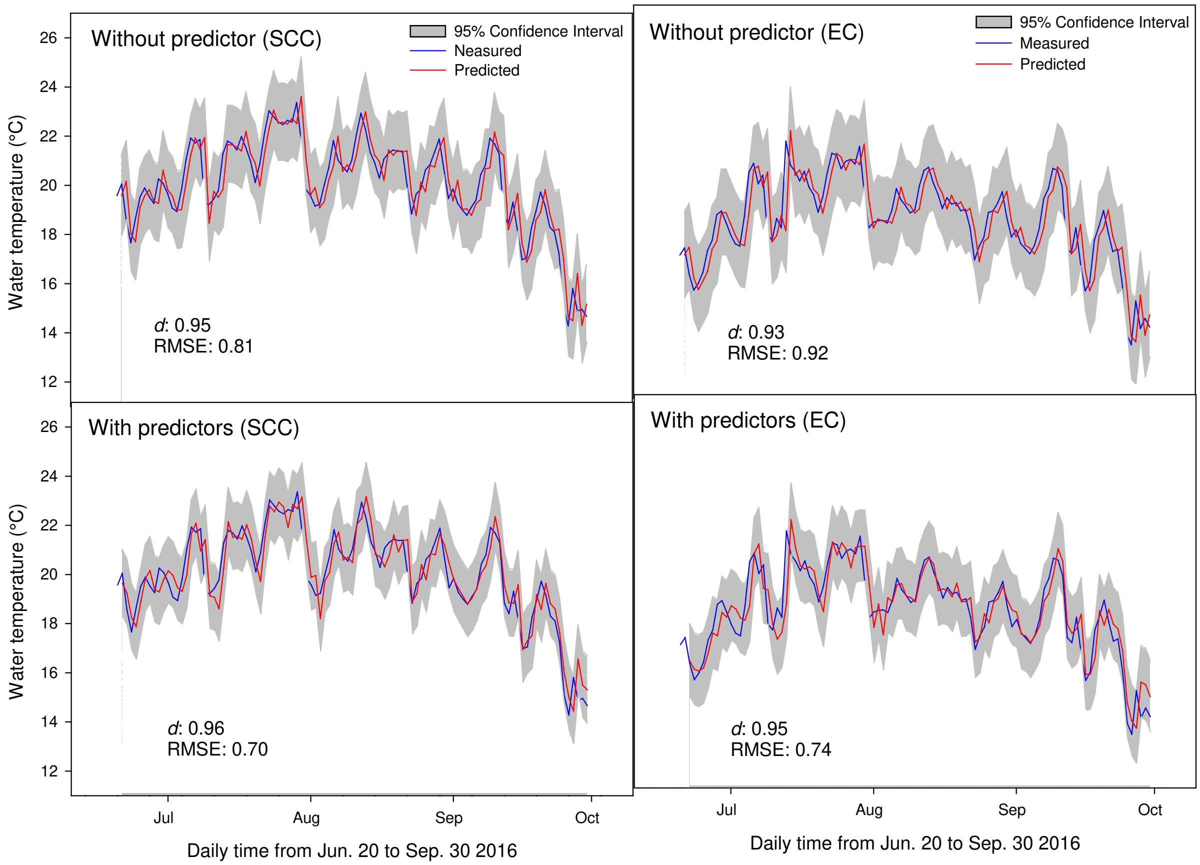

Figure 3: Model forecasting for daily mean water temperature ARIMA time series model at SCC and EC without and with predictors. Predictors at SCC includes Tave_lag0. Predictors at EC includes Tave_lag0 and Flow_lag0. Grey area is 95% confidence intervals.

DISCUSSION

Our results show that the basic ARIMA model for daily water temperature from 06/20/2015 to 06/19/2016 at both SCC and EC were (2, 1, 0), which suggests the original daily water temperature time series is not stationary in terms of mean and variance during the calibration period and one order of difference was necessary. Two orders of autoregressive means water temperature in previous 2 days significantly influence the current water temperature. The result implies the existence of memory in water temperature, which is very common in water quality data (Arya and Zhang 2015).

For daily water temperature at both SCC and EC, mean air temperature (Tave_lag0) was a significant environmental variable. The result was consistent with previous studies in which linear or nonlinear regression models relied solely on mean air temperature to predict water temperatures (Crisp and Howson 1982, Mohseni, Stefan, and Erickson 1998, Stefan and Preud'homme 1993). Mean air temperature is still important to predict water temperature in models incorporated with watershed hydrology (Ficklin et al. 2012). Air temperature was a dominant variable for modeling water temperature because the net heat exchange in streams can be approximated by adjacent air temperature (Smith 1981). This study was based on daily time series data, which suggested air temperature was significant on a daily time scale. Previous studies showed that the air-water temperature correlation has been effectively used at different temporal scales including daily, weekly, and monthly (Stefan and Preud'homme 1993, Mohseni, Stefan, and Erickson 1998, Webb, Clack, and Walling 2003, Webb et al. 2008, Pilgrim, Fang, and Stefan 1998, Erickson and Stefan 2000). No time lags of air temperature were found for water temperature time series at both SCC and EC. Time lag is caused by the delayed response of water temperature to the changed air temperature because of larger heat capacity of water. Time lag between air and water temperatures could increase with increasing streamflow and river depth (Neitsch et al. 2011, Stefan and Preud'homme 1993). Our results suggest that the time required to complete net heat exchange between air-water is less than a day at SCC and EC.

Streamflow is another significant variable for water temperature time series at EC, but not at SCC (Table 2). Streamflow is an important variable influencing water temperature. Increasing streamflow (more volume of water) may increase thermal capacity and cool water temperature through mixing water from different sources (Caissie 2006, van Vliet et al. 2011). Annual average streamflow from 1998 to 2016 is 4.80 cms and 2.78 cms at EC and SCC, respectively. With a larger drainage area at EC (164.98 km^2), more tributaries from high elevations in the Catskill Mountains (21 peaks higher than 3,000 feet above sea level) could contribute streamflow to cool down water temperature at EC, which suggests streamflow becoming more important with increasing area of watersheds. The results also imply that there should be different dominant variables at different watershed scales. Our results suggest that the impacts of streamflow on water temperatures should be incorporated to provide more accurate estimations of water temperatures at larger watershed scales (van Vliet et al. 2011).

During the process of selecting dominant variables, we found both maximum and minimum daily air temperature were significant to water temperature. However, maximum and minimum air temperature were not selected as dominant variables for water temperature at SCC and EC because both were serially correlated with mean air temperature. Additionally, the objective of this research focused on daily mean water temperature instead of daily maximum water temperature. Dominant variable may be changed to maximum air temperature from mean air temperature when the maximum water temperature was modeling (Mohseni, Stefan, and Erickson 1998, Caissie, El-Jabi, and Satish 2001). Using both maximum and minimum air temperature, the model complexity increased but the model performance did not significantly improve. This suggests water temperature models could be as parsimonious as possible to use just the dominant variables.

The dominant variables for water temperature found in the study is useful for agencies engaged in monitoring water quality and stream health. Due to the high expense of installing water temperature data loggers, models are important tools to estimate water temperature especially in ungauged watersheds (Risley, Roehl, and Conrads 2003). It is also labor intensive to collect all the input variables needed for physical water temperature. Under limited budgets, this study can direct the priority of variables collected for water temperature models.

CONCLUSIONS

Water temperatures were measured at SCC and EC located in the upper Esopus Creek watershed, NY. Different dominant variables were selected for the water temperature time series at SCC and EC using ARIMA time series model. The dominant variable represents the main hydrological process regulating water temperatures. In additional to mean air temperature, streamflow also influenced water temperature at EC. This suggests that researchers or decision makers should be cautious when applying a water temperature model for estimating water temperature at different stream orders even in the same watershed. Watershed heterogeneity and area may change the dominant variables and one model may not fit all streams to estimate water temperatures.

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