

Supplementary Material

Machine Learning Models for Prediction of Shade-affected Stream Temperatures

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Introduction

This supplementary material complements the manuscript titled "Machine Learning Models for Prediction of Shade-affected Stream Temperatures." The study assesses the selection of predictor variables for machine learning (ML) models predicting stream temperatures influenced by riparian shading. It explores two model development scenarios: *Forecasting ML Models* for predicting shade-affected stream temperatures at monitored locations and *Interpolation ML Models* for predicting at unmonitored locations using data from nearby monitored gauges. This document is organized into three appendices. Appendix 1 illustrates the categorization of predictor variables utilized in the study. Appendix 2 outlines the process of computing the "shade factor," incorporating key variables, diagrams, equations, and results. Appendix 3 provides in-depth tables and figures, offering detailed insights into specific aspects of the research results.

Supplementary material Appendix 1

1. Categorization of predictor variables

Table S1: Variables categorized into four classes—weather, stream & watershed characteristics, seasonality, and site-location characteristics—corresponding to each component of the mass and energy transfer process.

Class of variable	Sub-class	Mass transfer				Energy transfer		
		Surface flow	Lateral flow	Goundwater	Snow flow	Shortwave radiation	Longwave radiation	Evaporation & conduction
Weather		Precipitation	Precipitation	Precipitation	Max air temp	Solar radiation	Air temperature	Air temperature
		Air temperature	Air temperature	Groundwater temp.	Humidity		Humidity	Wind speed
		Streamflow*			Wind speed			
					Solar radiation			
Stream & watershed characteristics	Watershed	Drainage area	Drainage area		% Snow area			
			slope					
	Stream	Length (stream)	Length slope			Stream aspect		
		Slope				Channel width		
		n Manning channel				water depth		
		Sinuosity						
	Land cover	Land cover				Riparian vegetation		
		n Manning overland				(Tree height)		
	Soil	Hydrologic group	Hydrologic group	Baseflow recession				
			Available water storage	Drainage class				
			Drainage class	Available water storage				
Seasonality	Year				Day of the year	Day of the year		
Site location					Maritime location			
					Latitude	Latitude		
					Longitude	Longitude		
					Elevation			

Supplementary material Appendix 2

2. Shade factor modeling

2.1. Shade factor approach

The shade factor was calculated as the ratio of blocked solar radiation (due to topography and riparian vegetation) to potential solar radiation that would reach the stream surface. Key variables in the equations are outlined below.

Solar angle and solar azimuth

The solar angle is measured between the observer's horizon and the sun. It is a function of the stream latitude, declination of the sun, and the time of the day.

$$\alpha = \sin^{-1}(\sin \phi \sin \delta + \cos \phi \cos \delta \cos \tau) \quad (\text{S1})$$

$$\delta = 23.45 \left(\frac{2\pi}{360} \right) \cos \left(\frac{2\pi(172-JD)}{365} \right) \quad (\text{S2})$$

$$\tau = (180 - \text{long} - t_m - (360 \text{ hr}/24)) (2\pi/360) \quad (\text{S3})$$

Where: α is the solar altitude (solar angle), ϕ is the stream latitude, δ is the declination of the sun, τ is the local hour angle of the sun, JD is the Julian day (1-365), long is the stream longitude, t_m is the local time zone meridian (degrees), and hr is the hour of the day. These equations are explained in depth by Boyd (Boyd 2003).

The solar azimuth is the angle formed by the north and the horizontal projection of the sun (on the observer's horizon) measured clockwise.

$$\text{Sun}_{az} = \cos^{-1} \left(\frac{\sin \delta - \sin \alpha \cdot \sin \phi}{\cos \alpha \cdot \cos \phi} \right) \quad (\text{S4})$$

Stream azimuths were measured from the north to the stream center line in the flow direction.

Sub daily solar radiation

Solar radiation for sub-daily time scales was obtained using the Kaplanis approach (Kaplanis, 2006; Khatib & Elmenreich, 2015). This approach proposes solar radiation at any time as a cosine function limited by the sunrise and sunset and conditioned to the day.

$$h_{ij} = a \cdot n_j + b \cdot n_j \cos \left(\frac{2\pi t_{ss}}{24} \right) \quad (\text{S5})$$

Where h_{ij} is the solar radiation at any time within the day, t_i is the time in hours, n_j is the Julian day, and a and b are coefficients determined for any site and any day. The sub-daily solar radiation was determined for time intervals of 0.01 hours and accumulated during the day (from sunrise to sunset).

Shadow over the stream

The length of the shadow (L_{az}) (either by riparian or the topography) parallel to the solar azimuth, and length of the shadow normal to the streamflow are obtained by geometry (**Figure S1**).

$$L_{az} = \frac{h_{tree}}{\tan(\alpha)} \quad (S6)$$

$$L_n = L_{az} \cdot \sin(\text{sun}_{az} - \text{strm}_{az}) \quad (S7)$$

Where h_{tree} is the tree height in riparian vegetation, α is the solar angle, sun_{az} is the solar azimuth, and strm_{az} is the stream azimuth.

The normal shadow was then multiplied by the stream length. Thus, three shading scenarios on the stream can be observed: no shadow over the stream, partial shadow over the stream, and full shadow over the stream. In this calculation, the shade factor corresponding to the topography, left bank and right bank (defined in the direction of flow) has been identified and then calculated separately. The sum of these three components was the total SF at the control station.

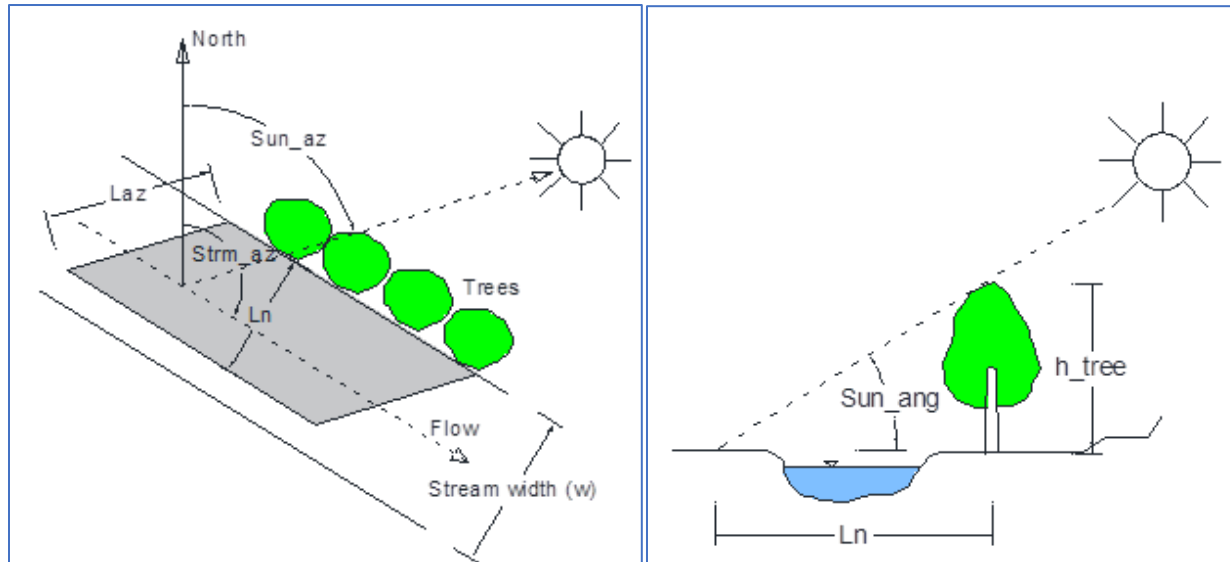
$$\text{Shade} = \text{Strm}_{length} \cdot L_n \quad (S8)$$

Finally, the shade factor for each day and each station was obtained by dividing the accumulated amount of blocked solar radiation by the potential solar radiation representing the solar heat flux (both diffuse and direct beam) that would reach the stream surface without barriers.

$$SF_{ijk} = \frac{\sum_{k=t_{sr}}^{t_{ss}} \text{Shade}_{ijk} \cdot h_{ijk}}{L_j \cdot W_j \cdot H_{ijk}} \quad (S9)$$

Where i indicates the station or sub-basin, j is the day in the year (from 1 to 365), k is the time in the day, Shade_{ijk} is the shade of the barrier on stream, h_{ijk} is the solar radiation at the time k , L_j is the stream length, W_j is the surface water width determined by the no linear equation suggested by Allen et al. (Allen et al., 1994), H_{ijk} is the registered daily solar radiation.

Figure S1. Diagram showing the variables used to calculate the length of the shadow parallel to the azimuth (L_{az}) and perpendicular to the streamline (L_n).

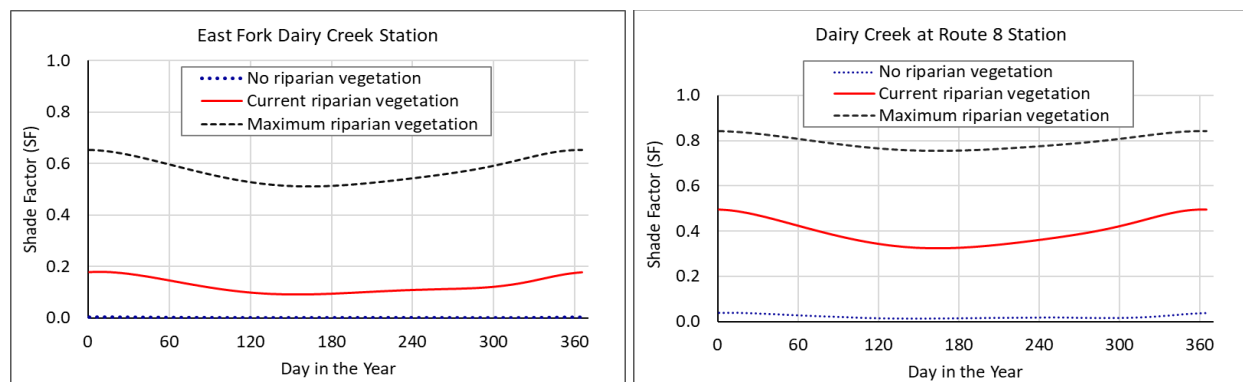


This calculation process was developed in the Python environment, which is available at https://github.com/noayarae/SF_model.git.

2.2. Shade factor results

In all three scenarios (No-riparian, current-riparian, and full-riparian vegetation), shade factors show similar patterns over the year with slightly higher SF values in winter than in summer. Shade factors in the non-riparian vegetation scenario are practically zero. Shade factors in the full riparian vegetation scenario are greater than the SFs in the current scenario (**Figure S2**).

Figure S2: Annual shade factor variations for (a) East Fork Dairy Creek station (left) and (b) Dairy Creek at Route 8 station (right), considering three riparian vegetation scenarios: No riparian, current riparian, and maximum riparian vegetation.



Supplementary material Appendix 3

Table S2. Top five models in best subset selection for EFDC and DCR8 stations across three ML models. Models with four predictors share common predictors, though not always in the same order.

# variables	XGB - ML model	MLP - ML model	CNN - ML model
East Fork Dairy Creek Station			
1	Ta	Ta	Ta
2	Ta, SF	Ta, flow	Ta, DY
3	Ta, SF, flow	Ta, flow, SF	Ta, DY, flow
4	Ta, SF, flow, DY	Ta, flow, SF, DY	Ta, DY, flow, SF
5	Ta, SF, flow, DY, pp	Ta, flow, SF, DY, SR	Ta, DY, flow, SF, pp
Dairy Creek at Route 8 Station			
1	Ta	Ta	Ta
2	Ta, SF	Ta, DY	Ta, DY
3	Ta, SF, DY	Ta, DY, SF	Ta, DY, SF
4	Ta, SF, DY, flow	Ta, DY, SF, flow	Ta, DY, SF, flow
5	Ta, SF, DY, flow, SR	Ta, DY, SF, flow, SR	Ta, DY, SF, flow, SR

Table S3. Variables included in the 6-predictor Interpolation ML Model.

# variables	Set of predictors
1	Ta
2	Ta, W_elev
	Ta, S_elev
	Ta, hg_cd
	Ta, SR
	Ta, DY
3	Ta, SR, W_elev
	Ta, SR, hg_cd
	Ta, DY, W_elev
	Ta, W_elev, SR
	Ta, hg_cd, SR
4	Ta, SR, hg_cd, W_elev
	Ta, SR, hg_cd, str_wd
	Ta, S_elev, RH, W_elev
	Ta, S_elev, RH, str_wd
	Ta, SR, W_elev, str_wd
5	Ta, SR, hg_cd, W_elev, DY
	Ta, S_elev, RH, W_elev, str_wd
	Ta, SR, hg_cd, W_elev, hg_b
	Ta, SR, hg_cd, W_elev, dc_3
	Ta, SR, hg_cd, W_elev, aws_150
6	Ta, SR, hg_cd, W_elev, DY, RH
	Ta, SR, hg_cd, W_elev, DY, W_area
	Ta, SR, hg_cd, W_elev, DY, W_slp
	Ta, SR, hg_cd, W_elev, DY, str_len
	Ta, SR, hg_cd, W_elev, DY, str_wd

Table S4: Variables featured in models with six predictors and their frequency of appearance.

Variable	Variable code	# of times in the model	Type of data
Air temperature	Ta	26	Weather data
Watershed elevation	W_elev	17	Stream/watershed feature
Solar Radiation	SR	17	Weather data
hydrological soil group C/D	hg_cd	14	Soil data
Day in the Year	DY	8	Seasonality
Stream width	str_wd	5	Stream/watershed feature
Site elevation	S_elev	4	Site-location feature
Relative Humidity	RH	4	Weather data
hydrological soil group B	hg_b	1	Soil data
Somewhat poorly drained soil	dc_3	1	Soil data
Available water storage	aws_150	1	Soil data
Watershed area	W_area	1	Stream/watershed feature
Watershed slope	W_slp	1	Stream/watershed feature
Stream length	str_len	1	Stream/watershed feature

Table S5: Categories of variables in six-predictor models, along with their respective frequencies.

Type of variable	# of times in the model
Weather data	21
Stream/watershed features	25
Soil data	17
Seasonality	8
Site-location features	4

Figure S3: DMW map displaying RMSE values achieved by the optimal Interpolation ML model with six predictors.

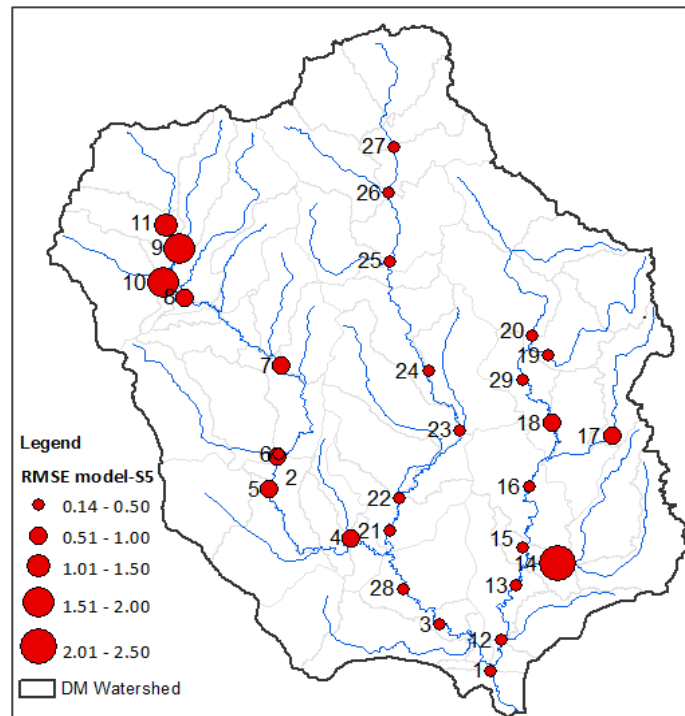


Figure S4: Validation of stream temperature forecasting at East Fork Dairy Creek (top) and Dairy Creek at Route 8 (bottom) stations.

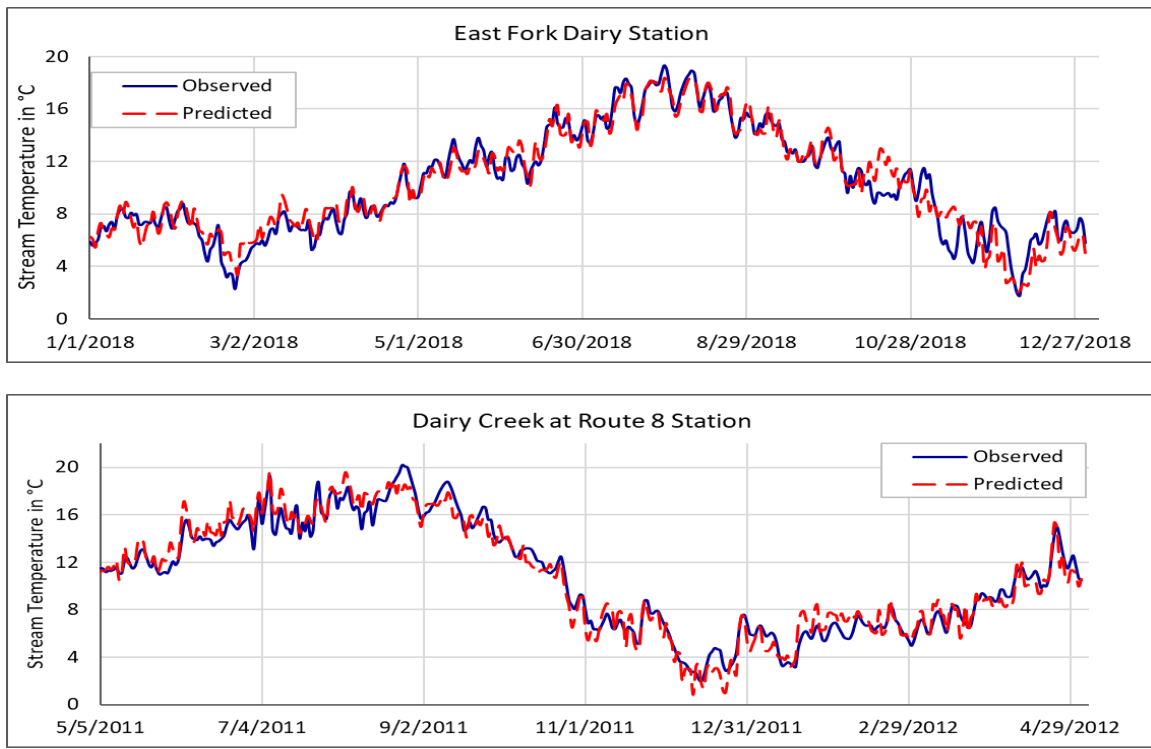
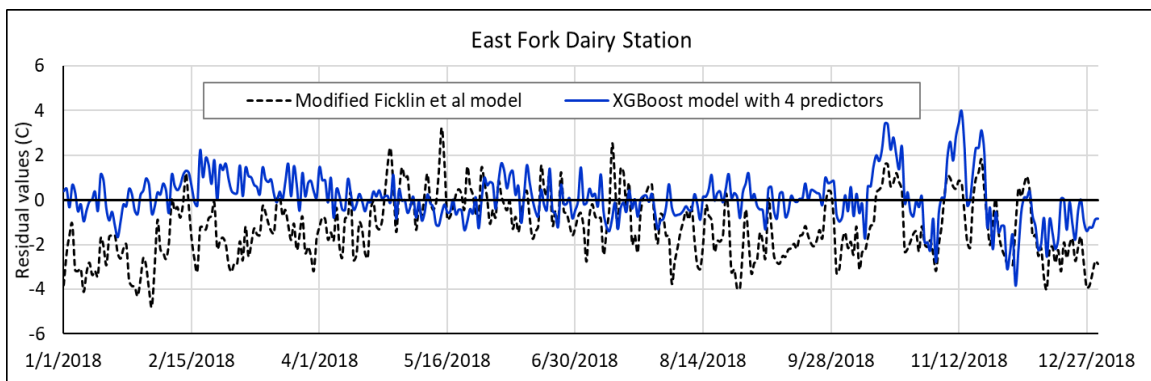


Figure S5: Residual stream temperature comparison between the XGB model with four predictors and the modified Ficklin et al. model at East Fork Dairy station (top) and Dairy Creek Route 8 station (bottom).



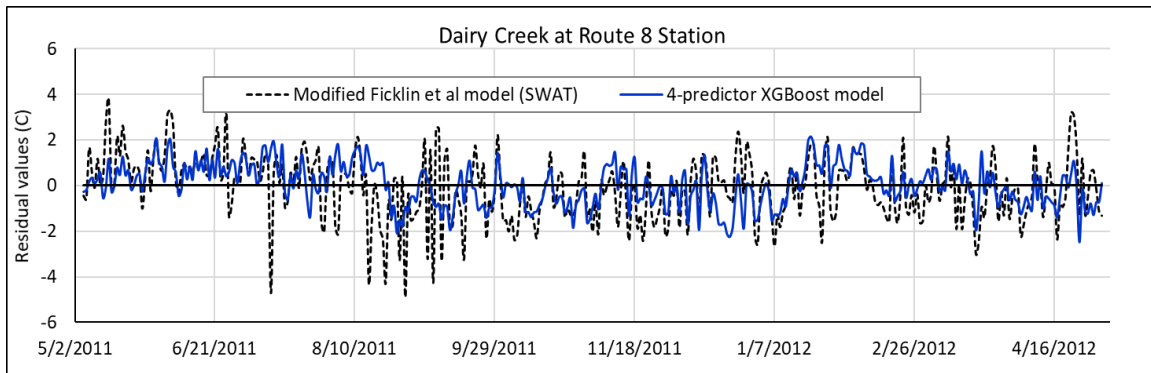


Figure S6. Predicted stream temperature for EFDC (top) and DCR8 (bottom) stations in summer validation, comparing different riparian conditions. Observed temperature shown as dashed line.

