An Application of Neural Networks to Improve Water Quality Forecasting in the Colorado-Big Thompson Project

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Abstract

The Bureau of Reclamation (Reclamation) manages the Colorado-Big Thompson Project (C-BT), which collects water in the headwaters of the Colorado River on the Western Slope of the Continental Divide and delivers it to the Big Thompson River on the Eastern Slope. Water primarily originates as snowmelt in Rocky Mountain National Park and Grand County, before flowing from Grand Lake through Shadow Mountain Reservoir and into Granby Reservoir, a group of water bodies collectively referred to as the Three Lakes. Water is primarily stored in Granby Reservoir, with additional inputs pumped from nearby Willow Creek and Windy Gap Reservoirs. To meet demands, the flow direction is reversed when the Farr Pump Plant lifts water to the Granby Pump Canal into Shadow Mountain Reservoir and the connected Grand Lake. The Alva B. Adams Tunnel carries water from Grand Lake to the Eastern Slope.

The unique interconnection and characteristics of the Three Lakes creates a complex physical, chemical, and biological system that ultimately controls the water quality in Grand Lake. Further, water quality predictions are needed to understand how operational alternatives and future summer weather conditions will impact the system. Historically, water quality in Grand Lake was monitored by measuring Secchi depth, or simply the depth below the water surface at which a Secchi disk is no longer visible. Secchi depth is a measure of the clarity of the water but is influenced by optical properties, dissolved constituents, and total suspended solids (TSS) including inorganic suspended sediment (ISS), particulate organic matter (POM), and algae.

An improved approach to estimating Secchi depth should consist of multiple operations extending from an initial water quality model – clustering, bias correction, and regression – to account for the stochastic nature of the system and uncertainty within estimation. Each of these operations builds upon the previous step to maximize the predictive skill. While these operations can be implemented separately within traditional regression-based approaches to achieve reasonable results, neural networks (NNs) can simultaneously handle all three operations within a single architecture to produce a more user-friendly product with potentially greater accuracy. This work describes the process for calibrating the initial water quality model and using the predicted water quality values from it as inputs to a NN which was constructed and trained to improve Secchi depth estimates within the C-BT.

Introduction

In the early 2000s, local interest in preserving the water quality in Grand Lake resulted in the development of a spreadsheet-based Three Lakes Water Quality Model. The Three Lakes region and model domain is shown in Figure 1. Hydros Consulting Inc. (Hydros) migrated this model to the CE-QUAL-W2 (W2) modeling platform, using version 4.0 (Cole and Wells, 2015) with custom modifications, ultimately resulting in the Three Lakes Water Quality Model v1.1

(3LWQM v1.1). The model documentation provides additional information on the background and development of the 3LWQM v1.1 (Hydros 2017). ECAO contracted with the Technical Service Center (TSC) to support updates resulting from external peer review of the 3LWQM v1.1 for its use in the Grand Lake Clarity National Environmental Policy Act (NEPA) process. This work summarizes the revisions to the 3LWQM v1.1 and re-calibration, resulting in a version of the model referred to in this document as the 3LWQM-TSC v1.0, the ultimate intent of which was to inform alternative comparison and management of the system to a water quality criterion defined by water clarity as measured by Secchi depth (Reclamation, 2021). As part of the effort, the TSC formulated a neural network-based approach to estimate Secchi performance from the model, described in the present work.

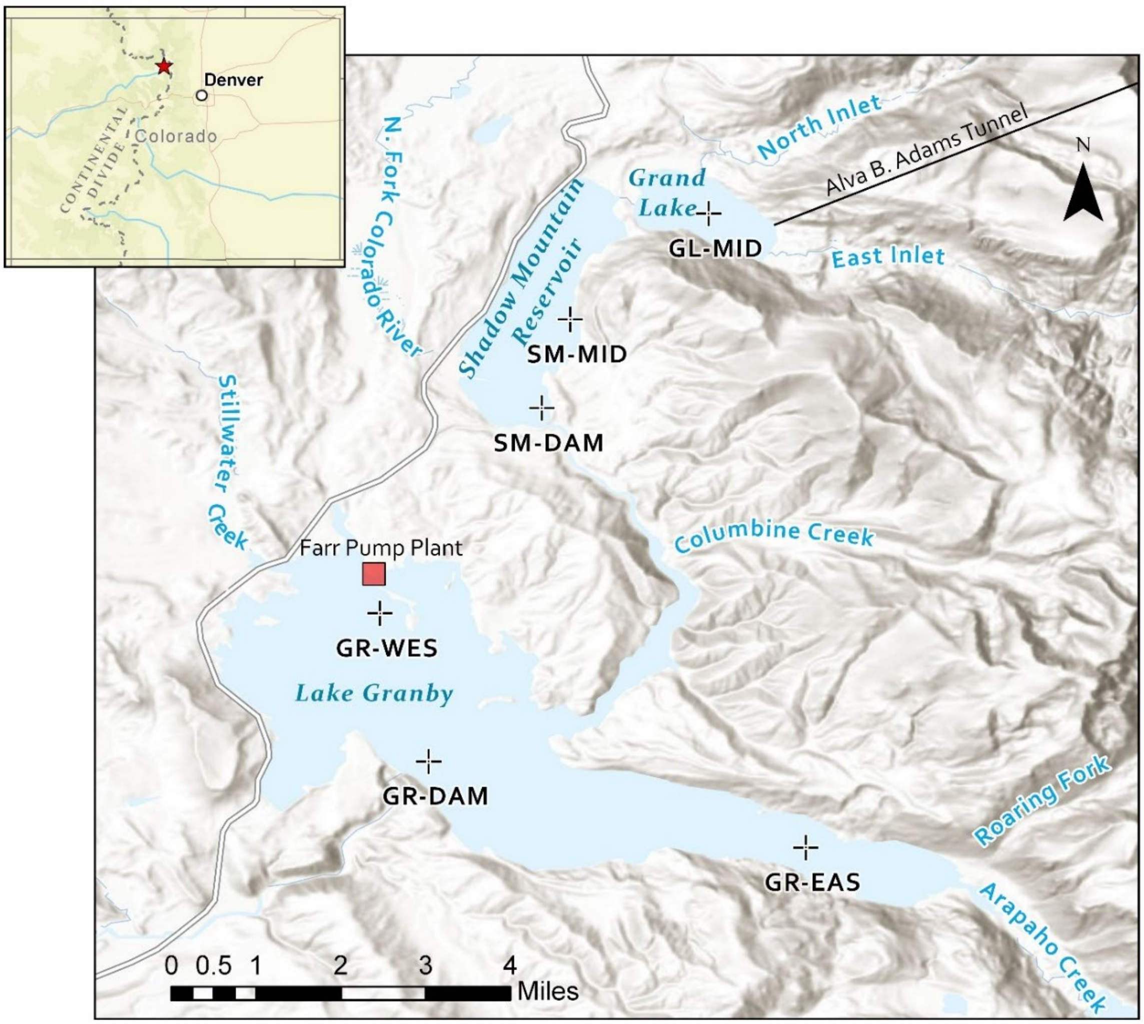


Figure 1. Map of the Three Lakes collection system and water quality sampling locations (+).

In response to external peer review of the 3LWQM v1.1 (Wells et al. 2018), the TSC prioritized model revisions from the reviewer recommendations that targeted sediment resuspension, model geometry, and model parameterization. Evaluating the most current version of the release version of W2 (v4.1 at the time of analysis) and the associated resuspension algorithm, the TSC determined that the necessary features needed to isolate resuspension algorithms from the larger sediment diagenesis package were not available and that the sediment diagenesis package was not ready for full implementation in this project (see release notes for version 4.2 in Wells 2020). The resuspension algorithm from the sediment diagenesis package was rewritten into a custom version of W2 v4.1. As further suggested by the reviewers, this algorithm is based on exceedance of a critical scour and is more generally applicable across all model segments. In the previous sediment resuspension formulation, the algorithm was only applied to user-selected segments and the model was calibrated with resuspension only in segments 12-16 in the northern portion of Shadow Mountain Reservoir. The new and more general approach is applied to all segments and therefore could support potential NEPA alternatives that alter the geometry of Shadow Mountain Reservoir. The vertical discretization in Grand Lake was refined to approximately 1 m from 2.5 m. The reviewers recommended using consistent reaeration formulae and turbulence closure for the waterbodies. The reviewers identified several corrections to model input file errors as well as coefficients that should be evaluated. These changes sufficiently altered the model, requiring recalibration to determine model performance.

Recalibration was conducted for 3LWQM-TSC v1.0 in line with modeling best practices (Palmer, 2001). It is considered best practice to conduct calibration when a model is initially created, the physical processes within the model are altered, or the domain of the model is modified in either space or time. Due to the changes to the 3LWQM model as described above, recalibration of model coefficients and parameters was required. Additionally, the availability of new data permitted a validation to be conducted to verify model performance. Calibration of the 3LWQM-TSC v1.0 was done in two phases to improve the understanding of the model and to limit computational requirements. Model variables that affect water clarity can be divided into first and second order variables based on the magnitude of their effect. Variables that are first order have a direct impact on clarity in the system (e.g., chlorophyll as a proxy for algae and TSS). Second order variables have less impact and may only have an indirect relationship to clarity (e.g., nutrients which act through their effect on algae). This distinction is useful to understand how physical processes interact within the model as well as for prioritizing processes for additional investigation and refinement. The initial calibration phase focused only on the first order clarity variables and model output errors that are directly predictive of Secchi depth, using the same values as the 3LWQM v1.1 for all other parameters. The subsequent calibration phase expanded the parameters and model output errors to include second order variables in addition to the first order variables. Automated calibration was conducted with the Optimization Software Toolkit for Research Involving Computational Heuristics (OSTRICH) platform (Loney et al., 2020) using the Particle Swarm Algorithm. For additional calibration details, see Reclamation 2021.

Secchi Depth Calculation

The stochastic nature of the relationship between physical or optical properties and Secchi depth is well established in the literature (Davies-Colley & Vant, 1988; Harvey et al., 2019; Castillo-Ramírez et al., 2020; Tilzer, 1988). Secchi depth values are a stochastic function of optical properties, and optical processes are a stochastic function of physical properties. Additionally, while the literature establishes what physical properties are anticipated to contribute to Secchi depth, it does not account for how a specific physical property value will affect Secchi depth at a particular system state nor the uncertainty associated with that transfer function (e.g., a function which converts from the independent to dependent variables).

As described in the model documentation (Hydros 2017), the 3LWQM v1.1 linear regression coefficients were determined using measured values of chlorophyll-a, ISS, POM to measured Secchi depth values. This regression then substitutes chlorophyll-a, ISS, and POM time series from the 3LWQM v1.1 model to obtain a Secchi depth prediction.

The regression modeling as described in the 3LWQM v1.1 model documentation can result in erroneous Secchi depth predictions. This is because application of any regression model developed from measurements to a modeled output does not account for model error and bias. The approach allows model error or bias to carry through the Secchi regression to manifest as error in the predicted Secchi depth values. If the measured regression were to be applied to the model estimated values, a bias correction step needs to be implemented to eliminate the propagation of model error into the Secchi depth prediction. Alternatively, the measured Secchi depth values can be regressed directly to the modeled values to account for any model error and bias. Either of these two methods explicitly account for the model error and would not propagate it forward to the Secchi depth values. Accounting for this error is particularly important when comparing to Secchi depth thresholds that are absolute, not relative to other model simulations.

Given the large uncertainties in the physical-optical-Secchi relationships and the limited skill of the 3LWQM v1.1 linear regression-based Secchi formulation during validation years, the TSC concluded that it is likely not suitable to impose a single deterministic relationship among these clarity variables, particularly if the modeling system is used to simulate conditions that differ from those used to calibrate the models. The TSC therefore determined based on these concerns that new approaches for predicting Secchi depth from model output should be explored to ascertain if performance improvements were possible.

Methods

An improved approach to estimating Secchi depth should consist of three operations – clustering, bias correction, and regression – to account for the stochastic nature of the system and uncertainty within the transfer function. Each of these components builds upon the previous step to maximize the predictive skill. While these operations can be implemented separately within traditional regression-based approaches to achieve reasonable results, neural networks (NNs) can simultaneously handle all three operations within a single architecture to produce a more streamlined product with potentially greater accuracy.

Clustering analysis groups data based on similarity. Used in the context of the Three Lakes system, a clustering analysis can identify when different physical processes are dominant. The subsequent operations of bias correction and regression can then account for the physical process regimes. An initial clustering analysis was performed using the 3LWQM v1.1 regression variables as well as hydrodynamic variables from the 3LWQM-TSC v1.0 model. The initial clustering analysis indicated a significant dependence on flow rate. Once flow rate dependency was removed, no clear clustering was visible from plotting the remaining parameters. To determine if the data clustered against any remaining parameters, a Hopkins test was utilized to quantitatively evaluate the distribution of each parameter (Holgate, 1965). The test identified a medium magnitude of clustering for the remaining parameters. Given that the data were clustered without a distinctive visual partitioning, more advanced data analytics methods, such as NN methods as is subsequently described, must be used to perform the clustering classification.

Bias correction accounts for and removes any systematic errors the model may exhibit against the observational data. Bias correction is necessary when using model output to prevent the systematic errors from carrying through subsequent calculations and propagating model bias. Correction of model bias is preferred by improving the accuracy of the model itself; however, post hoc removal of bias is acceptable if model bias remains or is associated with limited model regimes. Bias correction subsequent to clustering analysis gives visibility to model performance as different physical processes become dominant within the model. When taken over an entire period, a model may be unbiased, although it may be biased locally within physical process regimes. The combination of clustering followed by bias correction can identify and correct for biases related to a specific physical regime and improve model performance more than bias correction alone.

Regression is the process through which a transfer function is developed to convert an independent variable to a dependent variable. Numerous regression methods exist, such as linear, nonlinear, and statistical methods. Linear and nonlinear regressions assume a form of transfer function based on physical relationships. An optimization is conducted to determine coefficients that convert the independent values to the dependent values with the least error. Statistical regression approaches go further by not assuming a form of the transfer function but rather construct the transfer function during the regression process. All three methods can be supplemented with information gained through autocorrelation to determine if adding a lag between the independent and dependent variables would improve regression skill. Following clustering and bias correction, a regression can be created specific to each physical process regime. This allows the transfer function to more accurately account for the specific relationships happening within the regime without needing to generalize across regimes with reduced performance.

NNs are a machine learning method to create a nonlinear transfer function between input and output variables. NNs can perform data clustering, bias correction, and regression operations simultaneously within the network rather than through separate operations. Additionally, the NN training procedure can identify trends in the data that may be challenging to extract manually through visual inspection. With an appropriate, albeit more complex procedure, it is possible to obtain substantially similar results to a NN with the combination of classical clustering, bias correction, and regression methods (Mamun et al., 2019; Chen & Liu, 2015). Use of NNs are well established in a variety of scientific and engineering applications (e.g., Govindaraju, 2000; Yaseen, 2015; Abiodun, 2018). The TSC determined that the use of NNs could be beneficial for estimating Secchi depths given their ability to simultaneously perform all three operations.

The independent variables used in the NN were largely analogous to those in the 3LWQM v1.1 Secchi depth regression, except for extinction depth because it is colinear with the remaining chlorophyll, POM, and ISS variables. The W2 model uses these variables to estimate extinction depth. Flow rate was added as an input to the NN given it was shown to be a primary clustering variable, resulting in four variables used as input to the NN.

The structure of the NN was determined using an automated training approach. For a test network configuration, the NN was trained over the model calibration period. It was then used to predict Secchi depth for the seasonal validation runs, smoothed by a 7-day rolling average. The MAEs for the calibration and validation years were calculated and averaged to obtain a mean error. This training metric sought to distribute the error equally between the calibration and validation periods. This is analogous to the operations performed in a classical regression case. When formulating a regression, one seeks an expression that captures the calibration period with minimal error while not being too overfit to accurately describe the validation periods. In much the same way, a NN is constructed with a form that follows these three objectives.

The final selected NN configuration still benefits from human review of the network configurations. Balancing error between the calibration and validation periods neglects the difference in trend between the predicted and actual Secchi depth values. This can lead to portions of the validation period being poorly represented if the network performs better in other periods. This can be particularly apparent among the validation years if one year demonstrates large improvements at the expense of another. Each improved NN should be logged and reviewed to select a configuration which captures the correct trend in addition to minimizing error.

Results

The NN was developed using the scikit-learn MLPRegressor function in the Python programming language (Scikit-learn, n.d.). The rectified linear unit activation function was utilized with the limited-memory Broyden-Fletcher-Goldfarb-Shanno (LBFGS) solver. The regularization term was set to 0.001 with a maximum of 5,000,000 solver iterations per configuration. The MLPRegressor function requires specification of a random seed as part of its clustering operation. For each network configuration, the algorithm was repeatedly seeded with the integer values between 1 and 20 to minimize the effect of poor clustering on the evaluation of the network configuration.

Training was conducted on a Dell Precision 5820 tower with an Intel Xeon W-2135 and 32 GB of memory. A limitation of the NN approach is that the resulting NN can be machine dependent. Given an identical network configuration and random seed value, a user will not be able to reproduce the behavior of a network on different system. This issue can be minimized by saving a network once it is computed to produce a platform independent NN. Additionally, the automated training process can allow the network to be retrained as required, either on a new machine or as new data becomes available. A further limitation is the computational intensity of the NN training. Each potential network configuration must be solved with multiple random seeds to determine its performance. Automated training beyond approximately three network layers may require distribution among multiple workstations or use of HPC resources to make training tractable.

The model output from the second order calibration was used within the NN. The selected network was three layers with a (3, 11, 4) configuration and random seed of 3. This was the second-best network in terms of the output error metric and was selected based on its better trend resolution compared to the best case over the validation period. This configuration does not exclude the existence of additional network configurations not seen in the training configurations that would improve NN performance.

The NN transfer function performed equally well or better than the 3LWQM v1.1 regression approach in both the calibration and validation years based on MAE. Table 1 gives the comparison by year. Table 2 through Table 4 are intended to explicitly highlight the skill of the Secchi depth formulations over the clarity season (July 1 – September 11), using metrics consistent with the clarity goals of the 2016 Grand Lake Clarity Stakeholders Memorandum of Understanding. Figure 1 through Figure 3 show the continuous Secchi predictions for each of the validation years. The NN approach reduces error over the calibration period by approximately 20%. The 2017 performance of the revised model and Secchi NN is excellent, reducing MAE by 49% compared to the 3LWQM v1.1 model and regression. The 2018 performance of the revised approach lags behind the 3LWQM v1.1 regression by 5% and shows a 25% improvement again in 2019.

Both approaches find the 2018 management season challenging. In the early season, the NN approach better represents the trend seen in the Secchi observations. Around July 1st, pumping begins in a strong cyclic manner. This leads both approaches to predict a decrease in Secchi depth compared to the strong improvement witnessed in the observations. The decrease corresponds to the models predicting a large increase in TSS, shown in Reclamation 2021, that is not reflected in the observations. The error in TSS skews the prediction of both approaches for the remainder of the season. It is difficult to attribute the TSS overprediction to any specific feature of the 2018 model that could be altered a priori to improve forecast skill. The most likely explanation for the overprediction is the W2 engine being overly aggressive with sediment resuspension as large magnitude, sustained pumping begins for the year; however, more frequent TSS sampling would be needed to confirm this explanation or to assess other possibilities, such as errors in the inflow concentration input files.

The observed Secchi depth gradually declines until the late 2018 season when it becomes approximately constant. The 3LWQM v1.1 regression predicts a gradual improvement in clarity beginning around September 1st through the remainder of the model duration. The NN predicts a strong improvement centering on September 10th followed by an immediate correction toward the observations around September 22nd. The NN further predicts a worsening of clarity for the remainder of the season not covered by observations. While both prediction approaches perform poorly, the late season gradual improvement of the 3LWQM v1.1 regression corresponds with more observations producing slightly better performance compared to the NN approach.

Similarly, the approaches show a performance reduction in 2019 as pumping begins. Both the NN and the 3LWQM v1.1 regression overshoot the reduction in clarity seen in the observations; however, the NN does not fail the minimum Secchi depth goal of 2.5, as the 3LWQM v1.1 does. The 3LWQM v1.1 regression overshoots more strongly, leading to its worse performance overall in 2019. The NN predicts an earlier worsening of clarity but otherwise captures the trend better than the 3LWQM v1.1 in the later season. The earlier timing of the maximum clarity in the NN prediction is likely the result of the 7-day rolling average applied to the series. This will have the tendency to shift the timing of extremes when large changes in magnitude occur. While there is limited information to attribute the overshoot behavior, it is hypothesized that the 2019 year is the first year where the sediment boundary conditions become important. The 2019 modeled TSS timeseries, shown in Reclamation 2021, predicts large amounts of suspended sediment while the TSS observations are much lower as the pumps turn on. The pumps act to resuspend the sediment already in the water column within the model, causing the sharp performance decrease within the NN and 3LWQM v1.1 regression. This goes to the limitations of the model used in the annual forecast mode and its sensitivity to the input timeseries.

Table 1. Performance comparison between the 3LWQM v1.1 regression and 3LWQM-TSC v1.0 NN approaches

Model	**MAE [m]**			
	Calibration	2017	2018	2019
3LWQM v1.1	0.680	1.012	0.699	1.005
3LWQM-TSC v1.0	0.542	0.515	0.737	0.756

Table 2. Performance comparison between the 3LWQM v1.1 regression and 3LWQM-TSC v1.0 NN approaches for mean Secchi depths in 2017 over the compliance period (7/1/2017-9/11/2017)

Model	2017 Secchi Depth [m]			
	Model Mean	Observed Mean	Average Goal	Minimum Goal
3LWQM v1.1	3.684	3.503	3.8	2.5
3LWQM-TSC v1.0	3.433			

Table 3. Performance comparison between the 3LWQM v1.1 regression and 3LWQM-TSC v1.0 NN approaches for mean Secchi depths in 2018 over the compliance period (7/1/2018-9/11/2018)

Model	2018 Secchi Depth [m]			
	Model Mean	Observed Mean	Average Goal	Minimum Goal
3LWQM v1.1	3.434	4.155	3.8	2.5
3LWQM-TSC v1.0	3.368			

Table 4. Performance comparison between the 3LWQM v1.1 regression and 3LWQM-TSC v1.0 NN approaches for mean Secchi depths in 2019 over the compliance period (7/1/2019-9/11/2019)

Model	2019 Secchi Depth [m]			
	Model Mean	Observed Mean	Average Goal	Minimum Goal
3LWQM v1.1	3.137	4.391	3.8	2.5
3LWQM-TSC v1.0	3.706			

Conclusions

This work summarized the TSC effort to revise the 3LWQM v1.1 model based on reviewer comments and conduct recalibration, with emphasis given to the enhancement of the Secchi depth transfer function. This effort resulted in a model which, on the whole, slightly improved the ability to predict water quality within Grand Lake. However, inconsistent forecasting performance during the validation period continues to show the limitations of the water quality model. Resolution of the timing and magnitude of the TSS and chlorophyll peaks remain a challenge despite the improved physics and recalibration. While further revision to the initial and boundary conditions or adjustments to the calibration may improve model performance, it is unclear to what extent these improvements are available a priori during operations planning.

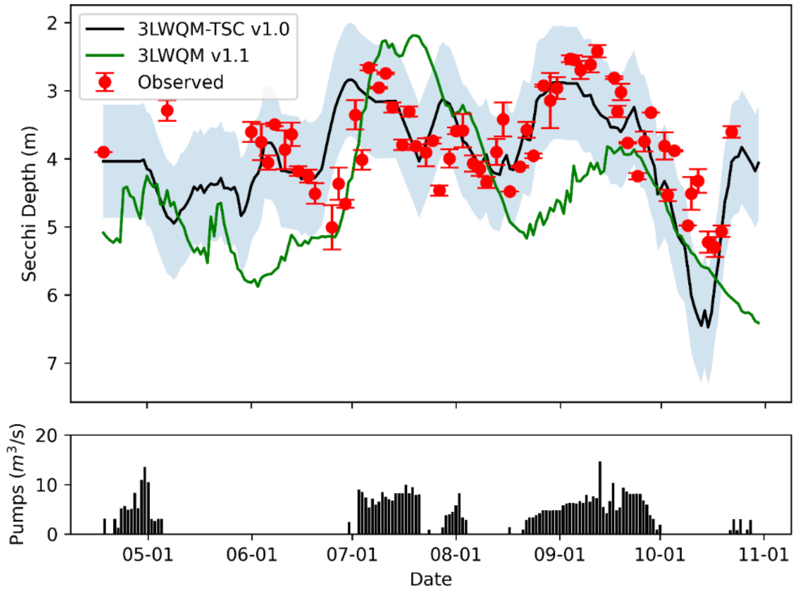
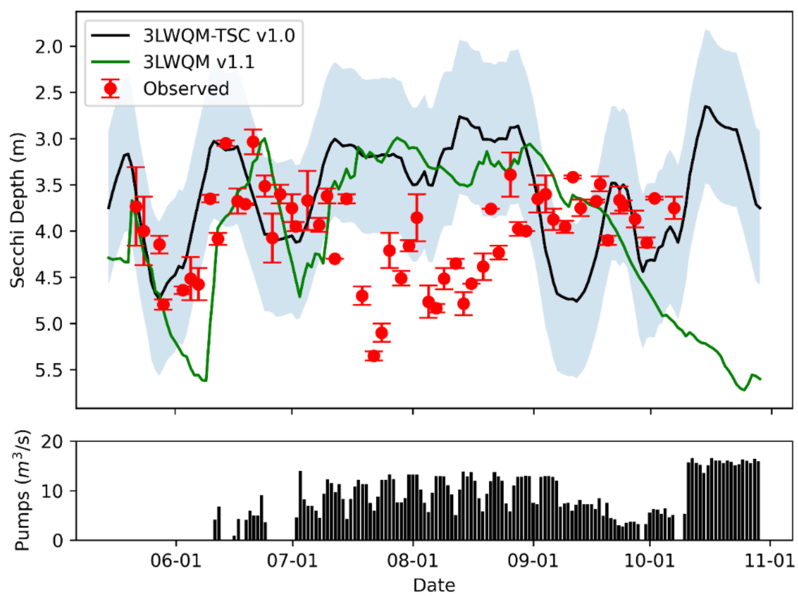


Figure 2. Comparison of the NN based Secchi depth forecast with the 3LWQM-TSC v1.0 model to the 3LWQM v1.1 prediction in 2017. Pump timing and magnitude is shown for reference. The red dots are the mean observed values for a given day, with the error bars showing the +/- one standard deviation around the mean if multiple values are available for the same day. The shaded blue around the 3LWQM-TSC v1.0 are +/- one standard deviation for the residual calibration error after training.



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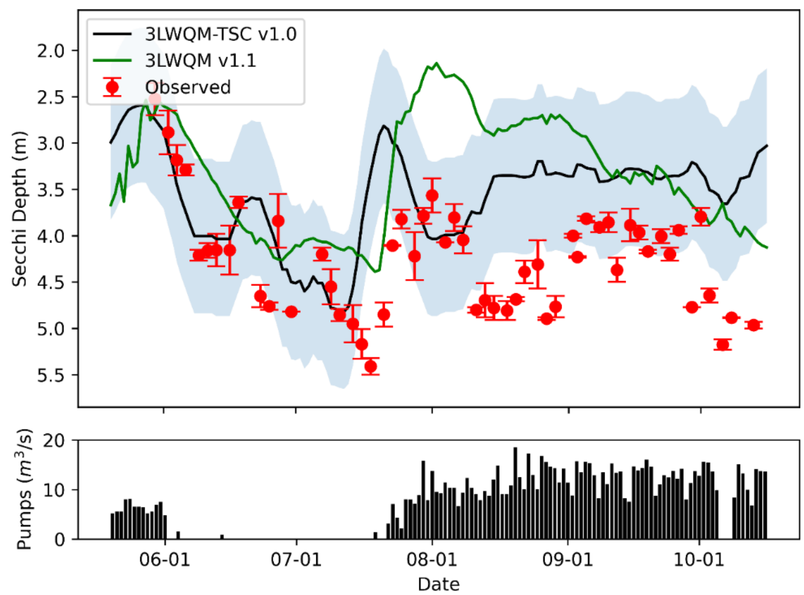

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The ability of the NN to compensate for model errors and improve the skill of Secchi depth forecasts is due to the robustness of machine learning methods. However, the performance of the NN ultimately remains tied to the performance of the W2 model. When the model accuracy is low, the NN is unable to provide significant corrections. NN performance could be improved with additional Secchi depth measurements to increase correction to the model output. However, improving the NN will likely be of diminishing returns as model accuracy becomes more limiting compared to the number of Secchi measurements available for NN training.

The performance of the 3LWQM-TSC v1.0 model indicates modest skill when looking at deterministic scenarios. Deterministic simulations are done to analyze specific cases and take model output as absolute quantities. However, the model may remain useful in comparing relative water quality under various operational scenarios. These cases would run multiple models and look at the relative performance among the scenarios. The extent to which this is possible is unclear and would require additional investigation.

In 2020, over 95% of the Willow Creek watershed feeding into the Three Lakes system was burned in the East Troublesome fire (US Forest Service, 2020). Wildfires can change the hydrology of the basin as they reduce runoff times and retention rates resulting in altered sedimentation processes (NRCS, 2016). Given the likely change to the hydrology, sedimentation, and nutrient loading within the Three Lakes and surrounding watersheds it will be necessary to revisit the TSC W2 model calibration and parameterization of physical processes.

Adapting either the 3LWQM-TSC v1.0 or the 3LWQM v1.1 model to the post-fire condition would be of limited operational benefit at this time. The development of a W2 model requires accurate initial and boundary conditions to model a system. However, the 2020 burn introduces such uncertainty regarding the initial and boundary conditions that output from the model may not meaningfully represent the system. Additionally, skill of a W2 model is determined using a calibration/validation procedure. As the burn is relatively new, limited information exists to develop a calibration and validation period for a set of new model parameters to represent the post burn condition, and existing validation runs have already challenged W2s predictive ability, without the drastic changes expected in runoff water quality from the burned areas.

The rapid hydrologic change anticipated in the post-burn Three Lakes system may require new approaches if water quality forecasts are to continue. Given that modeling skill will be limited for some time, using a direct, continuous measurement approach would be preferred. This should focus on the first order variables that have a direct impact on water quality – flow rate, TSS, and chlorophyll – to maximize their impact on clarity forecasts. Coupled with the NN based transfer function approach, a measurement based forecast system could provide reasonably accurate forecasts with a lead time meaningful to reservoir operations.

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