TMDLS: Statistical Correlations or Mechanistic Modeling?

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Abstract

In developing TMDL waste-load allocations for the Snake River-Reservoir system in Western Idaho and Eastern Oregon, determinations of the assimilative capacity of the system and the impact of pollutant reduction strategies has been performed using both a statistical-correlation approach and a mechanistic modeling approach. The system included the Lower Snake River, Brownlee Reservoir, Oxbow Reservoir, and Hells Canyon Reservoir with the focus was on Brownlee Reservoir.

The statistical approach used on Brownlee Reservoir divided the system into riverine and lacustrine zones. Field data were then averaged over season and location to provide statistical correlations, such as between total phosphorus (TP) and chlorophyll *a* (chl *a*), between an anoxic factor (AF) and TP, and between a hypoxic factor (HP) and TP. The anoxic factor is defined as the number of days when dissolved oxygen was less than 2 mg/l and the hypoxic factor was defined as the number of days when dissolved oxygen was less than 6.5 mg/l.

The mechanistic approach used a two-dimensional, unsteady, hydrodynamic and water quality model called CE-QUAL-W2. The model was calibrated to field data over a three year period for 1992 (a low flow year), 1995 (an average flow year), and 1997 (a high flow year).

Some of the important questions that the TMDL process was to answer included the following. What level of TP is necessary in the river coming into Brownlee Reservoir to reduce the number of days of hypoxia in the reservoir? What are the causes of low-

dissolved oxygen in Brownlee Reservoir and what management strategies can be implemented to improve water quality?

This paper examines the strengths and weaknesses of answering management questions using these two approaches. Recommendations are suggested for answering assimilative capacity questions that arise in TMDL studies.

Key Words

Brownlee Reservoir, CE-QUAL-W2, regression models, mechanistic models, TMDL

Introduction

With increasing TMDL requirements for surface water quality, water quality modeling approaches have been used to set water quality controls. Both a mechanistic modeling approach, based on the principles of conservation of mass and momentum, and regression models have been used to predict the impact of management strategies on water quality. Many different mechanistic models have been used for water quality studies, such as QUAL2E, CE-QUAL-W2 (Cole and Wells, 2000), and WASP/DYNHYD (Ambrose, R. B. et al., 1988). The regression models are developed by compiling water quality data and then postulating a cause-effect relationship between water quality parameters, such as between chlorophyll *a* (chl *a*) and total phosphorus (TP). Regression relationships between the independent and dependent variables are then developed. Are these approaches compatible? Do they yield similar predicted results? What are the strengths and weaknesses of each approach?

A case study comparing a deterministic water quality model and a statistical correlation model is presented for Brownlee Reservoir, Idaho/Oregon, USA (Figure 1). Water quality studies were initiated by the Idaho Power Company and the City of Boise, Idaho to examine causes of eutrophication and to make recommendations for TMDLs.

Brownlee Reservoir receives over 95% of its inflow from the Snake River and has a watershed drainage area of approximately 72,590 square miles (188,000 km^2) including drainage from the states of Nevada, Wyoming, Utah, Idaho and Oregon. The high flow rates are usually during the late spring snow-melt period (usually in May when historical average flows are 29,000 cfs or 800 cms), while the lowest flows are the late summer when precipitation is lowest and irrigation use is high. This usually occurs in August when average flows are approximately 10,000 cfs or 300 m^3 s^{-1}. The depth at the dam is almost 200 ft (60 m) with outlet structures consisting of 3 powerhouse intakes and several spillways. The length of the reservoir is approximately 50 miles (90 km) and consists of well defined riverine, transition, and lacustrine zones.

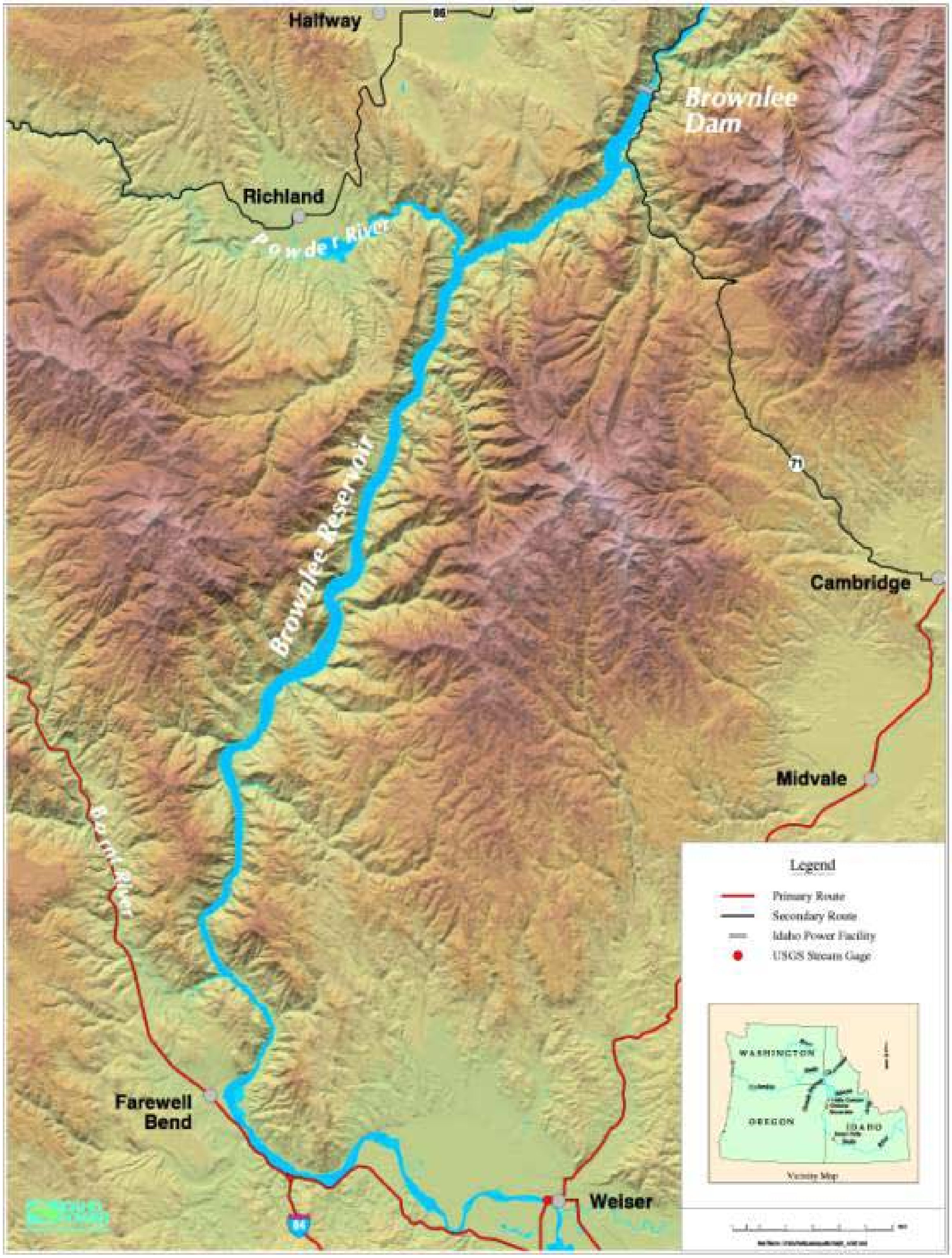

Figure 1 Brownlee Reservoir (Harrison et al., 2000).

CE-QUAL-W2 Modeling Study

CE-QUAL-W2 Version 3 (Cole and Wells, 2001) is a two-dimensional water quality and hydrodynamic model capable of modeling watersheds with interconnected rivers, reservoirs and estuaries. A typical model domain is shown in Figure 1. The model is based on solving the two-dimensional (longitudinal/vertical), unsteady hydrodynamic and advective-diffusion equations (Table 1).

The latest version of CE-QUAL-W2 has the following capabilities:

1. riverine branches in conjunction with reservoir/lake and estuary branches
2. hydraulic elements between branches including pipes, weirs, weirs with flashboards, pumps, spillways, and gates with dynamic gate openings
3. up-to-date theoretical reaeration (including spillway effects) and evaporation models
4. view model results graphically as they are being computed
5. use a variety of turbulence closure schemes
6. insert internal weirs in the computational domain
7. ULTIMATE-QUICKEST for advective transport of mass/heat
8. dynamic vegetative and topographic controlled shading
9. user-defined number of algal, epiphyton/periphyton, CBOD, suspended solids, and generic water quality constituents.

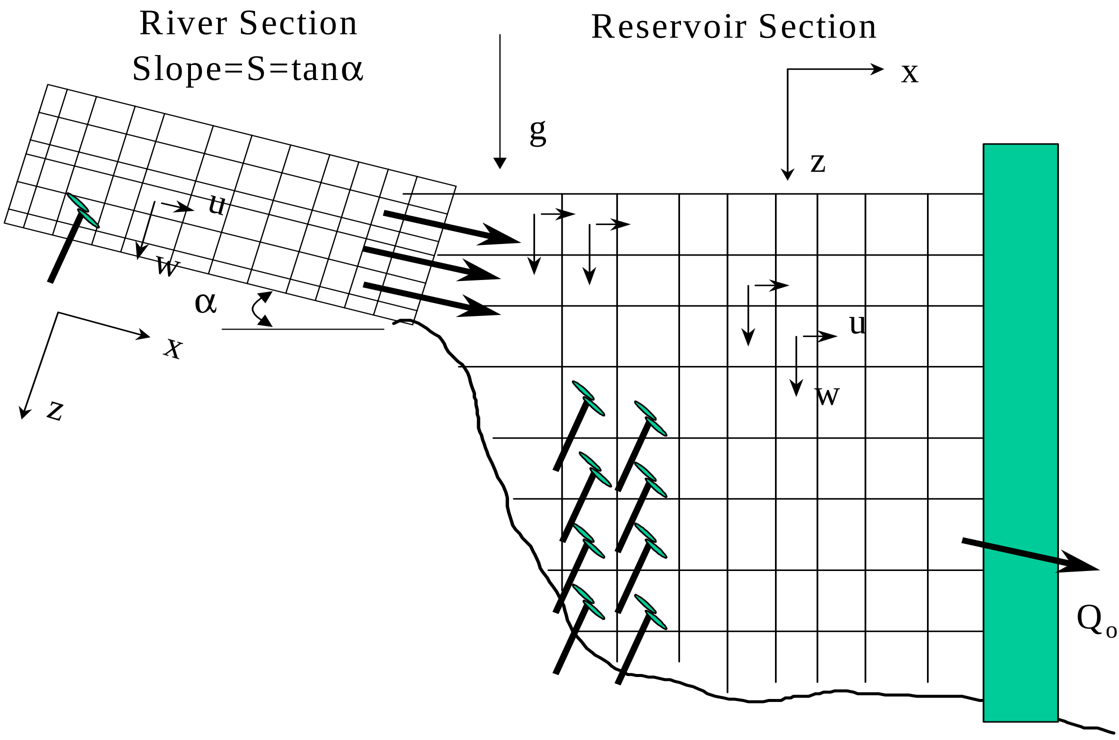

Figure 2. CE-QUAL-W2 Model Grid.

Table 1. CE-QUAL-W2 Governing equations.

Equation	Version 3 governing equations
x- momentum	$\frac{\partial UB}{\partial t}+\frac{\partial UUB}{\partial x}+\frac{\partial WUB}{\partial z}=gB\sin\alpha+g\cos\alpha B\frac{\partial\eta}{\partial x}-\frac{g\cos\alpha B}{\rho}\int_{\eta}^{z}\frac{\partial\rho}{\partial x}dz+\frac{1}{\rho}\frac{\partial B\tau_{xx}}{\partial x}+\frac{1}{\rho}\frac{\partial B\tau_{xz}}{\partial z}+qBU_x$
z-momentum	$0=g\cos\alpha-\frac{1}{\rho}\frac{\partial P}{\partial z}$
free surface equation	$B_\eta\frac{\partial\eta}{\partial t}=\frac{\partial}{\partial x}\int_{\eta}^{h}UBdz-\int_{\eta}^{h}qBdz$
continuity	$\frac{\partial UB}{\partial x}+\frac{\partial WB}{\partial z}=qB$
equation of state	$\rho=f(T_w,\Phi_{TDS},\Phi_{ss})$
Conservation of mass/heat	$\frac{\partial B\Phi}{\partial t}+\frac{\partial UB\Phi}{\partial x}+\frac{\partial WB\Phi}{\partial z}-\frac{\partial\left(BD_x\frac{\partial\Phi}{\partial x}\right)}{\partial x}-\frac{\partial\left(BD_z\frac{\partial\Phi}{\partial z}\right)}{\partial z}=q_\Phi B+S_\Phi B$
where B is the width, U is the longitudinal velocity, W is the vertical velocity, q is the inflow per unit width, α is the channel angle, Φ is the concentration or temperature, η is the water surface elevation, P is the pressure, h is the depth, T_w is the water temperature, Φ_{TDS} is the concentration of TDS, Φ_{ss} is the concentration of suspended solids, ρ is the density	

Mechanistic Modeling

CE-QUAL-W2 was applied by Idaho Power Company to Brownlee Reservoir to examine management strategies to achieve water quality goals (Harrison, et al., 2000). The numerical grid from their work is shown in Figure 3. Calibration years included 1992, 1995, and 1997, which represent low, average, and high flow conditions, respectively. The model was calibrated to observed data during each year for the following parameters: water surface elevation, temperature, dissolved oxygen, algae, ammonium, nitrate+nitrite, and inorganic phosphorus. Labile and refractory dissolved and particulate organic matter, suspended solids, and a 0 and 1st order sediment model were also included in the simulations.

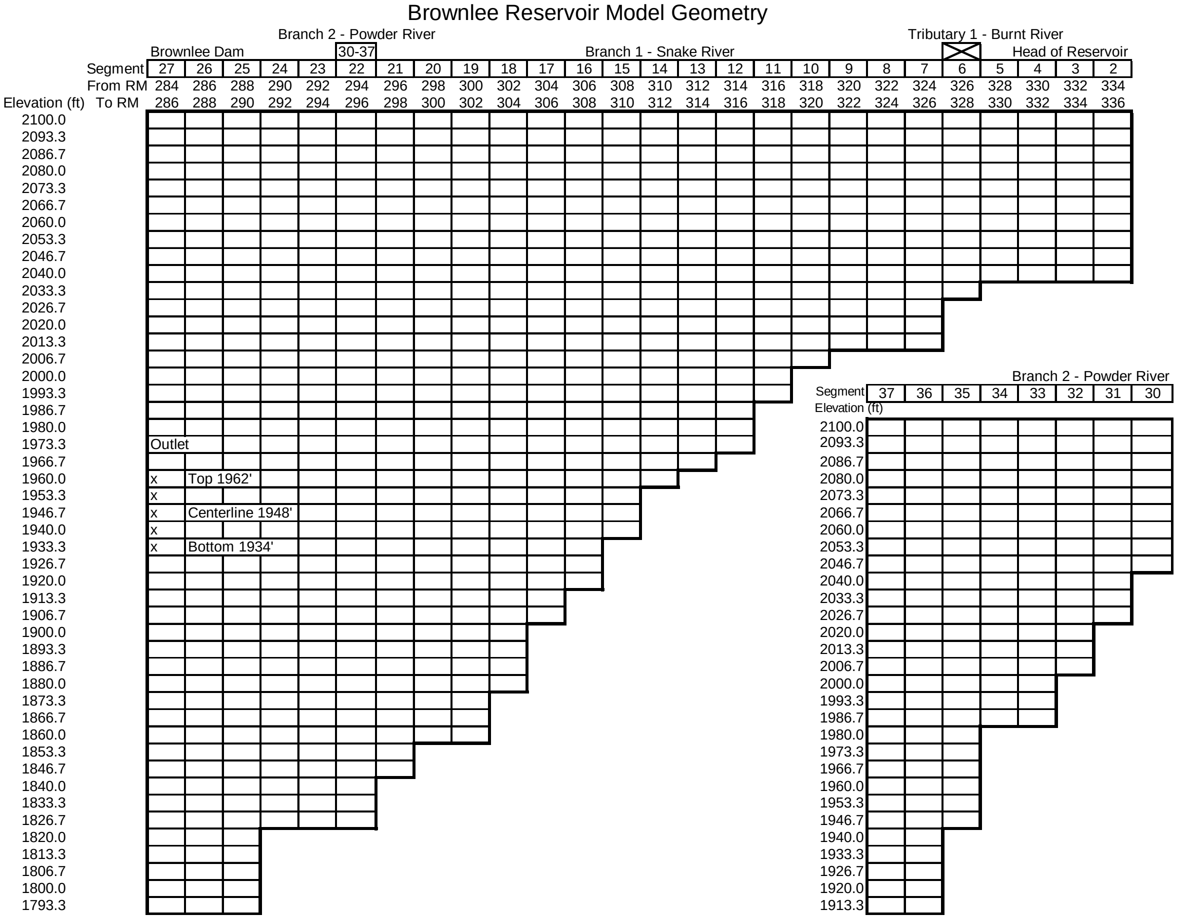

Figure 3. Model grid from Harrison et al. (2000) for Brownlee Reservoir.

Typical model results for temperature and dissolved oxygen are shown in Figure 4 and Figure 5. The absolute mean error (AME) for 71 temperature profiles is 0.6°C, which means that, on the average, the model was within ±0.6°C of the observed data. The AME for dissolved oxygen near the reservoir is about 1.5 mg/l for each year of calibration. Nutrient concentrations for inorganic phosphorus and nitrate+nitrite were also well represented (Figure 6 and Figure 7). A comparison of epilimnetic algal concentrations with field data is shown in Figure 8. The model reproduces the spatial and temporal variations in algal biomass in Brownlee Reservoir. In general, model-data agreement was good for all 3 years of calibration.

A typical criticism of deterministic models is the number of model coefficients available for adjustment during model calibration. In these simulations, default values of model parameters were generally used for the simulations that reproduced water quality data under three very different hydrologic years. The only parameter adjusted during calibration was the zero-order sediment oxygen demand. The lack of accurate boundary conditions is the major cause of poor model-data agreement in nearly all CE-QUAL-W2 applications.

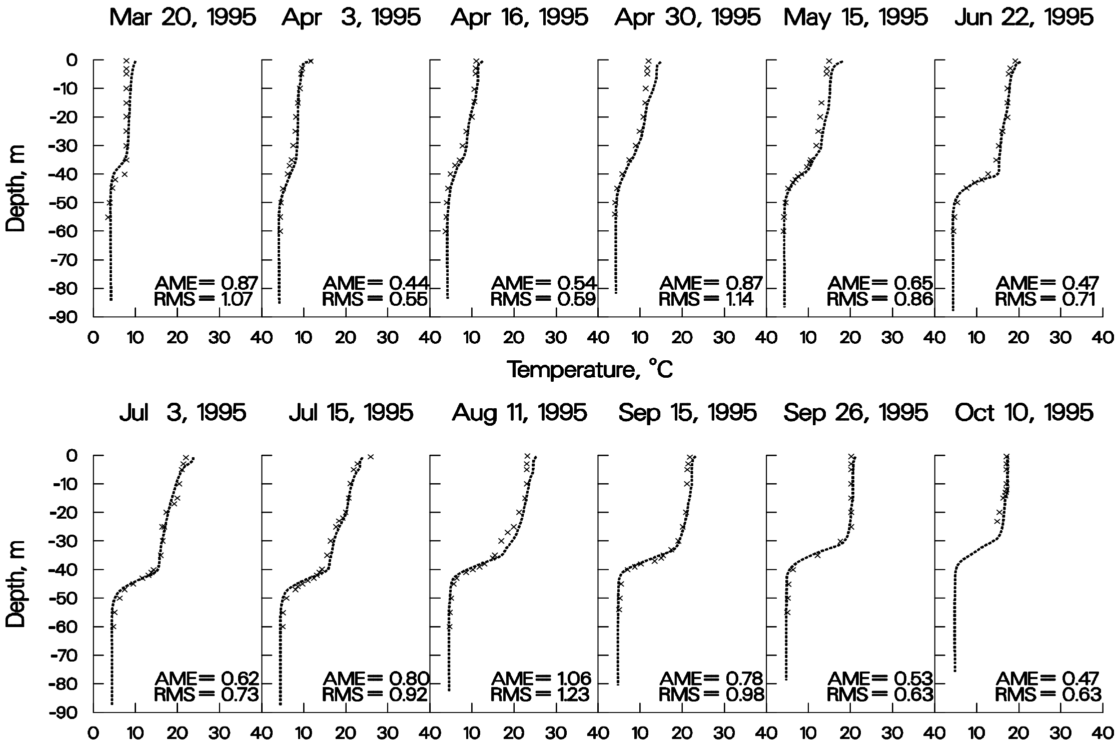

Figure 4. 1995 Brownlee Reservoir computed versus observed temperatures (AME is the absolute mean error and RMS is the root-mean square error).

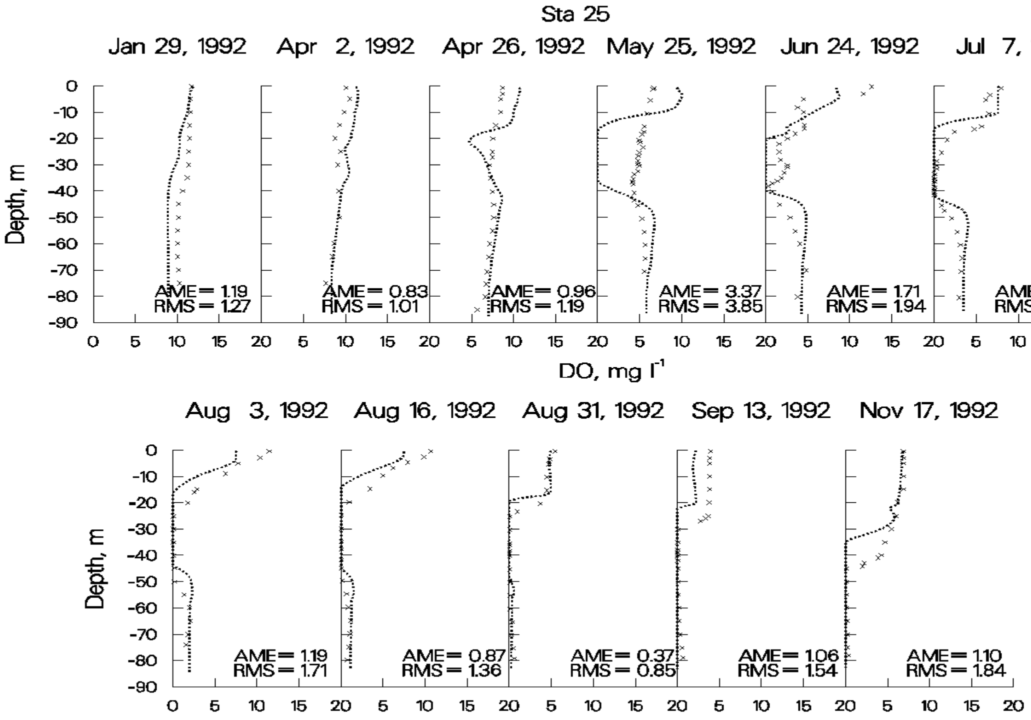

Figure 5. Brownlee Reservoir computed vs. observed DO in 1992 (AME is the absolute mean error and RMS is the root-mean square error).

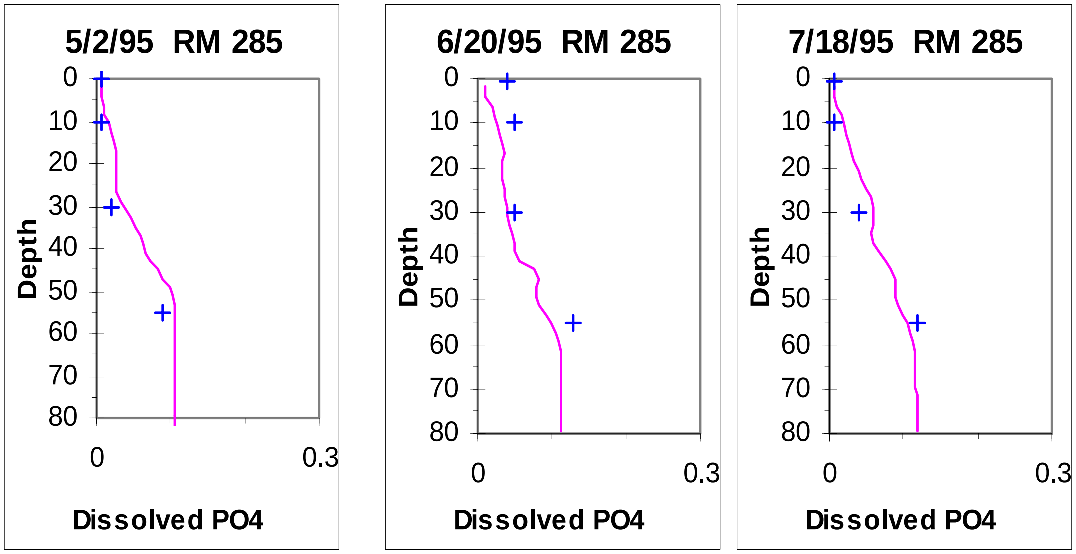

Figure 6. Comparison of model predictions (smooth line) and data (plus symbols) of vertical profiles of dissolved ortho-phoshorus. Depth is in m and dissolved PO4 is in mg/l.

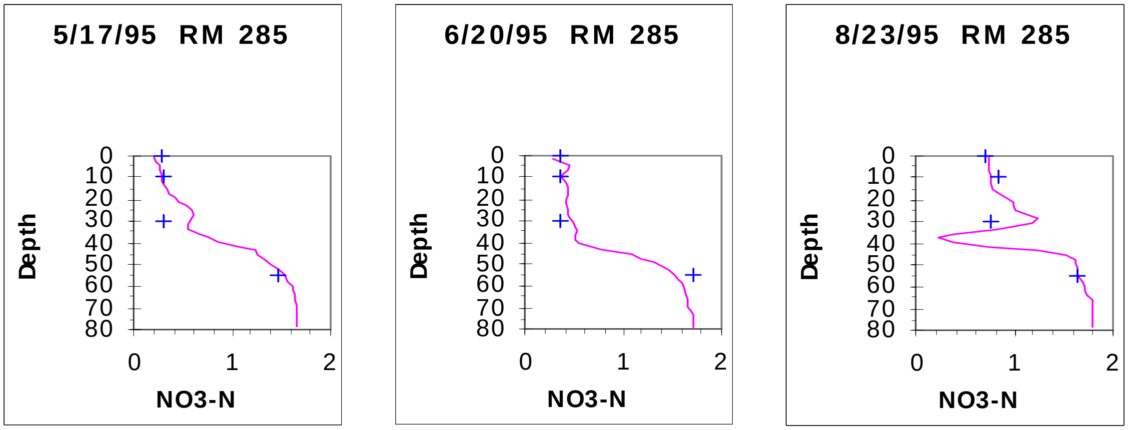

Figure 7. Comparison of model predictions (line) and data (+) of vertical profiles of nitrate+nitrite. Depth is in m and NO3-N is in mg/l.

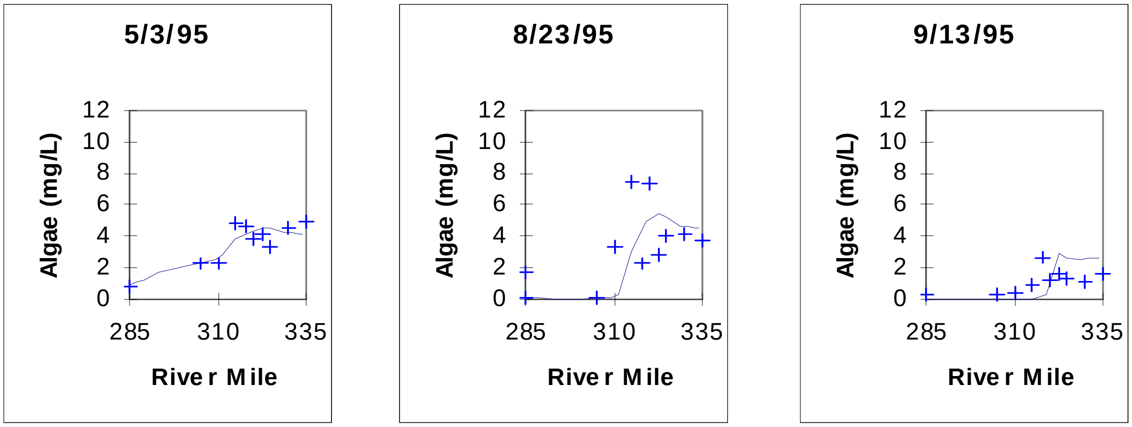

Figure 8. Comparisons of model predictions (line) of algae at the surface with field data (+) as a function of River Mile along the reservoir (the dam is at RM 285).

Regression Modeling

In a two-year study of water quality in Brownlee Reservoir by Nurnberg and Brown & Caldwell (2001), a regression model approach was undertaken to predict the effect of management strategies on water quality. This project attempted to develop statistical correlations between water quality variables in order to predict the impact of management strategies. The over-riding concept was to minimize the complexity by 'keeping it simple, stupid!"

The approach consisted of the following:

- ❑ Hydrologic and nutrient budgets
- ❑ Evaluation of seasonal epilimentic Phosphorus
- ❑ Predict water quality through data correlations
- ❑ Verify these correlations with data
- ❑ Predict the effect of scenarios

The data correlations that were developed were between TP and P loading, TP and chlorophyll, an Anoxic Factor and TP, algal bloom frequency and chlorophyll a, and Secchi disk depth and chlorophyll a.

Also, in the interest to simplify the system, the Brownlee Reservoir system was divided into the shallow part and deeper part and data in these areas were averaged. This divison is shown in Figure 9.

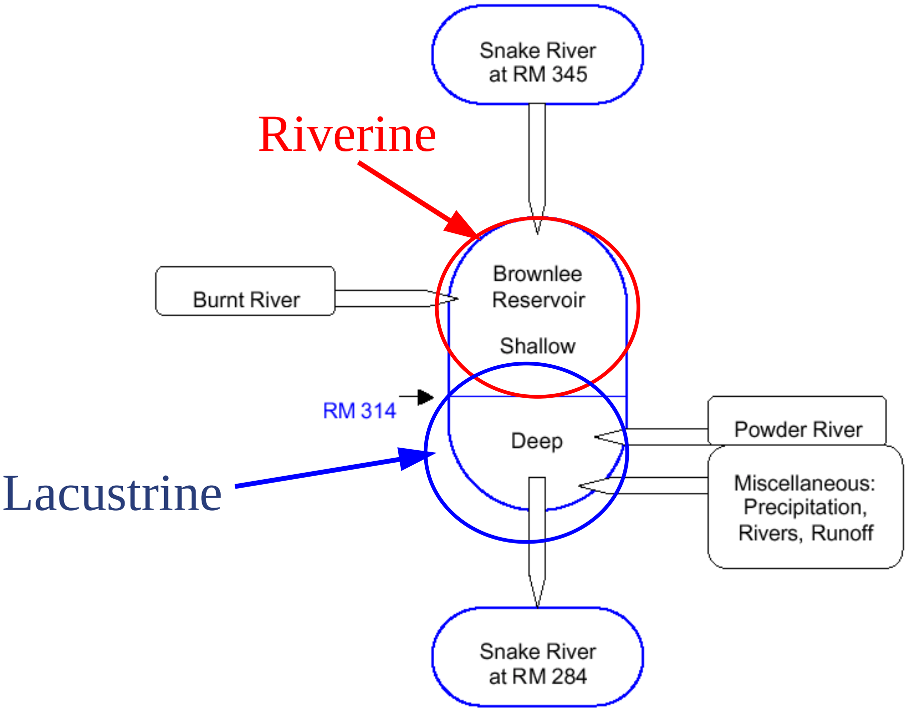

Figure 9. Division of Brownlee Reservoir into riverine and lacustrine zones for data correlations.

The regression relating an Anoxic Factor (AF) and TP is shown in Figure 10, and the regression between chlorophyll *a* and TP is shown in Figure 11. AF is defined by Nurnberg and B&C (2001) as “a measure of anoxia in lakes and reservoirs, based on DO…and morphometric data” and “is a ratio that represents the number of days in a year or season that a sediment area equal to the lake surface area is anoxic”.

Nurnberg and B&C indicate that the amount of hypolimnetic anoxia is a function of “Total P, morphology and hydrology.” The authors claim that the model of TP versus AF used for 73 North American lakes is also applicable to Brownlee Reservoir since the average TP for Brownlee falls on the best fit line. As shown in Figure 10, the riverine data for Brownlee Reservoir fall far below the correlation line and the lacustrine data fall above it. When averaged, the correlation data fall on the line. The statistical correlation model was determined based on using the annual whole lake average AF-TP as

- $AF = -35.4 + 44.2 \log (TP) + 0.95\, z/A^{0.5}$ (1)

  where z is the mean depth in m and A is the surface area in km^2. This correlation is based on data from 73 stratified lakes where the goodness of fit is $R^2 = 0.65$.

The chl *a* – TP relationship is based on the observation that algal growth is dependent on the limiting nutrient, which in freshwaters is usually phosphorus. As a result, the following regression model was developed based on Figure 10:

- $\log (\text{chl } a) = -0.25 + 0.799 \log (TP)$ (2)

  where chl *a* and TP are based on the summer epilimnetic chl *a*. This correlation is based on data from 180 lakes where the goodness of fit is $R^2 = 0.64$.

However, analysis of the Brownlee data indicated that chl *a* showed no correlation with TP loadings and AF showed a negative correlation, as remarked upon by Nurnberg and Brown & Caldwell in their analysis. Years of lowest inflow (thus low TP loadings) resulted in the highest values for chl *a* and AF, not the lowest as predicted by equations 1 and 2. Years of highest inflow (thus high TP loadings) resulted in the lowest values for chl *a* and AF, not the highest as predicted by the equations.

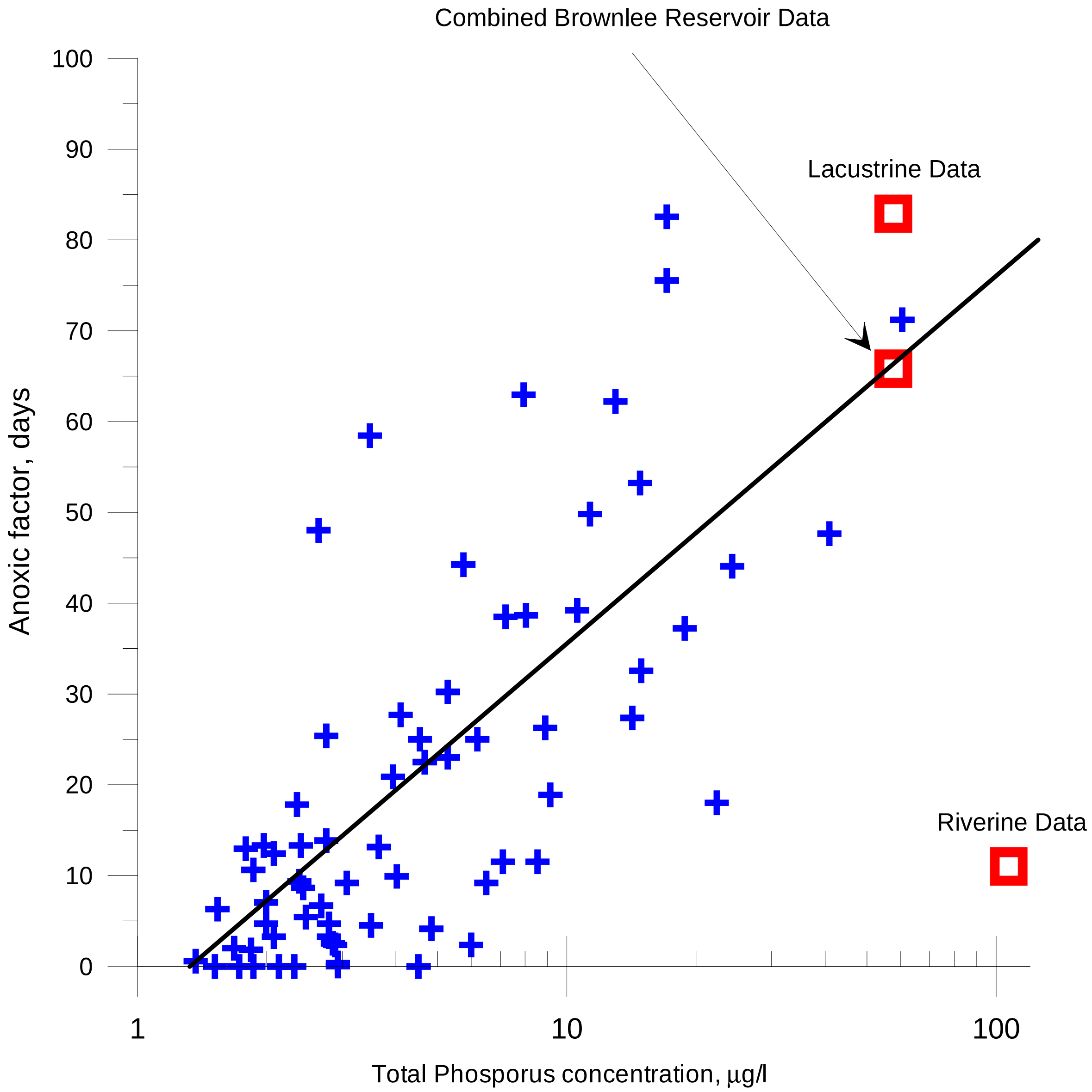

Figure 10. Correlation between AF and TP for Brownlee Reservoir and 73 other lakes (after Nurnberg and B&C, 2001).

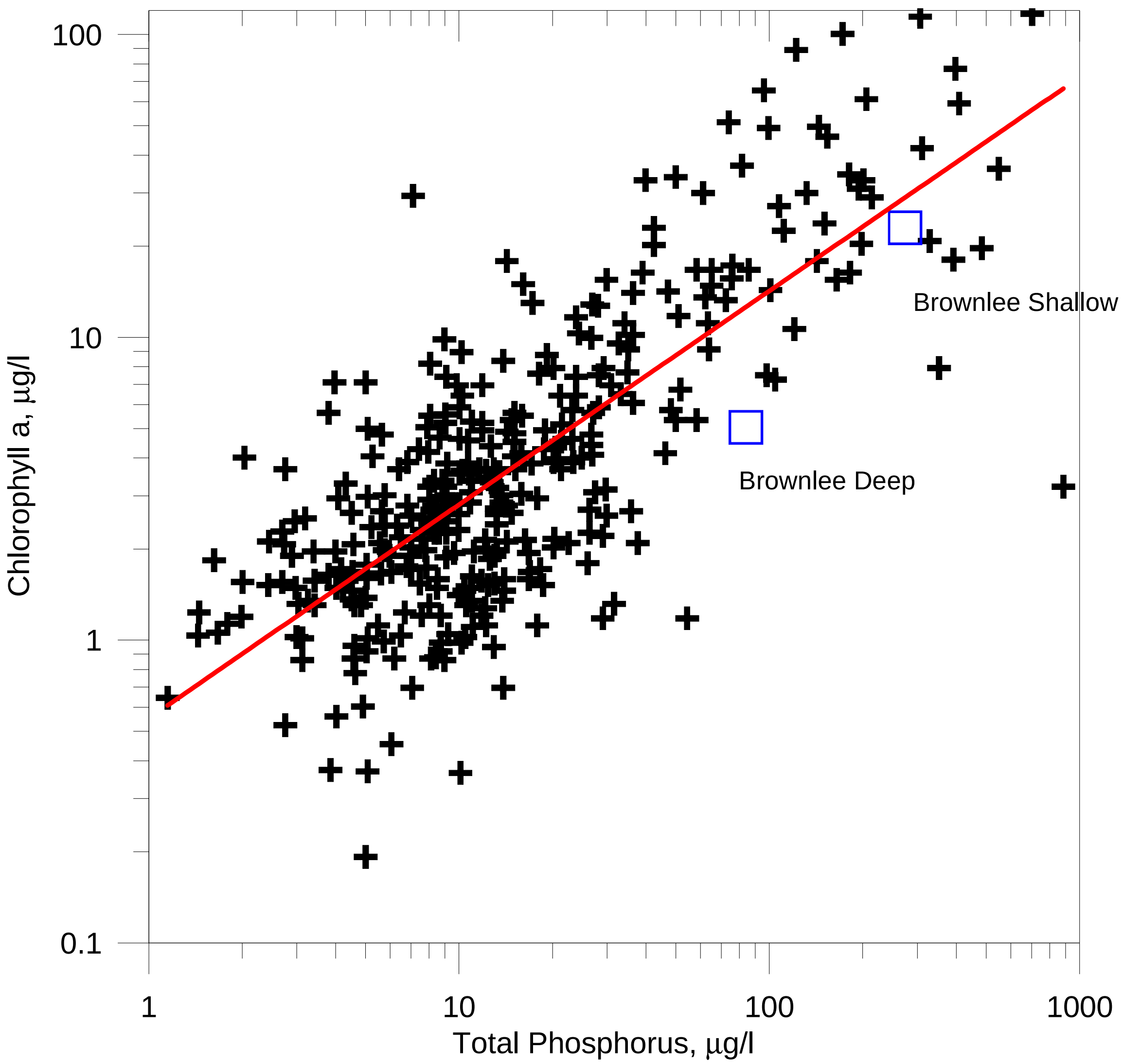

Figure 11. Correlation between chl *a* and TP (after Nurnberg and B&C, 2001).

In point of fact, algae do not respond to nutrient mass loadings but rather to water column concentrations, hence the observed relationship between high/low inflow and low/high chl *a* and high/low dissolved oxygen. Additionally, algae utilize only the bioavailable form of phosphorus, commonly measured as ortho-phosphate or soluble reactive phosphorus, rather than TP.

So, the basic premise or cause and effect relationship the regression models are based upon is flawed. Any forcing function that serves to increase the water column concentration of bioavailable phosphorus will increase algal biomass that will eventually lead to an increase in the AF, but the regression equations do not include this relationship. Additionally, longer residence time in the riverine zone allows for greater algal growth in a given location as the algae are not advected downstream as quickly when compared to years with short residence times. Again, the regression equations cannot account for varying hydrology as the mechanism is not included in their formulation.

For Brownlee Reservoir, low flow years resulted in higher bioavailable phosphorus levels in the inflowing Snake River as a result of decreased dilution of inputs from agricultural and urban runoff. Additionally, the increased residence time in the riverine zone allowed for greater degradation of organic matter resulting in lower oxygen levels. Further complicating matters, warmer inflowing waters with their higher nutrient and organic matter loads entered higher in the photic zone thus making more nutrients available for algal growth for a longer time period. The end result was periodic fish kills in the riverine zone during low flow years. None of these mechanisms that affect algal growth and oxygen uptake in Brownlee Reservoir were included in the regression models. All of them and more are included in the mechanistic model CE-QUAL-W2.

The reason why Nurnberg's and other similar regression models have yielded statistically significant relationships between TP and chl *a* and dissolved oxygen on a number of lakes is due to several serendipitous occurrences. First, the relationships were developed for lakes where long residence times generally prevail thus making hydrology in the form of short residence time much less of a factor in algal and dissolved oxygen dynamics.

Secondly, because of the long residence time, most of the TP entering the lakes can be recycled into a bioavailable form that can be utilized by algae, particularly for lakes with anoxic hypolimnions where phosphorus release from the sediments back to the water column is common. However, equations 1 and 2 are still fundamentally flawed when applied to systems outside the range of their development as their development is not based on a clearly defined cause and effect relationship unlike mechanistic models such as CE-QUAL-W2. Since residence time and water column inorganic phosphorus concentrations and their effects on dissolved oxygen and algal growth are built into the mechanistic model, any changes to forcing functions that affect these two variables are explicitly included. Additionally, equations 1 and 2 completely ignore the impacts of inflowing organic matter on dissolved oxygen levels, but their effects are included in the mechanistic model. Finally, TP and chl *a* are autocorrelated.

However, in spite of the clear evidence that chl *a* showed no correlation with TP and AF showed a negative correlation with TP in Brownlee Reservoir both in terms of actual data and a limnological analysis of the system, the regression models were still used to predict the impact of reducing TP loadings to Brownlee Reservoir and their effects on dissolved oxygen and chl *a*. This was in spite of the fact that "none of the available information indicates any relationship between oxygen conditions and TP or chlorophyll concentration in Brownlee Reservoir on an annual basis".

The reasoning given for using equations 1 and 2 is that "even though there is no correlation between phosphorus and annual oxygen depletion found for Brownlee Reservoir data over the short term, it is *likely* (emphasis added) that long-term average anoxia is influenced by phosphorus concentration because the regression model found on worldwide lakes predicts the Brownlee Reservoir's long-term average AF well". As pointed out previously and as shown in figure 9, the regression model does not predict any actual AF for the different portions of Brownlee very well at all, only the average between the riverine and lacustrine AF, which has no correspondence to reality. So, in spite of all evidence to the contrary, flawed regression models were applied to the system with the following conclusion: reduction in TP loadings to the system would have minimal impact on the AF in Brownlee Reservoir and that changes to operations that resulted in more flushing would have a substantial reduction in anoxia. When all you have is a hammer, the whole world looks like a nail.

CE-QUAL-W2, on the other hand, reproduced the variation in algal biomass and hypoxia/anoxia between the various flow years.

Conclusions

The purpose of this paper is not to try to demonstrate the superiority of mechanistic modeling over statistical modeling for all TMDLs. Indeed, egregious examples of inappropriate usage of mechanistic models could just as easily have been shown. It is also recognized that appropriate use of statistically based models can yield useful information in a short time frame and in a cost effective manner. The purpose of this paper is to show that whatever type of model is used for developing a TMDL, it should be applied appropriately with full knowledge of its capabilities and limitations and should be able to address in a meaningful way the TMDL requirements.

In the case study presented here, regression models were applied inappropriately to Brownlee Reservoir and recommendations regarding phosphorus reductions to be used in the TMDL process were presented as being firmly established in sound science, when such was clearly not the case. Obtaining the wrong answer more quickly and/or more cheaply does not bode well for our water resources.

On the other hand, the mechanistic model CE-QUAL-W2 was able to reproduce very complicated dissolved oxygen and algal dynamics over both a short and long term time frame as well as the impact of increased inorganic phosphorus concentrations on algal growth and increased/decreased inflow on anoxia. The reason why is that CE-QUAL-W2, unlike the regression models, included the ability to simulate these effects in its formulations. The tradeoff to obtaining more scientifically sound results to base TMDL decisions on in this case is the additional time and expense involved in the application of a mechanistic, numerical model. It is up to the stakeholders to decide if the effort is warranted.

It is important to realize that both approaches can provide valuable information for developing TMDLs and that neither method should necessarily be preferred over the other but should be used where appropriate. Deciding where the two methods should be appropriately applied is what separates the wheat from the chaff in the TMDL modeling game. That said, it is our belief that mechanistic models such as CE-QUAL-W2 that have a proven track record are more universally applicable and can address a wider range of issues for a given system than regression models based on small and/or inappropriate data sets. CE-QUAL-W2 has now been applied to more than twice the number of reservoirs that were used to develop the AF-TP regression relationship (Equation 2).

As an example, one of the conclusions drawn by Nurnberg and B&C is that a substantial reduction in anoxia could be achieved through operational changes that maximize flushing although no regression model was used as a basis for this opinion. In fact, the exact opposite might happen if in the process of maximizing flushing, hypolimnetic temperatures were increased causing a more rapid decay rate of organic matter in the hypolimnion, which is typical of reservoirs with short residence times. CE-QUAL-W2 could easily address this issue in a few minutes, whereas the regression models would be completely inappropriate.

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