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Nutrients dynamics simulation of two lakes in Albania utilizing CE-QUAL-W2 model

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Abstract: Two lakes in Albania are modeled to simulate the nutrients dynamics in the water column. Nutrients characteristics for each of the two lakes were simulated using the CE-QUAL-W2 model, which is a carbon-based, laterally averaged, two-dimensional water-quality model. The modeling effort was supported with data collected in the field for a 2-year period for both lakes. At each lake monitoring site, nutrients profile measurements were taken from the surface through the water column. The validation process consisted of comparisons of predicted in-lake concentrations to those observed during the monitoring period, which extended from May through November 2013 and March through October 2014 with a 2-week offset. The focus for evaluating the model validation was given to three constituents of nitrogen and two constituents of phosphorus: nitrate plus nitrite, ammonia, total nitrogen, orthophosphorus, and total phosphorus. The sample data for each nutrient parameter was statistically analyzed on the basis of the four metrics of mean errors (ME), mean absolute errors (MAE), root mean square errors (RMSE), and relative error of the mean in percentage (REM), using measured inputs of nutrients. The taken results showed that the CE-QUAL-W2 model was able to accurately simulate nutrients, with relative error of the mean less than 10%. Model results revealed that model simulated concentrations of key nutrients indexes matched well with the measured values. The results and conclusions from this study are not intended for use on Prespa and Ohrid Lakes alone. The concepts of model development can potentially be applied and also broaden its usefulness to other systems.

Key words: Lake Prespa, Lake Ohrid, CE-QUAL-W2 model, nutrients, water quality, hydrodynamics.

I. INTRODUCTION

The CE-QUAL-W2 models address the interaction between nutrient cycling, primary production, and trophic dynamics to predict responses in the distribution of temperature and oxygen in lakes (Smith et al., 2014). CE-QUAL-W2 is a two dimensional, longitudinal/vertical, hydrodynamic, and water quality model. Because the model assumes lateral homogeneity, it is best suited for relatively long and narrow water bodies exhibiting longitudinal and vertical water quality gradients (Cole and Wells, 2003). The CE-QUAL-W2 model is capable of predicting water surface elevations, velocities, temperatures, and several water quality constituents. The input data used in the model are the best available and are assumed to be accurate representations of meteorology, flow, and water quality parameters.

Development and evolution of CE-QUAL-W2 has spanned three decades. Modifications to the model have included improvements to computational efficiency and accuracy, transport and mixing schemes as well as additional water quality algorithms, hydraulic structures, and the ability to connect multiple water bodies. The model has been successfully applied to lakes, lakes, rivers, and estuaries around the world. There are many application examples to water systems of CE-QUAL-W2 model (Bowen and Hieronymus, 2003; Ha and Lee, 2007; Galloway and Green, 2006; Green et al., 2003; Kurup et al., 2000; Smith et al., 2014; Sullivan et al., 2011; Sullivan and Rounds, 2005; Wells, 1999).

Water quality constituents represented by the model are complex interactions. The methods used to solve these are simplistic descriptions but have replicated observed processes in various systems with impressive results (Cole and Wells, 2003). Several water quality processes are not simulated including sediment transport and accumulation, toxics, and dynamic sediment oxygen demand (Cole and Wells, 2003). This paper will discuss the nutrients dynamics in two lakes and will present results from nutrients simulations. Conclusions from the modeling will be presented and used to recommend future research and monitoring as they relate to improving model performance and lake operations.

II. MATERIALS AND METHODS

A. Study Areas

The Region of Ohrid and the Prespa Lakes, situated in south-eastern Europe (40°40' - 41°2' N latitude; 20°23' - 21°16' E longitude), extends across the borders of Albania, Greece, and Macedonia (Fig. 1). In 2014, the Ohrid-

Prespa Transboundary Reserve between Albania and Macedonia was added to UNESCO's World Network of Biosphere Reserves. UNESCO recognizes the biosphere reserves as areas where human activities are focused on sustainable use of natural resources and provision of adequate conditions for humans to live in harmony with fauna and flora.



Fig 1. Ohrid-Prespa Region

Lake Ohrid

Lake Ohrid is the deepest lake of the Balkans, with a maximum depth of 288 m and a mean depth of 164 m. The lake has an area of 358 km², and a volume of 55.4 km³ of water (Matzinger et al., 2006). Of the total surface area, 248 km² belongs to Republic of Macedonia and 110 km² belongs to Albania. Ohrid Lake is 30.4 km long by 14.8 km wide at its maximum extent with a shoreline length of 87.53 km, shared between Macedonia (56.02 km) and Albania (31.51 km).

The lake drains an area of around 2600 km² and is fed primarily by underground springs on the eastern shore (about 50% of total inflow), with roughly 25% shares from rivers and direct precipitation. Over 20% of the lake's water comes from nearby Lake Macro Prespa. The water leaves Lake Prespa trickling through underground watercourses in the karstic landscape, where it is joined by mountain range precipitation and eventually emerges in numerous springs along the eastern shore and below the water surface of Lake Ohrid. The water leaves Lake Ohrid by evaporation (~40%) and through its only outlet, the Black Drin River, which flows in a northerly direction into Albania and thus to the Adriatic Sea. The relatively dry, Mediterranean climate and the small drainage basin of 2600 km² (catchment/lake surface ratio of about 7) of Lake Ohrid results in a long hydraulic residence time of about 70 years.

Both in terms of nutrient concentration, as well as biological parameters Lake Ohrid qualifies as oligotrophic. Thanks to this oligotrophy and the filtered spring inflows, the water is exceptionally clear with transparencies to a depth of as much as 22 meters. Lake Ohrid lacks an annual deep water exchange which in other lakes can bring complete overturn; plunging rivers are also absent. Despite this, dissolved oxygen never drops below 6 mg L⁻¹.

Lake Prespa

Prespa is the name of two interconnected freshwater lakes (Macro Prespa and Micro Prespa) in southeast Europe. They are the highest tectonic lakes in the Balkans, standing at an elevation of 853 m. Prespa Lake is 28.6 km long by 16.9 km wide at its maximum extent with a shoreline length of 105.5 km, shared between Macedonia (45 km), Albania (39 km) and Greece (21.5). The lake has an area of 309.6 km², and a volume of 2.05 km³ of water. Of the total surface area, 176.3 km² belongs to the Republic of Macedonia,



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52.2 km² to Albania and 81.1 km² to Greece with a maximum depth of 55 m. The lakes drains an area of around 1,218.1 km² and its hydraulic residence time is about 11 years.

The Micro Prespa Lake is shared only between Greece (138 km² drainage area; 43,5 km² water mirror surface) and Albania (51 km² drainage area; 3.9 km² water mirror surface). Because Macro Prespa Lake sits about 150 m above Lake Ohrid, which lies only about 10 km to the west, its waters run through underground channels in the karst and emerge from springs which feed streams running into Lake Ohrid.

Both in terms of nutrient concentration (have a moderate supply of nutrients, is prone to moderate algal blooms, and have occasional oxygen depletions at depth), as well as biological parameters Lake Prespa may be regarded as mesotrophic lake with seasonal variations, which may pass to eutrophic character (Sarafiloska and Patceva, 2012).

B. Model Description

Both models for the lakes (Prespa, and Ohrid) are constructed using CE-QUAL-W2, version 3.7 (Cole and Wells, 2011), which is a two-dimensional, laterally averaged, hydrodynamic and water-quality model originally developed by the U.S. Army Corps of Engineers (USACE) Waterways Experiments Station (Cole and Buchak, 1993) for rivers, estuaries, lakes, reservoirs and river basin systems. It is applied in this study to simulate nutrients in Prespa and Ohrid Lakes.

The water quality algorithms incorporate 21 constituents in addition to temperature including nutrient / phytoplankton /dissolved oxygen interactions during anoxic conditions. Any combination of constituents can be simulated. The water quality algorithm is modular allowing constituents to be easily added as additional subroutines. The CE-QUAL-W2 model is a data intensive application. The data required for an application include bathymetric data, meteorological data (air temperature, dew point temperature, wind speed, wind direction, cloud cover, solar radiation, and precipitation), inflow and outflow volumes, inflow temperatures, evaporation, water quality constituent concentrations, and hydraulic and kinetic parameters. The availability and quality of these data directly affect model accuracy and limit usefulness.

Although the lateral averaging of CE-QUAL-W2 is better suited for long, narrow water bodies, such as reservoirs, rivers, and estuaries, CE-QUAL-W2 has been successfully applied in lake settings (Sullivan and Rounds, 2005; Sullivan et al., 2007). Lake Prespa has a relatively long and narrow body appropriate for CE-QUAL-W2. Both of these lakes exhibited enough homogeneity in water-quality and water-temperature data such that laterally averaging did not compromise the integrity of the model. Vertical variations captured with CE-QUAL-W2 are important for distinguishing temporal variations in the lake epilimnion and hypolimnion. The capability of the model to predict changes in nutrients in two dimensions (longitudinally and vertically) were among the characteristics which made CE-QUAL-W2 particularly suited to simulation of Prespa and Ohrid Lakes.

The individual lake models were developed in several phases. First, data were collected to determine the hydrological, thermal, and water-quality boundary conditions for the calibration year. Information from a digital elevation model (DEM) and available bathymetric data were used to generate bathymetric cross sections for the CE-QUAL-W2 model. Next, the model grid was constructed based on available lake bathymetry data.

The success of the model largely depended on a high data density of biological, chemical, and physical lake characteristics from which lake parameters could be calculated, and the model could be calibrated and validated. Several continuous flow and water-quality monitoring systems were installed to calculate the initial and boundary conditions for the models and to provide a robust calibration and validation dataset. Datasets necessary to run CE-QUAL-W2 were formatted to fit the input data structure.

C. Nutrients Data Collection and Laboratory Analysis

Limnological characteristics, including properties that could affect trophic state, were examined at one limnological site for each of the two lakes: Lake Prespa at Pusteci Point, and Ohrid Lake at Pogradeci Point. The sites were sampled monthly from May through November 2010 and March through October 2011 with a 2-week offset, so that biweekly sampling was accomplished for both the 2010 and 2011 field seasons for selected



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parameters. Samples for the analysis of total phosphorus, orthophosphate, nitrate plus nitrite, total Kjeldahl nitrogen, and ammonia, were collected near the surface and at depth, respectively (1 m and 20 m in Lake Prespa, 2 m and 20 m in Ohrid Lake, using a Van Dorn (Van Dorn, 1956) sampler and were analyzed to determine concentrations of nutrients. Two samples were taken from each depth. Water samples were filtered and preserved as required. Dissolved concentrations are those analyzed for a 0.45-micron filtered sample, whereas total concentrations were determined for a whole water sample. Total nitrogen, total phosphorus, orthophosphate and dissolved phosphorous were analyzed by U.S. Environmental Protection Agency (USEPA) method 365.1 (U.S. Environmental Protection Agency, 1993). Dissolved nitrate, as nitrogen was analyzed by Calorimetry method (Fishman, 1993); dissolved nitrate plus nitrite, as nitrogen enzyme reduction-diazotization (Patton and Kryskalla, 2011); dissolved ammonia as nitrogen was analyzed by Calorimetry, salicylate-hypochlorate method (Fishman, 1993); dissolved ammonia plus organic nitrogen, as nitrogen was analyzed by Calorimetry, microkjeldahl digestion method (Patton and Truit, 2000); dissolved orthophosphorous was analyzed by Calorimetry, phosphomolyddane method (Fishman, 1993).

D. Data and Statistical Analysis

An often overlooked step in model applications is plotting and analyzing observed data for all stations and times for which data are available. Another important task in data development and analysis is to analyze the data for reasonableness. So, all time-varying input data were plotted and screened for errors. The degree of fit between the simulated results and measured lake values was considered during model calibration. A number of model error statistics were computed and aggregated by parameter, season, and location to evaluate the spatial and temporal prediction capability of the model. The goodness-of-fit statistics for the comparison of modeled and measured values include annual mean errors (ME), mean absolute errors (MAE), root mean square errors (RMSE), and relative error of the mean in percentage (REM), which are calculated as:

$$ME = \frac{1}{N} \sum_{i=1}^N (O_i - S_i)^2 \quad (1)$$

$$MAE = \frac{1}{N} \sum_{i=1}^N |O_i - S_i| \quad (2)$$

$$RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^N (O_i - S_i)^2} \quad (3)$$

$$REM = \frac{1}{N} \sum_{i=1}^N \left| \frac{O_i - S_i}{O_i} \right| \quad (4)$$

where S_i and O_i are the simulated and observed (measured) values as samples taken along the season (e.g., biomass and CC), or at the end of the season (e.g., grain yield), N is the number of observations, and \bar{O} is the mean value of O_i . The RMSE in Eq. 1 represents a measure of the overall, or mean, deviation between observed and simulated values, that is, a synthetic indicator of the absolute model uncertainty. In fact, it takes the same units of the variable being simulated, and therefore the closer the value is to zero, the better the model simulation performance.

Linear regression analysis was also made with measured data as dependent variable and the modeled data as independent variable. The coefficient of determination, slope, and intercept of the linear regressions between for sampling data for each nutrient consistent were calculated.

III. RESULTS AND DISCUSSION

A. Model Calibration

Calibration consisted of setting model parameters to literature values or to values used by other models (Cole and Buchak, 1995; Cole and Wells, 2003; Cole and Wells, 2011, DeGasperi, 2009) and refining them in a logical and organized fashion until modeled and measured concentrations matched reasonably well. The degree



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Volume 4, Issue 4, July 2015

of fit between the modeled results and measured lake values was considered during model calibration. The four quantities utilized to evaluate the degree of fit were mean errors (ME), mean absolute errors (MAE), root mean square errors (RMSE), and relative error of the mean in percentage (REM).

The first step in the calibration process for two lake models was the water balance based on water-surface elevation. Before the temperature and water-quality calibration could proceed, the differences between the simulated and measured water-surface elevations were rectified. A water balance was considered complete when the AME and RMSE quantities were less than 0.01 m for the simulated water-surface elevation.

One of the main calibration tools for CE-QUAL-W2 model development was the vertical profile temperature data, available for two lakes. Simulated water temperature in lakes also was compared to lake profile data. For two lakes, the absolute mean error and root mean square error were less than 1.0 °C and 1.2 °C, respectively, for the different depth ranges used for vertical profile comparisons.

Additional calibration targets included water temperature and DO depth profiles, in addition to discrete measurements of ammonia, nitrate plus nitrite, total nitrogen, total phosphorus, orthophosphorus, and chlorophyll *a*.

In addition to water temperature, the CE-QUAL-W2 models for two lakes successfully predicted dissolved oxygen concentration based on the two metrics of absolute mean error and root mean square error. Simulated dissolved oxygen concentration generally tracked the measured dissolved oxygen concentration for the calibration periods.

Additional calibration targets included algal dynamics captured by three general groups: (1) diatoms, (2) green algae, and (3) blue-green algae. Simulated algal-growth temperature coefficients were consistent across all three lakes, in addition to the algal-growth rates and the light saturation intensity at the maximum photosynthetic rate.

A specific focus for evaluating the model calibration was given to three constituents of nitrogen and two constituents of phosphorus: nitrate plus nitrite, ammonia, total nitrogen, orthophosphorus, and total phosphorus. Ammonia, nitrate plus nitrite, and orthophosphorus concentrations in all three lakes were largely affected by the inflows and the lake hydrodynamics. In general, the simulated concentrations compared well to the measured data. Simulated total nitrogen and total phosphorus concentrations did not compare as well to measured data, particularly in the hypolimnion.

The available data and methods used to develop hourly water quality model boundary condition inputs and available calibration testing procedures are not described in this paper.

B. Model Validation

The validated model for Lake Prespa was run for the period 2012 - 2013, and for Lake Ohrid was run for the period 2013 - 2014.

Nutrient constituents used in the validation of the model include total phosphorus, orthophosphate, total nitrogen, ammonium-N, and nitrate-N.

The mean errors (ME), mean absolute errors (MAE), root mean square errors (RMSE), and relative error of the mean in percentage (REM) are used to evaluate the degree of fit between the simulated results and measured values.

A summary of the current model's performance along with summary statistics in graphic and tabular form follows for key nutrients components.

Total Phosphorous and Orthophosphate

Phosphorus levels in the Prespa and Ohrid lake were low overall (total phosphorus typically < 0.06 mg/L, orthophosphate typically < 0.02 mg/L as P). The greatest deviation between modeled and measured phosphorus

concentrations typically occurred in the fall, when the model predicted higher total phosphorus than was measured.

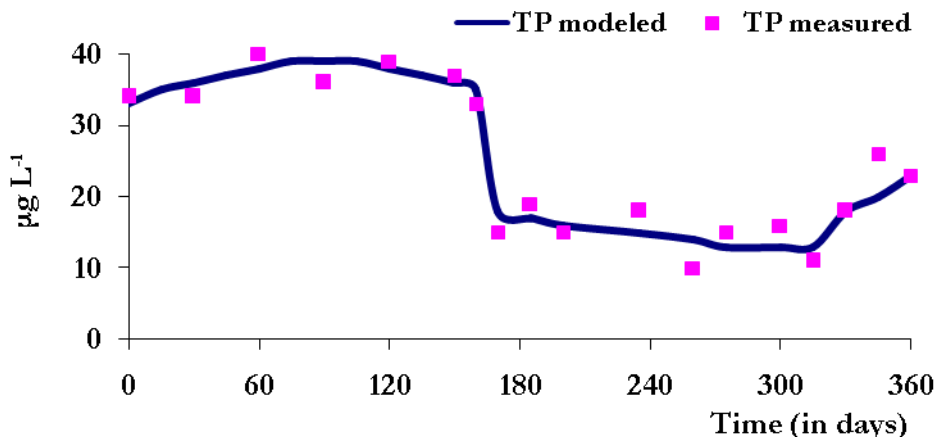


Fig. 2. Comparison between modeled and measured values for total phosphorous (TP) in Prespa lake

Modeled and measured total phosphorus temporal profile at the Pusteci monitoring site, for the representative year 2013 is shown in figure 2. Measured and modeled total phosphorus temporal profile at the Pogradeci monitoring site, for the representative year 2014 is shown in figure 3.

The temporal pattern in figure 2 and 3 illustrates several important processes affecting phosphorus concentrations in Prespa and Ohrid lakes. First, the overall phosphorus concentrations were fairly low and typical of an oligotrophic system. The low phosphorus concentrations could be limiting algal growth and primary productivity. Second, when algal blooms occurred (late spring through summer), orthophosphate concentrations (the bioavailable phosphorus) decreased to levels below detection near the surface of the lake where the algae were growing. Lastly, when the lake’s hypolimnion was anoxic from late August or September through mid-November, phosphorus concentrations increased near the lake bottom - a typical result of the dissolution of iron oxides in the lake sediments. Ammonia should also be released from the sediments under anoxic conditions, and this was in fact observed in the ammonia data each year.

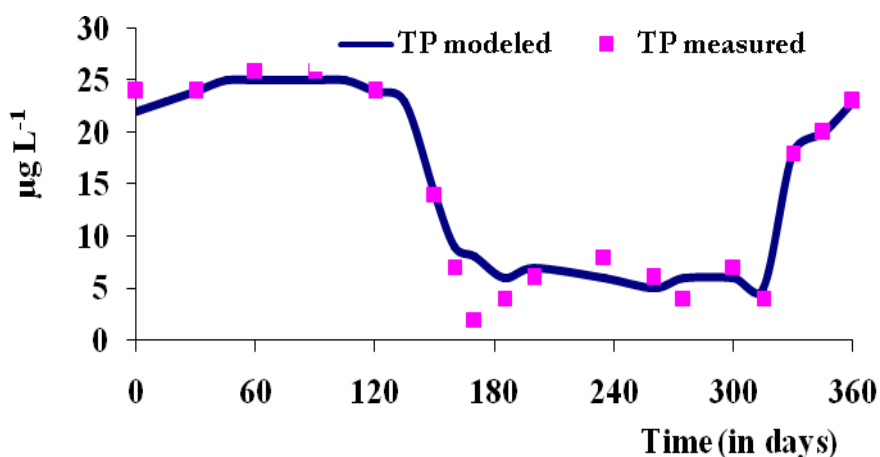


Figure 3. Comparison between modeled and measured values for total phosphorous in Ohrid Lake

A summary of model-prediction error statistics based on sampling data collected at the Pusteci and at Pogradeci monitoring sites for the representative years are provided in Table 1 and Table 2.



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ISO 9001:2008 Certified

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Volume 4, Issue 4, July 2015

Table 1. Summary of model prediction error statistics for sampling data, Lake Prespa

Parameter	n	ME	AME	RMSE	REM
Total Phosphorus	126	0.004	0.009	0.012	8.6
Orthophosphate	126	0.003	0.004	0.006	9.7
Total Nitrogen	126	0.006	0.009	0.014	9.6
Ammonium-N	126	0.009	0.042	0.043	9.3
Nitrate-N	126	0.005	0.008	0.008	8.5

Table 2. Summary of model prediction error statistics for sampling data, Lake Ohrid

Parameter	n	ME	AME	RMSE	REM
Total Phosphorus	90	0.005	0.009	0.015	17.3
Orthophosphate	90	0.002	0.003	0.005	15.3
Total Nitrogen	90	0.005	0.008	0.013	14.3
Ammonium-N	90	0.008	0.015	0.038	16.2
Nitrate-N	90	0.004	0.007	0.009	16.8

Calculating goodness-of-fit statistics between measured and modeled total orthophosphate produced annual MEs between 0.001 and 0.005 mg/L, MAEs between 0.003 to 0.006 mg/L, and RMSEs between 0.004 and 0.008 mg/L for 2013 through 2014 (table 1, 2). For total phosphorus, annual MEs ranged from 0.008 to 0.002 mg/L, MAEs ranged between 0.006 and 0.012 mg/L, and RMSEs were between 0.009 and 0.014 mg/L. The fact that the ME is near zero and the MAE and RMSE show errors of less than 0.012 mg/L indicates that the model accurately captured the phosphorous budget of Prespa Lakes.

Table 3. Summary of modelled versus predicted linear regression results for sampling data, Lake Prespa

Parameter	n	Intercept	Slope	R ²	P
Total Phosphorus	126	0.96	0.64	0.9049	**
Orthophosphate	126	1.02	0.31	0.8864	**
Total Nitrogen	126	0.96	0.24	0.9283	**
Ammonium-N	126	1.01	0.52	0.9677	**
Nitrate-N	126	0.87	0.64	0.8108	**

** = significant at $p < 0.005$; * = significant at $p < 0.05$; R² = regression coefficient; p = significance level.

Table 4. Summary of modelled versus predicted linear regression results for sampling data, Lake Ohrid

Parameter	n	Intercept	Slope	r ²	p
Total Phosphorus	90	0.92	0.59	0.8455	**
Orthophosphate	90	1.01	0.16	0.8746	**
Total Nitrogen	90	0.98	0.20	0.9138	**
Ammonium-N	90	1.03	0.38	0.9757	**
Nitrate-N	90	0.86	0.52	0.7857	**

** = significant at $p < 0.005$; * = significant at $p < 0.05$; ns = not significant ($p > 0.05$); r² = regression coefficient; p = significance level

Linear regression statistics results of measured versus modeled at the Pusteci and Pogradeci monitoring sites for the representative years are provided in Table 3 and Table 4, respectively.

The comparison of measured and modeled phosphorus concentrations in figure 2 and 3, table 1, 2 and table 3, 4 is reasonable. The model kept track of the phosphorus relatively well, and with sufficient accuracy to meet the needs of this investigation.

Ammonia and Nitrate

Measured and modeled total nitrogen (TN) profile at the Pusteci monitoring site, for the representative year 2013 is shown in figure 4. Measured and modeled total nitrogen profile at the Pogradeci monitoring site, for the representative year 2014 is shown in figure 5.

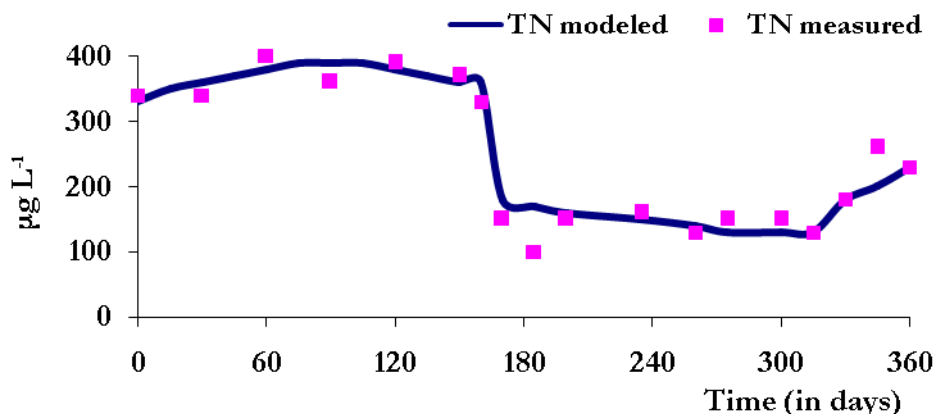


Fig. 4. Comparison between modeled and measured values for total nitrogen (TN) in Prespa Lake

Ammonia was below or close to its analytical detection limit (0.01 mg/L as N), but measurable concentrations of ammonia were found to accumulate in the hypolimnion at concentrations up to 0.68 mg/L as N once that layer became anoxic in late September. Ammonia can accumulate in the anoxic hypolimnion because no oxygen is present to support nitrification. Sources of ammonia to the hypolimnion include ground-water discharge and the deamination of organic material in the lake sediments. Nitrate can be reduced by bacterial communities to N₂ under anoxic conditions, but further reduction to ammonia is not favoured. When the lake turned over in the fall, the accumulated ammonia was mixed and diluted into the larger volume of the lake, and the entire lake became oxygenated, diminishing the production and stopping the accumulation of ammonia, and increasing the production of nitrate.

Nitrate was included in the both Lake models. It appeared that concentrations of nitrate in summer were depleted near the surface and were highest in the hypolimnion. This is consistent with the trend observed by Zyfi (2008). That study found the highest concentrations of nitrate in Prespa Lakes during winter (0.569 mg/L as N), and depletion in surface waters during the summer (less than 0.037 mg/L as N).

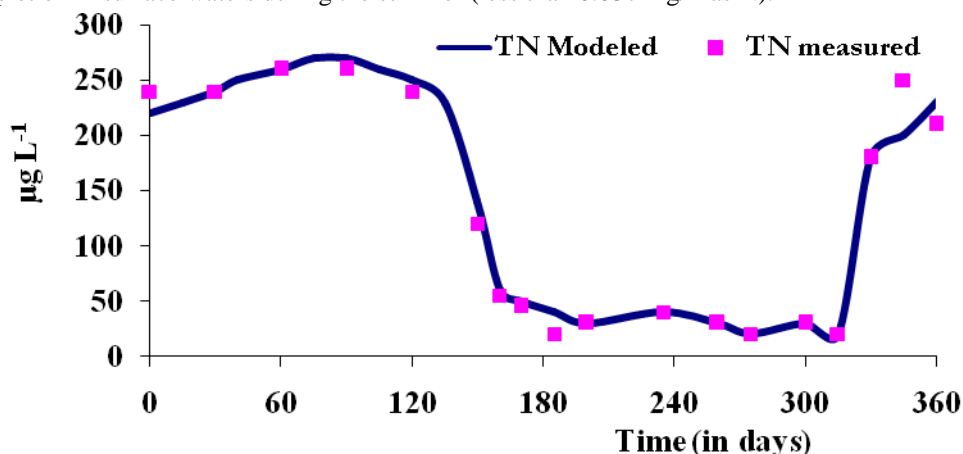


Fig. 5. Comparison between modeled and measured values for total nitrogen (TN) in Ohrid lake

Concentrations of nitrate in the hypolimnion remained relatively high (greater than 0.157 mg/L as N) except for the period of hypolimnetic anoxia in the fall. These trends were not always mimicked by the Lake model, possibly due to inaccurate boundary conditions, inaccurate capture of one or more limnological processes, or both. This is an area where additional data collection, research and additional model refinement may be required for the future. Nitrate is not a critical parameter in characterizing this lake's water quality (recall that blue-green



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algae can fix atmospheric nitrogen), however, so some error in its representation is acceptable for the purposes of this investigation.

Comparing measured and modeled ammonia profiles at the same location, date, and time produced annual MEs between 0 and 0.02 mg/L as N, MAEs between 0.02 and 0.05 mg/L as N and RMSEs between 0.04 and 0.06 mg/L as N for 2013 through 2014 (table 1). Concentrations of ammonia typically were low (< 0.06 mg/L as N), with the exception of samples collected from an anoxic hypolimnion. Therefore, it is not surprising that the goodness-of-fit statistics report a relatively small overall error. The model's overall ability to predict the lake's ammonia concentrations, in addition to the correct timing and general magnitude of ammonia accumulation in the lake's hypolimnion, suggests that the most important influences on ammonia were captured by the model with sufficient accuracy.

IV. CONCLUSIONS

Nutrient constituents (orthophosphorus, total phosphorus, nitrate plus nitrite, ammonia, and total nitrogen) for each of the two lakes are simulated using the CE-QUAL-W2 model. The limited number of pollution sources in combination with the high refresh rate of the lakes water and the inflow of clean karstic groundwater are the main reasons that the water quality remains good.

Simulation results indicated that the model adequately predicted the seasonal dynamics of nutrient concentrations in the epilimnion and the hypolimnion. The model has been shown to be robust in the simulation of nutrients characteristics data examined here.

Further improvements in the model's capabilities will only come with additional data collection and further model testing and development.

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