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Use of principal component scores in multiple linear regression models for simulation of chlorophyll-a and phytoplankton abundance at a karst deep reservoir, southwest of China

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ABSTRACT

The relationships between chlorophyll-a, phytoplankton abundance and 20 chemical, physical and biological water quality variables were studied by using principal component scores (PCs) in stepwise linear regression analysis (SLR) to simulate chlorophyll-a and phytoplankton abundance at a karst deep reservoir, southwest of China. Score values obtained by PC scores were used as independent variables in multiple linear regression models. The following models were used to simulate chlorophyll-a and abundance of Cyanobacteria, Chlorophyta, Bacillariophyta, and Pyrrophyta respectively: chlorophyll-a1 = 10.501 + 1.390 (score 1) ($P < 0.01$), chlorophyll-a 2 = 10.501 + 1.102 (score 1)−0.877 (score 2) ($P < 0.05$), $\log_{10}$ (Cyanobacteria) = 1.277−0.726 (score 2) ($P < 0.05$), $\log_{10}$ (Chlorophyta) = 3.927−0.150 (score 2) ($P < 0.01$), $\log_{10}$ (Bacillariophyta) = 4.872−0.131 (score 4) ($P < 0.01$) and $\log_{10}$ (Pyrrophyta) = 2.463 + 0.578 (score 1) ($P < 0.05$). The models could be used to simulate chlorophyll-a and phytoplankton abundance levels successfully, and revealed that DO, WD, Tem, TD, pH, NH_4–N and TSS were the most important factors regulating the composition of chlorophyll-a and Pyrrophyta abundance. ORP, Cl^-, SO_4^{2-}, TN were the main factors affecting Chlorophyta and Cyanobacteria abundance. F^- and Ca^{2+} were the main factors influencing the Bacillariophyta abundance.

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1. Introduction

Principal components analysis (PCA), which is widely used in the aquatic environmental and ecological modeling, offers an objective method for handling large sets of biotic and abiotic data by reducing the complexity of multidimensional systems through the maximization of component loading variance and elimination of invalid components [17,2,11]. Another advantage of PCA is it further enables one to extract interpretable information on physical–chemical features of a system [8,3,4] by explaining the variance–covariance structure of the original variables. Recently, PCA has been employed either alone or in combination with other methods to model biological and ecological processes [15,18,20,19]. A model can be useful to eliminate multi-colinearity, to remove indirect effect of variables and to reduce the number of variables in multiple regression models, it also can simulate aspects of biology [1,5]. To date, models for predicting chlorophyll-a had been studied infrequently using different ways [10,14,7,6]. The study stations were in a deep karst reservoir. The experiments enabled us to identify the significant factors influencing water quality in the reservoir, and to explore the relationships between the major environmental factors and chlorophyll-a with phytoplankton abundance. The aim of this study is to combine principal component analysis and stepwise linear regression models to identify the main factors affecting changes in chlorophyll-a and phytoplankton and simulate chlorophyll-a and phytoplankton abundance in the karst reservoir.

2. Material and methods

2.1. Study sites

Hongfeng Reservoir(HR) is a deep karst reservoir, located in the southwest of China (105°58′06.34″E–106°38′04.03″E, 26°09′00.42″N–26°41′37.87″N) with a drainage area of 1596 km^2, a volume of 6.01×10^8 m^3, an average water depth of 10.52 m and maximum depth 45 m. It was built on the river in 1960 year in order to generate hydroelectricity and irrigation, but recently, the reservoir is to supply drinking water for Guiyang city. The

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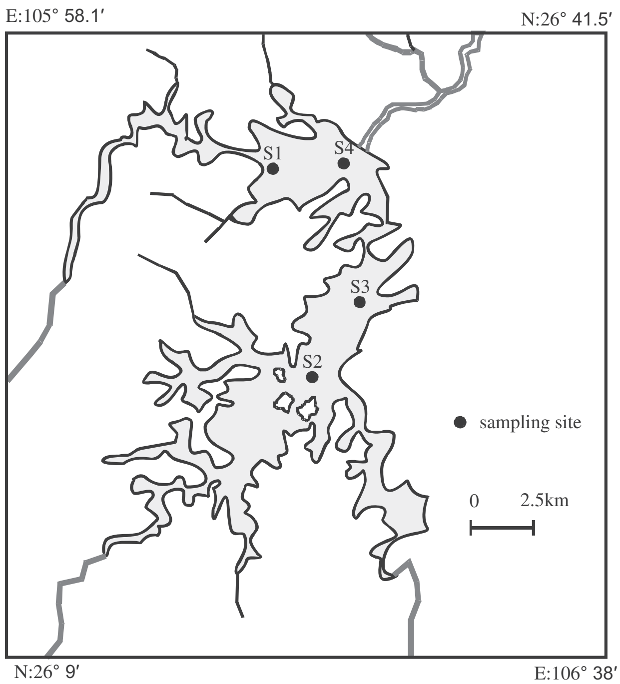

Fig. 1. The sampling stations at the Hongfeng Reservoir.

reservoir is filled by four rivers including Yangchang River, Maxian River, Houlu River and Taoyuan River. Most precipitation occurs during the summer monsoon season (from early May to late September). The water level in the reservoir fluctuates seasonally, with the lowest water level occurring in early summer and the highest in early winter. The reservoir is mesotrophic and even water bloom appeared in summer two years ago. HR is one of the main drinking water sources of Guiyang city, and also plays a role as power generation, flood control, irrigation, aquaculture, tourism and the regulation of natural ecological comprehensive function. Four sampling sites were selected (Fig. 1).

Table 2
Results of principal component analysis.

	Loading of variables				
	PCA1	PCA2	PCA3	PCA4	PCA5
EC	**−0.887**	−0.053	0.251	0.141	−0.016
DO	**0.807**	−0.188	0.529	−0.026	−0.012
WD	**−0.801**	0.289	−0.291	0.213	0.022
pH	**0.766**	−0.265	0.528	−0.078	0.059
TD	**0.736**	0.230	0.039	0.385	0.312
Tem	**0.717**	0.618	0.054	−0.146	0.035
NH_4–N	**−0.689**	0.060	−0.232	0.063	0.551
TSS	**0.635**	0.337	0.375	0.059	−0.003
ORP	−0.363	**−0.877**	0.071	0.077	−0.055
Cl^-	−0.145	**0.751**	0.243	0.426	0.030
SO_4^{2-}	−0.245	**0.702**	0.303	0.486	−0.029
TN	−0.470	**0.579**	−0.026	−0.537	−0.042
Na^+	0.202	**−0.351**	−0.026	−0.330	0.262
TP	0.233	0.526	**−0.738**	−0.079	−0.082
NO_3–N	−0.657	0.249	**0.663**	−0.182	−0.083
K^+	0.576	−0.198	**−0.655**	0.289	−0.165
Mg^{2+}	−0.388	−0.467	**0.564**	0.288	−0.045
F^-	0.107	0.168	0.103	**0.669**	−0.286
Ca^{2+}	−0.022	−0.569	−0.337	**0.599**	0.060
TOC	0.085	0.046	0.084	0.133	**0.872**

Note: Bold numbers represent the highest correlation coefficient of PCA.

2.2. Dates and analytical methods

Water samples were taken in January (winter) in 2010 at four stations (Fig. 1). Temperature (*T*), pH, dissolved oxygen (DO), electricity conductivity (EC) were measured in situ at all locatlities by YSI-6600V2. In the laboratory, the water samples were further analyzed for total phosphorus (TP) and total nitrogen (TN) using potassium persulfate digestion. Water samples were filtered through a 47 mm/45 μm Whatman GF/C filter for ammonium (NH_4–N), nitrates (NO_3–N) were determined colorimetrically, other environmental factors were further analyzed by Chinese Standard Methods of Water Quality Analysis (GB3838-2002). 400–1000 mL water was obtained for chlorophyll-a by filtering on a Whatman GF/A filter, and its concentration was determined within 8 h after

Table l
Descriptive statistics of selected PCs total variance explained.

Component	Initial eigenvalues			Extraction sums of squared loadings		
		% of Variance	Cumulative%	Total	% of Variance	Cumulative%
PCA1	6.062	30.311	30.311	6.062	30.311	30.311
PCA2	3.977	19.885	50.196	3.977	19.885	50.196
PCA3	2.926	14.630	64.827	2.926	14.630	64.827
PCA4	2.100	10.500	75.326	2.100	10.500	75.326
PCA 5	1.371	6.854	82.180	1.371	6.854	82.180
PCA 6	0.929	4.647	86.827			
PCA 7	0.797	3.987	90.814			
PCA 8	0.515	2.574	93.388			
PCA 9	0.394	1.969	95.357			
PCA 10	0.245	1.227	96.584			
PCA 11	0.163	0.815	97.398			
PCA 12	0.134	0.668	98.066			
PCA 13	0.117	0.586	98.652			
PCA 14	0.089	0.443	99.094			
PCA 15	0.072	0.359	99.453			
PCA 16	0.051	0.253	99.706			
PCA 17	0.035	0.176	99.882			
PCA 18	0.015	0.073	99.955			
PCA 19	0.006	0.031	99.986			
PCA 20	0.003	0.014	100.000			

Extraction method: principal component analysis.

Table 3
Results of regression analysis for chlorophyll-a ($n = 36$).

Included Independent variables		Regression coefficients		Standardized coefficients	t	P
		B	Std. error	Beta		
A	Constant	10.501	0.336		31.231	0.000**
	REGR factor score 1 for analysis 1	1.390	0.341	0.573	4.076	0.000**
B	Constant	10.501	0.310		33.845	0.000**
	REGR factor score 1 for analysis 1	1.102	0.333	0.454	3.307	0.002**
	REGR factor score 2 for analysis 1	−.0877	0.333	−0.362	−2.633	0.013*

Dependent variables: chlorophyll-a.

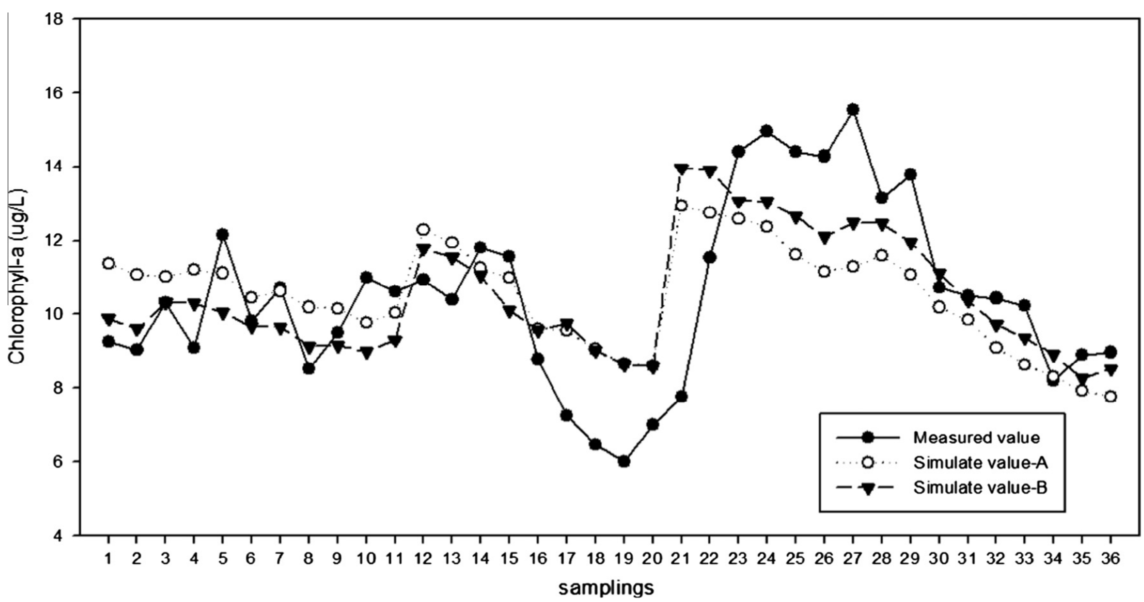

Fig. 2. Measured and simulated chlorophyll-a concentrations in the Hongfeng Reservoir(HF: Hongfeng). *Note:* 1–11 for HFS1-0.5 m, HFS1-2 m, HFS1-4 m, HFS1-6 m, HFS1-8 m, HFS1-10 m, HFS1-12 m, HFS1-14 m, HFS1-16 m, HFS1-18 m, and HFS1-20 m; 12-20 for HFS2-0.5 m, HFS2-2 m, HFS2-4 m, HFS2-6 m, HFS2-8 m, HFS2-10 m, HFS2-12 m, HFS2-14 m, and HFS2-16 m; 21-27 for HFS3-0.5 m, HFS3-2 m, HFS3-4 m, HFS3-6 m, HFS3-8 m, HFS3-10 m, and HFS3-12 m; 28-36 for HFS4-0.5 m, HFS4-4 m, HFS4-8 m, HFS4-12 m, HFS4-16 m, HFS4-20 m, HFS4-24 m, HFS4-28 m, and HFS4-32 m.

Table 4
Results of regression analysis for Cyanobacteria ($n = 36$).

Included independent variables		Regression coefficients		Standardized coefficients	t	P
		B	Std. error	Beta		
C	Constant	1.277	0.278		4.599	0.000**
	REGR factor score 2 for analysis 1	−0726	0.282	−0.404	−2.578	0.014*

Dependent variables: Cyanobacteria.

its extraction in 90% acetone. Phytoplankton was fixed with formalin 3–5% in the field and identified and enumerated (random fields) under the microscope using the settling technique in the laboratory. In addition, the cells colonies and filaments were enumerated to at least 300 specimens of the combined species [9].

2.3. Statistical methods

A Kolmogorov–Smirnov normality test was applied to all 20 water quality variables, chlorophyll-a and phytoplankton abundance of identified species. The abundance data for each species were normalized using a $\log_{10}(X + 1)$ function prior to their use in PCA. Communalities (CO) of variables in the selected PC were found to be greater than 0.70.

2.4. Multiple linear regression analysis

Multiple linear regression analysis with stepwise method was conducted with chlorophyll-a and phytoplankton abundance as dependent variables, respectively, and the PC scores as the independent variable. The model can be generalized as the following:

$$Y_{\text{chlorophyll-a (phytplankton abundance)}} = a + \sum b_k S_k + e$$

where a is a constant term; b_k is the regression coefficient of score values of kth PC; S_k is the score values of kth PC; and e is the error term of the mode; $k = 1$–20. A t-test was used to test the regression coefficients to determine the significance of the coefficient ($P < 0.01$). Weight of variables and values of standardized variables were multiplied to obtain the score values of PCs. Different combi-

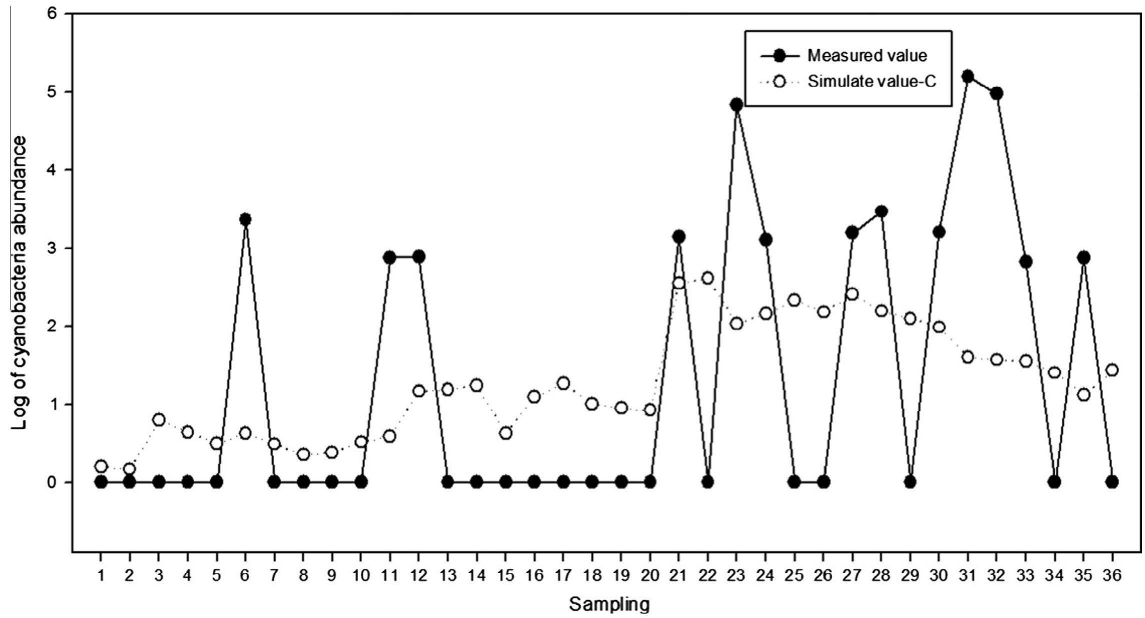

Fig. 3. Measured and simulated Cyanobacteria abundance in the Hongfeng Reservoir. *Note:* The numbers are the same to those in Fig. 2.

Table 5
Results of regression analysis for Chlorophyta (n = 36).

Included independent variables		Regression coefficients		Standardized coefficients	t	P
		B	Std. error	Beta		
D	Constant	3.927	0.067		58.455	0.000**
	REGR factor score 2 for analysis 1	−0.150	0.068	−0.354	−2.204	0.034*

Dependent variables: Chlorophyta.

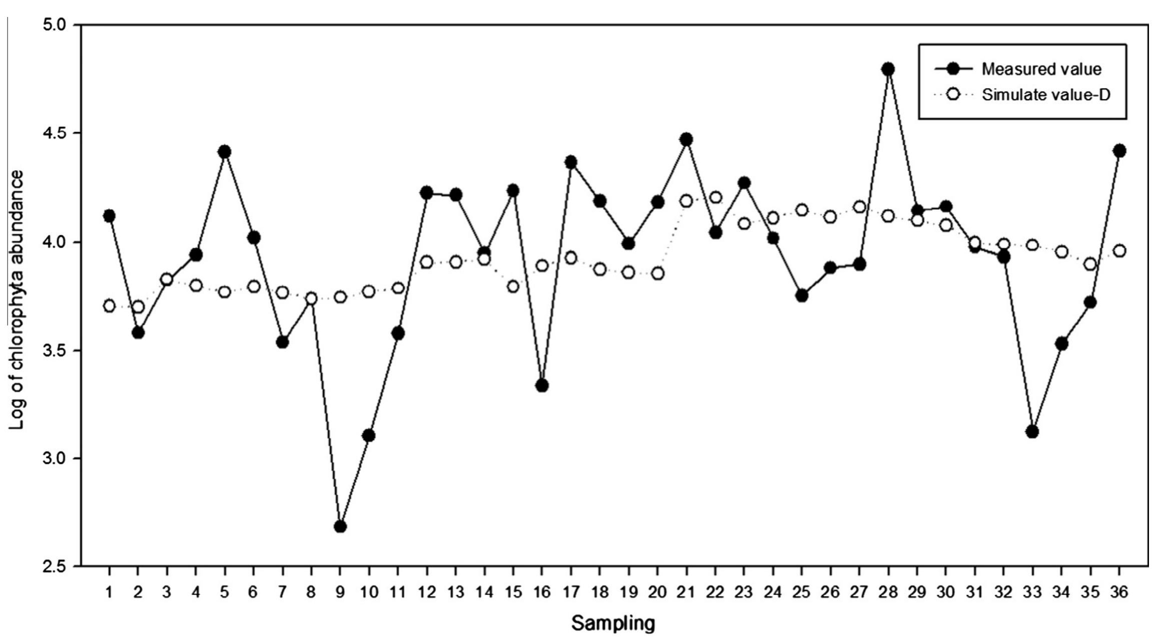

Fig. 4. Measured and simulated abundance of Chlorophyta abundance in the Hongfeng Reservoir. *Note:* The numbers are the same to those in Fig. 2.

nations of the principal component scores (PCs) were used as independent variables ($[X_i]$, $i = 1,2,\ldots 20$) in the stepwise linear regression analysis. These score values were used as independent variables in the stepwise multiple linear regression analysis to determine the most significant PCs for chlorophyll-a and phytoplankton abundance. All the analysis was done using SPSS (18.0).

Table 6
Results of regression analysis for Bacillariophyta ($n = 36$).

Included independent variables		Regression coefficients		Standardized coefficients	t	P
		B	Std.error	Beta		
E	Constant	4.872	0.043		114.079	0.000**
	REGR factor score 4 for analysis 1	−0.131	0.043	−0.461	−3.030	0.005**

Dependent variables: Bacillariophyta.

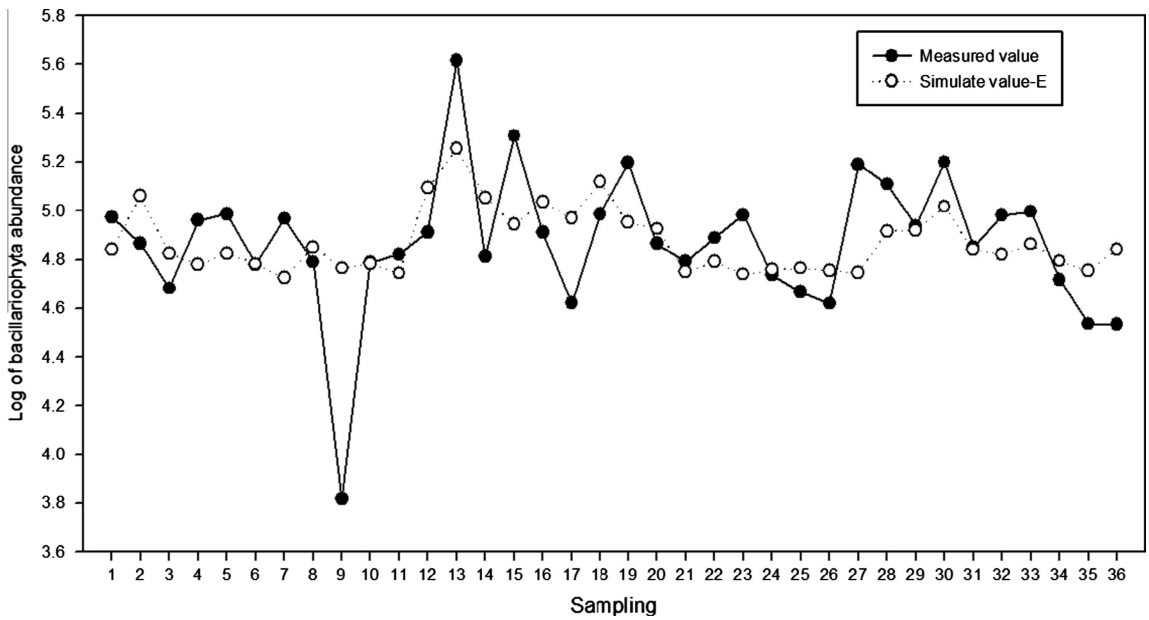

Fig. 5. Measured and simulated abundance of Bacillariophyta abundance in the Hongfeng Reservoir. *Note:* The numbers are the same to those in Fig. 2.

Table 7
Results of regression analysis for Pyrrophyta ($n = 36$).

Included independent variables		Regression coefficients		Standardized coefficients	t	P
		B	Std. error	Beta		
F	Constant	2.463	0.231		10.647	0.000**
	REGR factor score 1 for analysis 1	0.578	0.235	0.389	2.464	0.019*

Dependent variables: Pyrrophyta.
* $P < 0.05$.
** $P < 0.01$.

3. Results and discussion

3.1. Principal component analysis

The principal component analysis selected five components which explained 82.18% of the total variance (Table 1). As suggested by their loadings (Table 2), EC, DO, water depth (WD), pH, turbidity (TD), temperature (Tem), NH_4–N and TSS showed the highest loadings with PC1, while ORP, Cl^-, SO_4^{2-}, TN and Na^+ were grouped in PC2. TP, NO_3–N, K^+ and Mg^{2+} in PC3, $F^-$and Ca^{2+} were in PC4. In PC5, the only meaningful load was TOC.

3.2. Simulation of chlorophyll-a

In model-A, which the PCs was used as the independent variables, only PCs1 was selected as the variable to explain the variance in chlorophyll-a ($P < 0.01$, $R = 0.573$). It appears that with only PCs1, we can simulate chlorophyll-a reasonably well using the following model-A:

$$\text{chlorophyll-a} = 10.501 + 1.390\ (\text{score } 1)$$

Based on the signs of the correlation coefficient of PCs1 in the above model-A and the PCA results where PCs1 was mainly associated with 8 variables, we could further infer that increase in DO, pH, TD, Tem and TSS would lead to increase in chlorophyll-a level, while increase in EC, WD and NH_4–N would lead to decrease in chlorophyll-a level.

With model-B, chlorophyll-a was mostly explained by PC score 1, PC scores 2 ($P = 0.013$). Unlike in model-A, PC scores 2 was also important to simulate chlorophyll-a in model-B. The final model-B can be defined as following (Table 3, Fig. 2)

$$\text{chlorophyll-a2} = 10.501 + 1.102\ (\text{score } 1) - 0.877\ (\text{score } 2)$$

There are many methods to simulate chlorophyll-a. Pérez-Ruzafa forecasted the chlorophyll-a and the relationship between the environmental factors by using the way of differential equation and correlation [16]. French also successfully simulated the chlorophyll-a contents by TP and Tem, there was a strong correlation [7]. In our models, the chlorophyll-a concentrations had been relatively successful forecasted and found out the main environmental factor to influence on chlorophyll-a. In the Hongfeng Reservoir, EC, DO, WD, Tem, pH value, TD, NH_4–N and TSS were the main environment factors to influence chlorophyll-a. EC, WD and NH_4–N were the obvious negative correlation. On one hand, it revealed that chlorophyll-a would reduce with the increase of the depth at karst deep reservoir; On the other hand, nutrients were not the main factors of influence changes of chlorophyll-a, reflected the water eutrophication bodies, hydrological conditions and other environment factors affected phytoplankton change.

3.3. Simulation of phytoplankton abundance

Using similar method for chlorophyll-a, we also modeled the phytoplankton abundance which may give us additional information on the relationships between eutrophication and water blooms.

3.3.1. Simulation of Cyanobacteria abundance

Weight of variables and values of standardized variables were multiplied to obtain the score values of PCs, the result of model-C (Table 4) suggests that PC scores 2 was significant simulation of Cyanobacteria abundance. Fig. 3 showed the measured and simulated values of Cyanobacteria abundance. Simulated Cyanobacteria abundance was calculated from:

$$\log_{10}\ (\text{Cyanobacteria}) = 1.277 - 0.726\ (\text{score } 2)$$

The model-C suggested that increase in score 2 variables, such as Cl^-, SO_4^{2-} and TN would contribute to decrease in Cyanobacteria abundance. However, the boosted ORP and Na^+ brought forth an improved response (a similar varied trend) for Cyanobacteria abundance.

3.3.2. Simulation of Chlorophyta abundance

Weight of variables and values of standardized variables were multiplied to obtain the score values of PCs. but the result of model -D (Table 5) suggests that PC scores 2 was significant predictor for Chlorophyta abundance. Fig. 4 showed the measured and simulated values of Chlorophyta abundance. Simulated Chlorophyta abundance was obtained from:

$$\log_{10}\ (\text{Chlorophyta}) = 3.927 - 0.150\ (\text{score } 2)$$

The model revealed that increase in score 2 variables, such as Cl^-, SO_4^{2-} and TN would lead to decrease in Chlorophyta abundance. However, increase in ORP and Na^+ would lead to increase in Chlorophyta abundance. Fig. 4 showed that our model could predict Chlorophyta abundance only by score 2 ($R = 0.345$, $P < 0.05$); many factors affected Chlorophyta, and Cl^-, SO_4^{2-}, ORP, Na^+ and TN were the main ones.

3.3.3. Simulation of Bacillariophyta abundance

Only score 4 had a significant linear relationship with Bacillariophyta abundance. As seen from Table 6, simulated (model-E) values of Bacillariophyta abundance and observed (empirical) values were given in Fig. 5. Predicted Bacillariophyta abundance was gained from:

$$\log_{10}\ (\text{Bacillariophyta}) = 4.872 - 0.131\ (\text{score } 4)$$

score 4 had a negative impact on Bacillariophyta abundance. Bacillariophyta would be expected to decrease as the values of score 4 increased. Consequently, a total increase in significant variables of score 4, which was, F^- and Ca^{2+} would lead to a decrease in Bacillariophyta abundance. We concluded that the model could predict Bacillariophyta abundance only by score 4 ($R = 0.461$, $P < 0.01$). This meant that many factors affected Bacillariophyta, and F^- and Ca^{2+} were the main ones.

3.3.4. Simulation of Pyrrophyta abundance

Only score 1 had a significant linear relationship with Pyrrophyta abundance. As seen from Table 7, simulated (model-F) values of Pyrrophyta abundance and observed (empirical) values were displayed in Fig. 6. Simulated Pyrrophyta abundance was obtained from:

$$\log_{10}\ (\text{Pyrrophyta}) = 2.463 + 0.578\ (\text{score } 1)$$

score 1 had a positive impact on Pyrrophyta abundance. Pyrrophyta would be expected to increase as the values of score 1 increased. Consequently, a total increase in significant variables of score1, namely, we can further infer that increase in DO, pH, TD, Tem and TSS would lead to increase in chlorophyll-a level, while increase in EC, WD and NH_4–N would lead to a decrease in Pyrrophyta

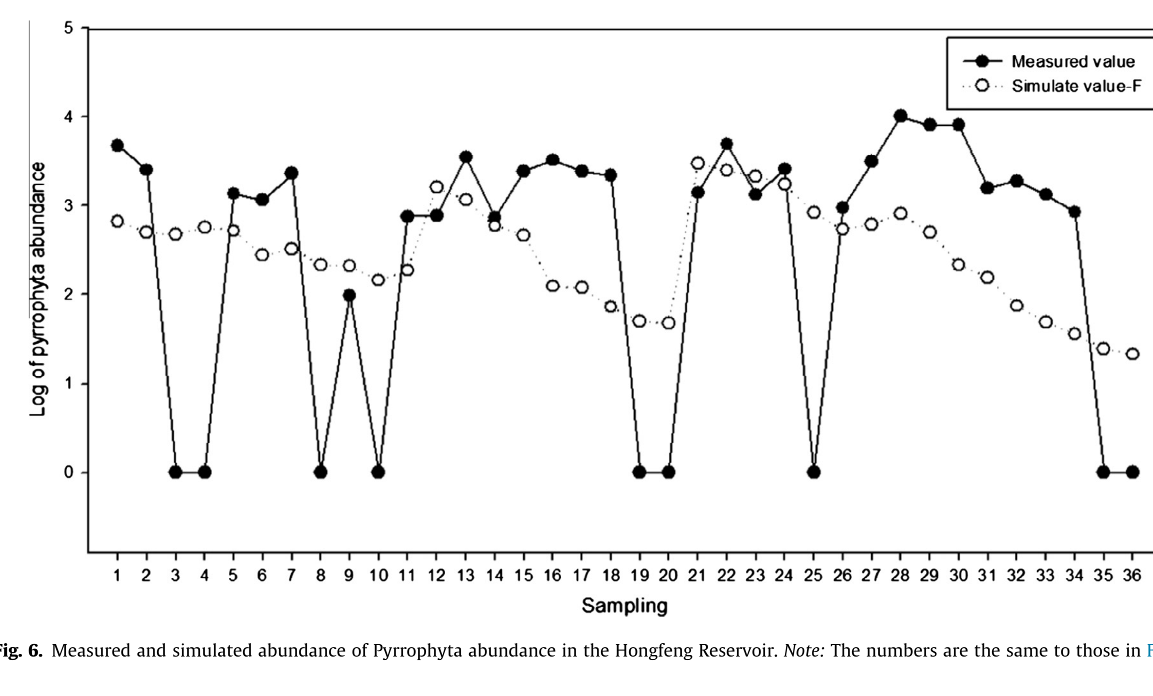

Fig. 6. Measured and simulated abundance of Pyrrophyta abundance in the Hongfeng Reservoir. *Note:* The numbers are the same to those in Fig. 2.

abundance. We arrived at the result that the model could predict Pyrrophyta abundance only by score1 ($R = 0.389$, $P < 0.05$), though many factors affected Pyrrophyta.

At present, the methods to forecast phytoplankton abundance were relatively less. CCA analysis revealed the relationships between the phytoplankton community and environmental factors [13]. This way could reflect the phytoplankton distribution pattern based on phytoplankton abundance, but could not simulate phytoplankton abundance. From the models, relatively successful forecast phytoplankton abundance dynamic changes in the Hongfeng Reservoir, especially in the diatom abundance, showed a strong correlation. On one hand, the phytoplankton qualitative and quantitative study in the Hongfeng Reservoir, diatom was the common type and relatively stable, so it was easy to simulate; on the other hand was Cyanobacteria and other algae changed quickly, increased the difficulty to simulate phytoplankton abundance, but these models still showed a good results [12].

4. Conclusion

It occurs for complex interactions between environmental factors which affect chlorophyll-a and phytoplankton abundance in reservoirs and lakes. In the Hongfeng Reservoir, the phytoplankton community was dominated by Cyanobacteria, Chlorophyta and Bacillariophyta in different seasons. This principal component analysis identifies DO, WD, Tem, TD, pH, NH_4–N and TSS as the critical factors regulated dynamics of chlorophyll-a. DO, WD, Tem, TD, pH, NH_4–N and TSS were the most important factors regulated the composition of Pyrrophyta abundance. ORP, Cl^-, SO_4^{2-}, TN were the main factors affected Chlorophyta and Cyanobacteria abundance. Finally, F^- and Ca^{2+} were the main factors affecting the Bacillariophyta abundance. In the models, we can simulate chlorophyll-a and phytoplankton abundance successfully. It is of critical importance for water resources management at the Hongfeng Reservoir.

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