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1 **Parameter Uncertainty and Sensitivity Analysis of**
2 **Water Quality Model in Lake Taihu, China**

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16 **Abstract:** Lake Taihu was chosen as a case for parameter uncertainty and
17 sensitivity analysis of water quality simulation in large shallow lakes. Forty
18 parameters in Environmental Fluid Dynamic Code model (EFDC) were filtered and
19 analyzed. The results showed that parameters had a considerable influence on
20 simulation and three groups of parameters related to algal kinetics (i.e. PMc, BMRc
21 and PRRc), light (KeChl) and temperature (KTG1c) were very sensitive. For shallow
22 lakes with frequent algal blooms, light extinction due to Chlorophyll-a is also a
23 sensitive parameter. While the temperature effect coefficient for algal growth is
24 sensitive for lakes with seasonal temperature variation. Sensitive parameters and their
25 relevant uncertainty varied spatially. For high nutrients and algae concentration
26 subareas, temperature was more likely to be a limiting factor, whereas sensitive
27 factors could be light in lower concentration subareas. Since most sensitive
28 parameters were related to algae, uncertainty in simulation increased with increasing
29 algal kinetic processes over time and varied in different subareas. Lower nutrients and
30 algae concentration subareas were more easily influenced by model parameters while
31 nearshore areas were highly influenced by boundary conditions. For better simulation
32 of water quality, variable stoichiometry phytoplankton models should be considered
33 and zooplankton need to be integrated into the model explicitly rather than a fixed
34 predation rate.

35 **Key words** Lake Taihu; Sensitivity analysis; Uncertainty analysis; Water quality
36 models;

37 **1 Introduction**

38 Water quality models (WQMs), valuable tools of supporting water quality
39 predictions, have been widely applied in environmental management in recent years
40 (Arhonditsis and Brett 2005; Li and Zhang et al. 2015; Xu et al. 2013; Cerco and Cole
41 1993). However, the inherent uncertainty of these models is greatly influenced by
42 factors including model-structure uncertainty, model-input uncertainty,
43 model-parameter uncertainty and measurement errors (Radwan et al. 2002). With the
44 development and application of performance computing technology, many water
45 quality models with good structure and complex parameters have been developed
46 (Wang, Li and Jia et al. 2013). However, an increasing number of parameters has
47 resulted in a sharp increase in computational requirements and thus exacerbated the
48 complexity of these models. Highly interactive parameter spaces and the nonlinear,
49 non-monotonous objective spaces have increased the difficulty of calibration. (Gupta
50 et al. 2000; Herman et al. 2013; Yi et al. 2016).

51 In order to improve the accuracy and rationality of model predictions and study
52 the parametric uncertainty and sensitivity of models, we conducted several
53 uncertainty and sensitivity studies in different water bodies such as rivers, lakes,
54 reservoirs, estuaries and coasts to identify subsets of important model parameters that
55 significantly influence model outputs have been carried out (Muleta et al. 2005;
56 Neumann 2012; Yi et al. 2016). Amongst these studies, large shallow lakes are often
57 accompanied with complex hydrodynamic and eutrophication problems. The
58 simulation of water quality is difficult and few studies were conducted on parameters
59 under different situations.

60 The hydrodynamic conditions in large shallow lakes are highly influenced by
61 wind-wave. They are not like other deep lakes or reservoirs which may be driven by
62 thermal stratification. Parameters related to wind and wave like wind drag coefficient
63 were supposed to be sensitive parameters in simulation (Li and Tang et al. 2015).
64 Some large shallow lakes also face serious eutrophication and algal bloom problems

65 like Lake Taihu. Parametric uncertainty is considerable with parameters related to
66 growth, respiration and death of algae and zooplankton generally sensitive in lake
67 eutrophication models (Omlin et al. 2001; Missaghi et al. 2013). Three factors (i.e.
68 nutrients, temperature and light) are considered to control the algal growth but the
69 limitation factors are normally not so clear in many cases. For example, phosphorus
70 was thought to be the limitation factors in Lake Taihu before but the influence of
71 nitrogen is also quite important by recent researches (Tang et al. 2016; Paerl et al.
72 2011). Some typical large shallow lake models, which have been analyzed with
73 different methods, showed that parameters related to light and temperature were
74 significant, for example in the Venician Lagoon (Pastres and Ciavatta 2005; Pastres et
75 al. 1997), and Dian Lake, China (Yi et al. 2016). Parameters related to limitation
76 factors will change according to real situation and sensitivities of these parameters
77 need to be investigated. Sediment is also an important source of pollution, and
78 parameters related to settling velocity and mineralization were found to be sensitive in
79 some models (Missaghi et al. 2013). Researches on different models of shallow lakes
80 suggested that the adsorption constant was relatively important in the simulation of
81 total nitrogen, whereas mineralization and settling rates were sensitive to total
82 phosphorus (Janse et al. 2010).

83 Meteorological and hydrodynamic situations, pollutant inflow and bathymetric
84 variance in lakes and reservoirs results in inherent temporal and spatial variability in
85 water quality (Missaghi et al. 2013). In a multi-dimensional model formulated by
86 physical, chemical, and biological processes, model behavior may vary across the
87 spatial domain whilst time-dependency should also be considered because of
88 time-varying sensitivities (Herman et al. 2013; Wang, Li and Lu et al. 2013; Herman
89 et al. 2013). However, few studies involving complex water quality models of
90 multi-dimensional lakes or reservoirs have been conducted on this problem.

91 In this research, we choose Lake Taihu, a large shallow lake, the third largest
92 freshwater lake in China, as an example to make relevant analysis. The water quality

93 module of the Environmental Fluid Dynamic Code (EFDC) was chosen for the
94 simulation, and water quality indicators such as ammonia nitrogen, nitrate nitrogen
95 phosphate and chlorophyll-a as model outputs. The objectives of this study were thus
96 to: (1) quantify the sensitivity of parameters in simulation of water quality model and
97 evaluate uncertainty caused by it; (2) analyze the spatial-temporal variability of
98 uncertainty and sensitivity; and (3) compare with other lakes and extend the result to a
99 larger modelling community. The results can be utilized in the design of a reasonable
100 water quality model for large shallow lakes and improve the efficiency of calibration
101 of such models.

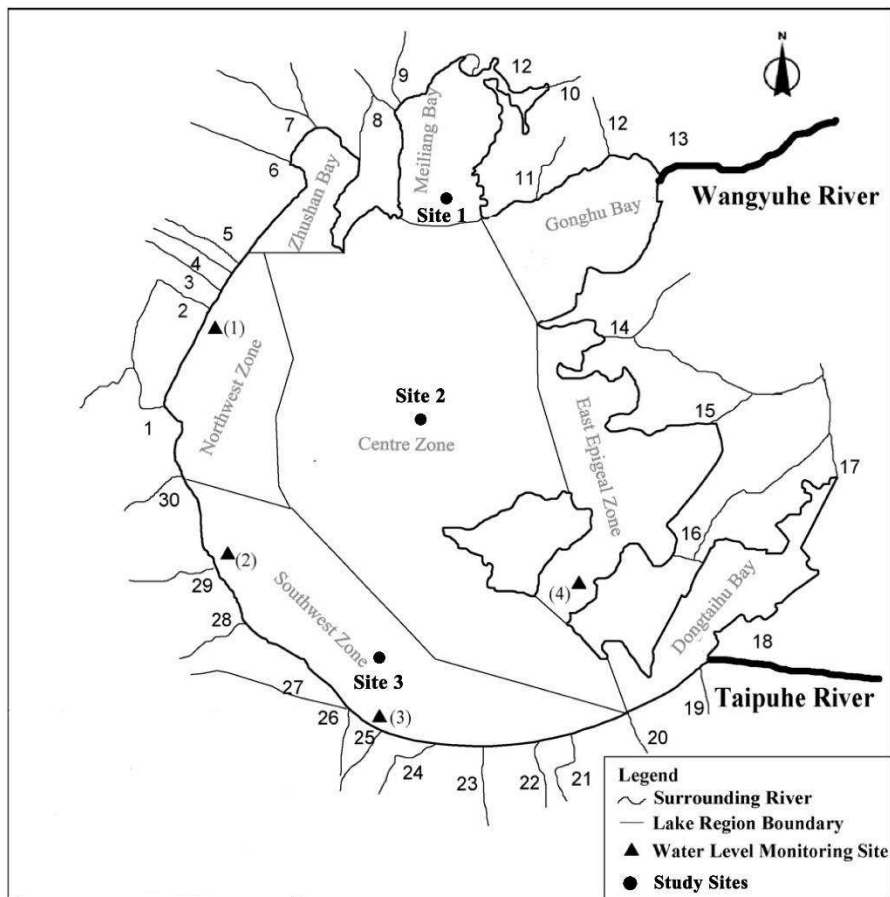
102 **2 Methods and materials**

103 **2.1 Study area**

104 Lake Taihu (longitude 119°08'–122°55'E, latitude 30°05'–32°08'N) is the third
105 largest shallow freshwater lake in China, with a surface area of 2,338 km² and a
106 catchment area of 36,500 km² (Zhu et al. 2007). The average depth of the lake is 1.9m
107 and the maximum depth is 2.6m, corresponding to an elevation of 3.0m a.s.l. (Qin
108 2009). The floor of the lake features flat terrain with an average topographic gradient
109 of 0°0'19.66". Lake Taihu has complex shoreline geometry and is connected to 172
110 rivers or channels (Qin 2009), and the mean hydraulic retention time is about 300d.
111 The water quality of the lake is seriously deteriorated. Nuisance algal blooms often
112 occur in summer and early fall in most lake areas, especially Meiliang Bay and
113 Zhushan Bay. The blooms are considered to be the result of a combination of high
114 nutrient loading and weak hydrodynamics (Mao et al. 2008). For the convenience of
115 management and monitoring, Lake Taihu have been divided into eight subareas (Liu
116 et al. 2014; Zhang et al. 2010). Three subareas (i.e. Meiliang Bay, Central Zone and
117 Southwest Zone) represent bay, central and nearshore zones respectively, and
118 represent different hydrodynamic and water quality situations for uncertainty and
119 sensitivity analysis in the water quality model (Fig. 1).

120 2.2 Model set-up and calibration

121 The Environmental Fluid Dynamic Code, a three-dimensional hydrodynamic
122 model originally developed by John Hamrick (Hamrick 1996), is utilized to
123 simulate water quality in Lake Taihu. The model is one of the most widely applied
124 advanced modeling frameworks for simulating hydrodynamics, water quality,
125 eutrophication, and dynamic changes and interactions in sediment transportation in
126 lakes, rivers and estuaries (Park et al. 2012; Kim et al. 2011; Li et al. 2011). A large
127 number of applications have demonstrated that the model has considerable generality,
128 convenient operation, and faster calculation times (Wu and Xu 2011; Youngteck and
129 Jinhyeog 2009).

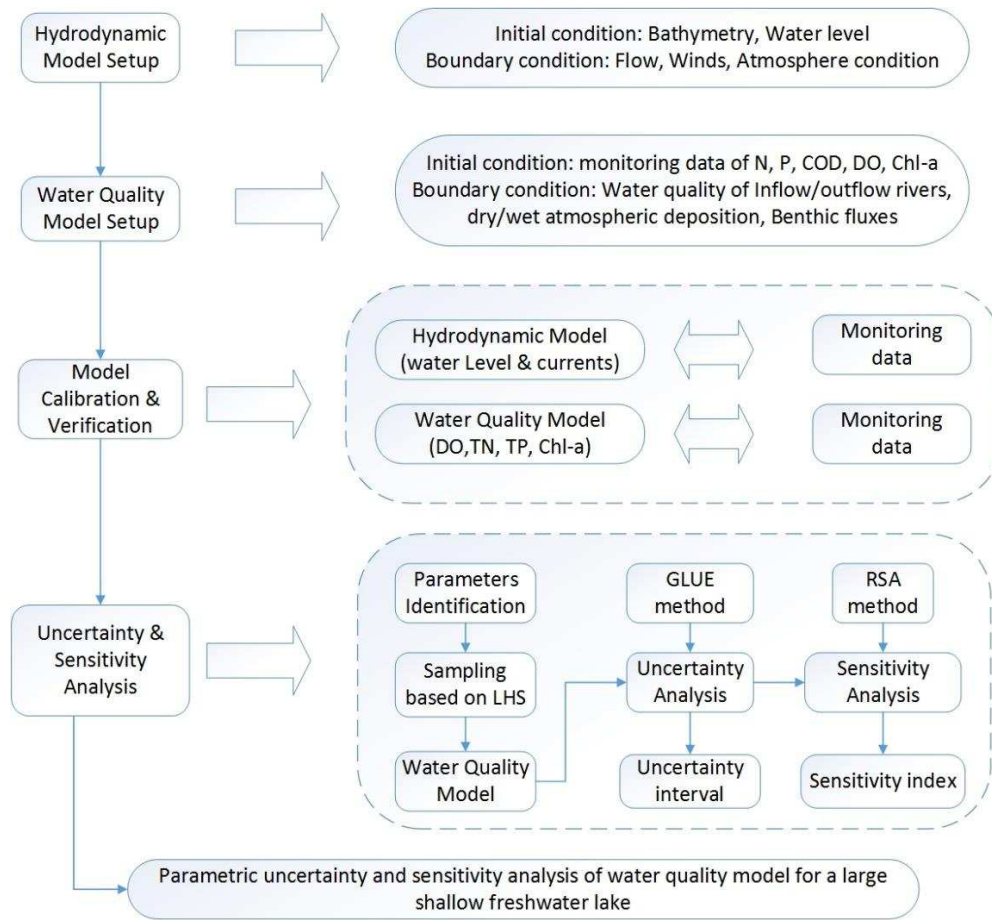


130
131 **Fig.1** Location of the study area, surrounding rivers and monitoring stations in and around Lake
132 Taihu, China. Water level monitoring stations (1) - (4) represent Dapukou, Jiapu, Xiaomeikou and
133 Xishan respectively.

134 Uniform rectangular grids were utilized to set-up the model for Lake Taihu in the
135 horizontal plane. In the vertical direction, vertical sigma coordinates with an evenly

136 distributed three-layer system were adopted as a trade-off between resolution and
137 stability issues (Li and Tang et al. 2015). The effect of temperature stratification was
138 ignored because the lake was shallow. The model was driven by atmospheric forcing,
139 surface wind stress, tributary inflow/outflow, and benthic fluxes (Fig. 2).
140 Inflow/outflow tributaries were generalized into 30 primary rivers (Fig. 1).
141 Atmospheric precipitation data was obtained by averaging data from eight monitoring
142 stations near the lake (Fig. 1). The wind data was collected from previous field
143 monitoring (Li and Tang et al. 2015). Benthic fluxes were set zonally by field
144 experiment and previous research (Pang and Wang 1994), and the dry/wet
145 atmospheric deposition was set by field experiment (Song et al. 2005; Yang et al.
146 2007). We try to run the model for several days with an assumption that the lake
147 surface was level and then the initial hydrodynamic conditions was set by the average
148 value of simulation on the first day. It is also applied in our previous study and can
149 help alleviate the influence of initial conditions on the simulation results. The initial
150 condition of water quality was set by the monitoring data in the first few days of
151 January from the 30 monitoring sites in Lake Taihu, including water temperature and
152 the concentrations of DO, COD, NO_3^- -N, NH_4^+ -N, TN, PO_4^- , TP and Chl-a. The
153 simulated time lasted for one year (From 1 Jan to 31 Dec), and a 10-s time step was
154 used as a trade-off between computational speed and stability issues.

155 Parameters concerned with the hydrodynamic processes were the same as those
156 used in previous studies (Li and Tang et al. 2015), and the results of current
157 calibrations have been presented in previous research (Li et al. 2011). Annual
158 monitoring data of water quality variables from 2005 was used to calibrate the water
159 quality module, and relative errors were less than 30% on the whole. The amount of
160 error remained significant after calibration, and therefore parametric uncertainty was
161 estimated and the most sensitive parameter(s) was investigated in order to improve the
162 model.



163

164 **Fig.2** Methodology flowchart of uncertainty and sensitivity analysis.

165 **2.3 Methods of uncertainty and sensitivity analysis**

166 Uncertainty and sensitivity analysis for the water quality module in EFDC for
 167 Lake Taihu was conducted based on the GLUE and RSA methods. The main analysis
 168 procedure is shown as follows.

169 **2.3.1 Parameter identification**

170 The simulation of water quality with EFDC involves a large number of
 171 parameters. It was not feasible or necessary to take all parameters into consideration
 172 (Muleta et al. 2005), so a reduction in the number of parameters based on the actual
 173 simulations was performed. Taking into account that the predominant type of algae in
 174 Lake Taihu is cyanobacteria, especially when algal blooms happened (Feng et al.
 175 2016; Lu et al. 2016; Yue et al. 2014), we excluded all parameters relating to other
 176 algal species, i.e. macroalgae, diatoms, and greens. The competitive relationships

177 between algal groups were omitted to reduce the number of parameters. Sediment is
 178 another factor that can have a great impact on the simulation result. The sediments
 179 module and water quality module were separated in EFDC model. It is difficult to
 180 calibrate the simulation results and the sampling quantity will increase exponentially
 181 if we include the sediments part. In our previous research, field observations with
 182 using of advanced devices were conducted on the lake to find behaviours of sediments
 183 settling and resuspension (Gao et al. 2017). Diffusive exchange of dissolved phase
 184 nutrients between water column and interstitial waters was investigated in many
 185 studies as well (Yu et al. 2016; Huang et al. 2015; Qiu et al. 2015; Kaiming et al.
 186 2014). Thus, we set the model with fixed benthic flux rates spatially by recent
 187 researches to simulate the processes of sediment instead (i.e. phosphate,
 188 ammonia-nitrogen, nitrate nitrogen, chemical oxygen demand, sediment oxygen
 189 demand). Since these processes were highly influenced by the hydrodynamic
 190 conditions driven by wind-wave in the lake, we set flux rates with considering about
 191 the influence of wind (Yu et al. 2016; Huang et al. 2015; Qiu et al. 2015; Kaiming et
 192 al. 2014). In addition, parameters about reference temperature, optimal depth for algal
 193 growth, and other parameters not likely to be modified in most cases were set to
 194 default values. Finally, 40 parameters were determined for further study and their
 195 descriptions are summarised in Table 1. The ranges of these parameters for
 196 uncertainty and sensitivity analysis were determined through a detailed investigation
 197 of the literature (He et al. 2011; Seo and Kim 2011; Wang and Zou et al. 2014; Wang
 198 and Jiang et al. 2014; Arhonditsis and Brett 2005).

199 **Table 1** Statistical features of the water quality module parameters for sampling.

Parameters groups	Parameters	Description	Units	Distribution	Min	Max
Algal Kinetic	PMc	Maximum growth Rate for Cyanobacteria	1/day	Uniform	2	5
	BMRc	Basal Metabolism Rate for Cyanobacteria	1/day	Uniform	0.01	0.06
	PRRc	Predation Rate on Cyanobacteria	1/day	Uniform	0.01	0.06
Nitrification	rNitM	Maximum Nitrification Rate	1/day	Normal	0.04	0.2
Dissolved Oxygen	KRO	Reaeration Rate Constant	-	Uniform	1.5	5.32
Chemical Oxygen Demand	KCD	COD Decay Rate	1/day	Uniform	0.01	0.15
Dissolution and Mineralization	KRN	Minimum Hydrolysis Rate of RPON	1/day	Normal	0.001	0.01

	KLN	Minimum Hydrolysis Rate of LPON	1/day	Normal	0.01	0.1
	KDN	Minimum Mineralization Rate of DON	1/day	Normal	0.01	0.08
	KRC	Minimum Dissolution Rate of RPOC	1/day	Normal	0.001	0.01
	KLC	Minimum Dissolution Rate of LPOC	1/day	Normal	0.01	0.1
	KDC	Minimum Dissolution Rate of DOC	1/day	Normal	0.005	0.15
	KRP	Minimum Hydrolysis Rate of RPOP	1/day	Normal	0.001	0.01
	KLP	Minimum Hydrolysis Rate of LPOP	1/day	Normal	0.01	0.1
	KDP	Minimum Mineralization Rate of DOP	1/day	Normal	0.01	0.3
Light	Keb	Background Light Extinction Coefficient	1/m	Uniform	0.45	0.55
	KeTSS	Light Extinction due to TSS	1/m per mg/l	Uniform	0.01	0.1
	KeChl	Light Extinction due to Chlorophyll a	1/m per mg/l	Uniform	0.01	0.07
	IsMIN	Minimum Optimum Solar Radiation	Langley /day	Uniform	40	60
Half-Sat Constant	KHNitDO	Oxygen Half-Sat Constant for Nitrification	gO ₂ /m ³	Uniform	0.5	1
	KHNitN	NH ₄ Half-Sat Constant for Nitrification	gN/m ³	Uniform	0.5	1
	KHCOD	Oxygen Half-Saturation Constant for COD Decay	mg/L O ₂	Uniform	1	1.5
	KHNc	Nitrogen Half-Saturation for Cyanobacteria	mg/L	Normal	0.01	0.25
	KHPc	Phosphorus Half-Saturation for Cyanobacteria	mg/L	Normal	0.001	0.05
	KHDNN	Half-Sat Constant for Denitrification	gN/m ³	Uniform	0.05	0.2
	KHORDO	Oxygen Half-Sat Constant for Algal Respiration	gO ₂ /m ³	Uniform	0.5	2
Temperature	KTHDR	Temperature Effect Coefficient for Dissolution	-	Normal	0.05	0.1
	KTMNL	Temperature Effect Coefficient for Mineralization	-	Normal	0.05	0.1
	KTCOD	Temperature Rate Constant for COD Decay	-	Uniform	0.03	0.05
	KNit1	Suboptimal Temperature Coefficient for Nitrification	-	Normal	0.002	0.006
	KNit2	Superoptimal Temperature Coefficient for Nitrification	-	Normal	0.002	0.006
	KTG1c	Suboptimal Temperature Effect Coefficient for Growth, Cyanobacteria	-	Uniform	0.001	0.01
	KTG2c	Superoptimal Temperature Effect Coefficient for Growth, Cyanobacteria	-	Uniform	0.001	0.01
	TMc1	Lower Optimal Temperature for Growth, Cyanobacteria	degC	Uniform	20	27
	TMc2	Upper Optimal Temperature for Growth, Cyanobacteria	degC	Uniform	27	30
	KTR	Reaeration Temperature Rate Constant	-	Normal	1	1.05
	KTBc	Temperature Effect Coefficient for Basal Metabolism, Cyanobacteria	-	Uniform	0.05	0.08
Settling Velocity	WSc	Settling velocity for cyanobacteria	m/day	Uniform	0.05	0.3
	WSrp	Settling velocity for refractory POM	m/day	Uniform	0.2	1
	WSlp	Settling velocity for labile POM	m/day	Uniform	0.2	1

200 2.3.2 Sampling of input parameters with the LHS method

201 Input parameters were sampled by using the Latin Hypercube Sampling (LHS)
202 method, a random sampling method which is commonly used for uncertainty and
203 sensitivity analysis (Manache and Melching 2008). The LHS method works by taking

204 the range of each independent parameter, dividing the range by the selected
205 realizations, rearranging the values into a random distribution, and then combining the
206 distributions for each independent parameter (Xu and Gertner 2008). As the variable
207 space was sampled with relatively few samples in LHS, the number of model runs
208 could be less compared with Monte Carlo sampling. In the study, 100, 300, 500, 1000
209 and 2000 realizations were generated by using LHS and were tested in order to obtain
210 their optimal realizations for analyzing model uncertainty and sensitivity.

211 Using the robustness test, we found that the results of the sensitivity analysis
212 were nearly stable when the sampling quantity was greater than 500. Therefore, taking
213 into consideration the computational cost and the stability of the result, we chose 500
214 Latin hypercube samples for uncertainty and sensitivity analysis.

215 **2.3.3 Uncertainty analysis with the GLUE method**

216 The GLUE methodology (Beven and Binley 1992) was utilized to quantify the
217 uncertainty of the model. The method, which avoided the optimal partial solution, was
218 suitable for the water quality model with equifinality of different parameter sets and.
219 It is commonly used in river, lake, and rainfall-runoff models (Blasone et al. 2008).

220 500 sets of parameters obtained from random sampling using the LHS method
221 were used in this model, and 500 sets of simulation results were obtained. The
222 following formula was used to calculate the likelihood measure of the simulated
223 results:

$$224 \quad L(\theta_i/Y) = 1 - \alpha_i^2/\alpha_0^2 \quad (1)$$

225 Where $L(\theta_i/Y)$ is the likelihood measure for the i th model conditioned on the
226 observations, α_i^2 is the error variance for the i th model (i.e. the combination of the
227 model and the i th parameter set), and α_0^2 is the variance of the observations.

228 To ensure that the group of parameters can represent the functional
229 characteristics of the model, a threshold was set to exclude these groups from the
230 results and normalized likelihood measure by using the linear function:

231
$$l(\theta_i/Y) = \frac{L(\theta_i/Y) - L_{min}(\theta_i/Y)}{L_{max}(\theta_i/Y) - L_{min}(\theta_i/Y)} \quad (2)$$

232 Where $L(\theta_i/Y)$ is the likelihood measure calculated by using formula (1),
 233 $l(\theta_i/Y)$ is the likelihood measure that has been normalized, $L_{min}(\theta_i/Y)$ and
 234 $L_{max}(\theta_i/Y)$ are the minimum and maximum likelihood measures respectively.

235 The normalized likelihood measure was sorted by value and the 97.5th and 2.5th
 236 percentiles were chosen as the upper and lower bounds of confidence intervals.
 237 Proportion of observations in uncertainty interval and ratio of uncertainty interval to
 238 mean concentration were calculated to evaluate the uncertainty of the model.

239 **2.3.4 Parametric sensitivity analysis with the RSA method**

240 The RSA methodology is utilized to analyze the sensitivity of parameters. The
 241 method overcomes the constraints of single factor analysis in traditional sensitivity
 242 analysis, and complex assumptions were not necessary.

243 Marginal cumulative distributions were calculated by likelihood measure, and
 244 sensitivity can be assessed qualitatively by examining differences between 10
 245 distributions of the parameter. The degree of dispersion of the lines is the visual
 246 measure of a model's sensitivity to an input parameter. To acquire the sensitivity
 247 accurately, the sensitivity indices (SI) of parameters in the three subareas were then
 248 calculated by adopting the Kolmogorov-Smirnov (K-S) test (Kottegoda and Rosso
 249 1997). The K-S test is a non-parametric test which can be used to compare different
 250 samples. The method is one of the most useful and general nonparametric methods for
 251 comparing the difference of samples and it is sensitive to differences in both location
 252 and shape of the empirical cumulative distribution functions of samples.

253 First, 500 sets of simulation results were divide into ten groups by the likelihood
 254 measure and the empirical distribution function F_n for n iid observations X_i in each
 255 group is defined as

256
$$F_n(x) = \frac{1}{n} \sum_{i=1}^n I_{[-\infty, x]}(X_i) \quad (3)$$

257 where $I_{[-\infty, x]}(X_i)$ is the indicator function, equal to 1 if $X_i \leq x$ and equal to 0

258 otherwise. The Kolmogorov–Smirnov statistic used to quantify a distance between the
259 empirical distribution functions of different groups is:

$$260 \quad D_{i,j} = \sup |F_{i,n}(x) - F_{j,m}(x)| \quad (4)$$

261 where $F_{i,n}(x)$ and $F_{j,m}(x)$ are the empirical distribution functions of two
262 samples respectively (i, j were the number of groups) and \sup is the supremum of the
263 set of distances. The maximum vertical distances (MVD) were then calculated as
264 Sensitivity Indices (SI) to quantify the sensitivity.

$$265 \quad MVD = SI = \max(D_{i,j}) \quad (5)$$

266 The parameters were divided into three levels by the sensitivity indices: very
267 sensitive parameters ($SI \geq 0.25$, $P < 0.05$), sensitive parameters ($0.1 < SI < 0.25$, $P \leq 0.05$),
268 and insensitive parameters ($SI \leq 0.1$, $P > 0.05$). The interval range of these parameters
269 was divided into 10 groups. Finally, the posterior distributions of these parameters
270 were calculated to discover suitable ranges in simulation.

271 In this research, a matlab toolbox for global sensitivity analysis (Pianosi et al.
272 2015) was utilized to analyze the output data.

273 **3 Results**

274 **3.1 Model uncertainty analysis**

275 The reliability and uncertainty of the model was studied by setting the threshold
276 of the Nash-Sutcliffe efficiency coefficient (NSE) to 0.5. The 2.5th percentile and the
277 97.5th percentile of the NSE were chosen to determine the lower and upper bounds of
278 likelihood measure. The simulated results with 95 percent confidence in the three
279 subareas of Lake Taihu are shown in Fig. 3 and Fig. 4.

280 Trends in simulated results were basically consistent with field observations in
281 the three subareas (Fig. 3 and Fig. 4), and the proportion of observations in
282 uncertainty interval (CR) was mostly higher than 66.7% (Table 2) meant that most
283 observations were within the confidence interval. The model was therefore deemed
284 feasible to be utilized in the simulation of water quality in Lake Taihu. The CR was

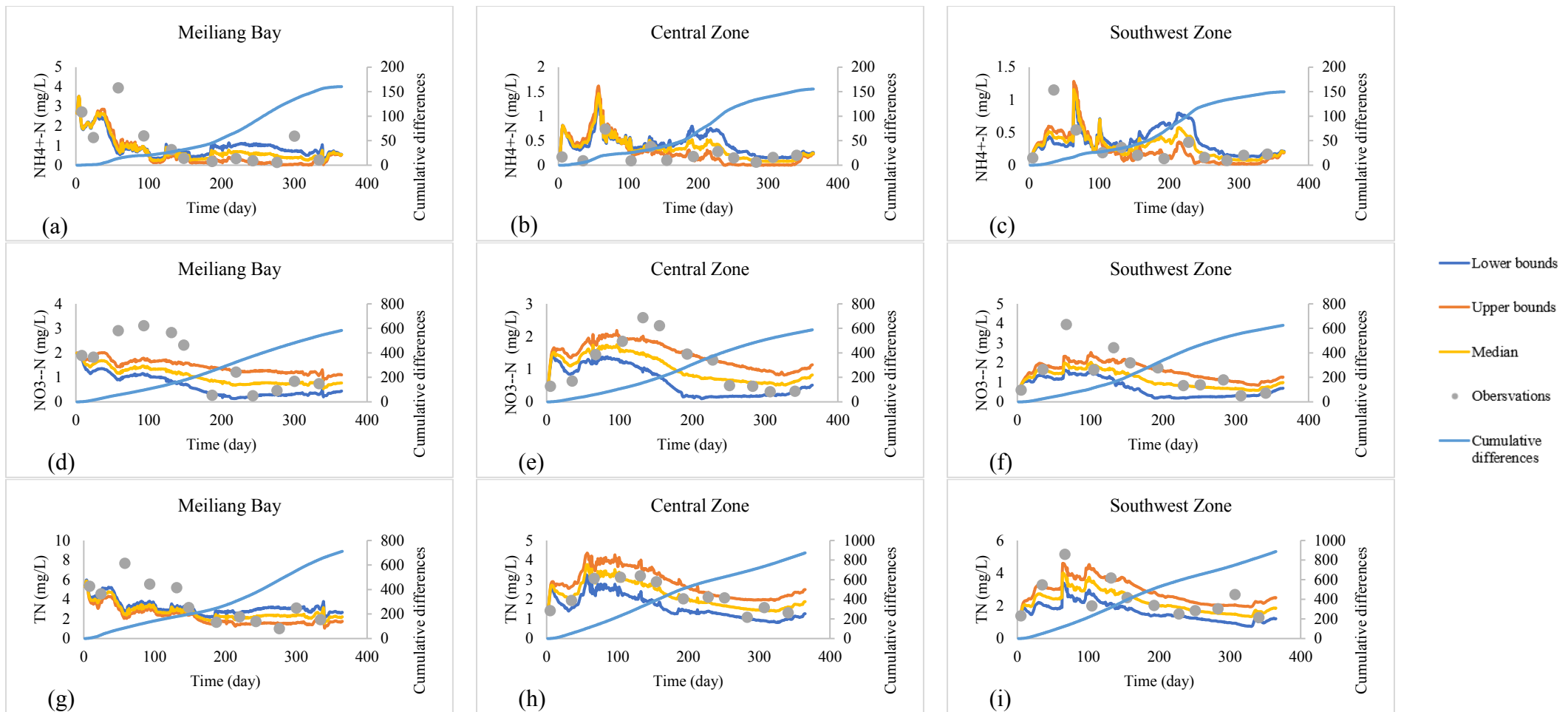
285 also distinguished between the three subareas. The average CR in Central Zone was
 286 the highest (84.7%) and higher than that of Southwest Zone (76.4%). The average CR
 287 in Meiliang Bay with a higher indicator concentration was the lowest (66.7%), which
 288 indicated that it is difficult to get accurate simulations in Meiliang Bay.

289 **Table 2** Statistics of simulated values and monitoring values for uncertainty analysis.

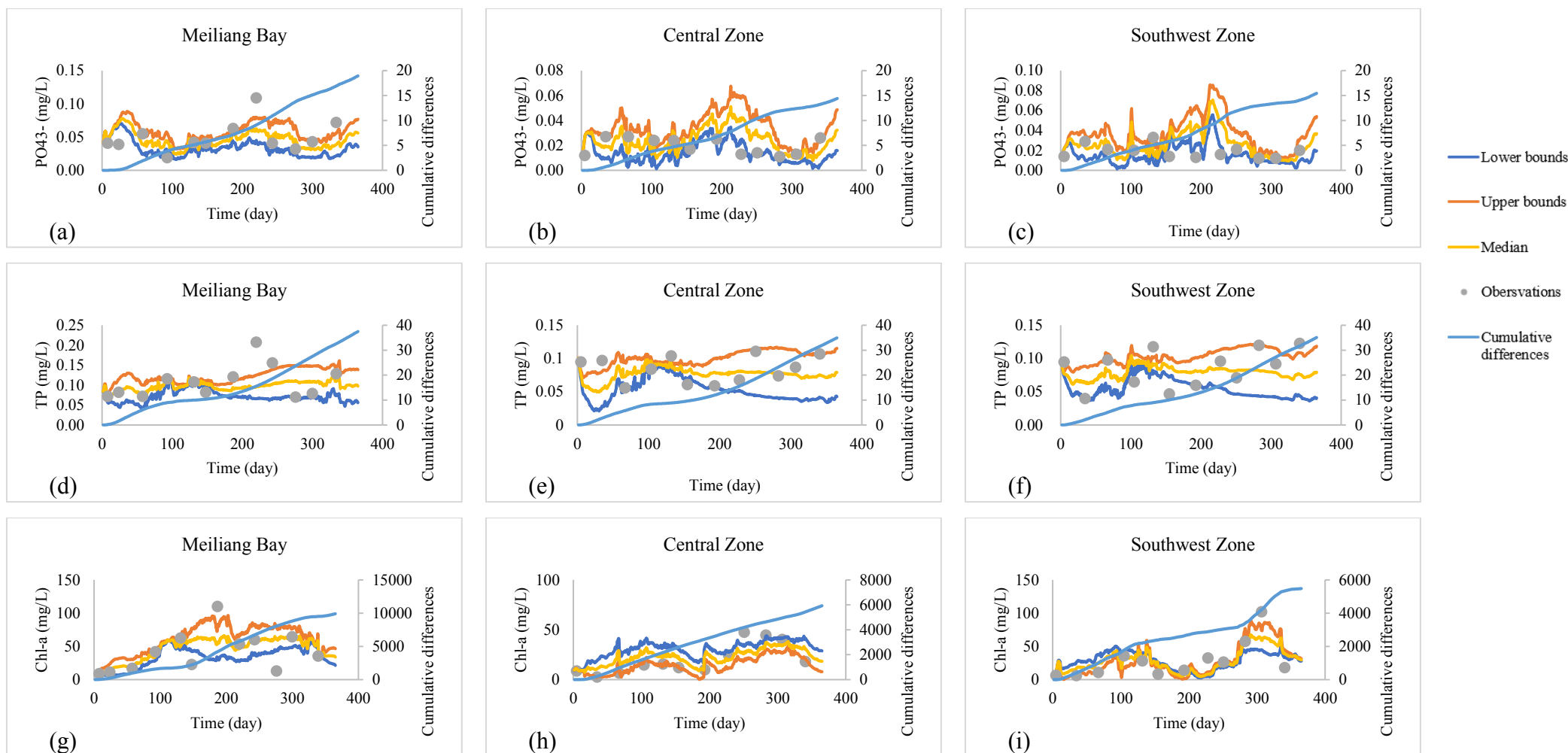
Indicators	Meiliang Bay				Central Zone				Southwest Zone			
	CR	UI	MC	RI	CR	UI	MC	RI	CR	UI	MC	RI
Ammonia nitrogen (mg/L)	66.7%	0.222	1.113	19.9%	75.0%	0.108	0.217	49.8%	75.0%	0.104	0.281	37.0%
Nitrate nitrogen (mg/L)	58.3%	0.407	1.554	26.2%	75.0%	0.411	1.138	36.1%	83.3%	0.435	1.492	29.2%
Total nitrogen (mg/L)	66.7%	0.497	3.593	13.8%	100.0%	0.610	2.153	28.3%	75.0%	0.620	2.420	25.6%
Phosphate (mg/L)	66.7%	0.014	0.050	27.0%	91.7%	0.010	0.019	52.6%	83.3%	0.011	0.019	57.9%
Total phosphorus (mg/L)	66.7%	0.027	0.108	24.5%	75.0%	0.025	0.084	29.2%	66.7%	0.025	0.085	28.8%
Chlorophyll-a ($\mu\text{g/L}$)	75.0%	15.59	41.75	37.3%	91.7%	12.28	23.76	46.1%	75.0%	13.00	28.80	45.1%

290 CR, Proportion of observations in uncertainty interval; UI, uncertainty interval between median and lower bounds;
 291 MC, Mean concentration of observations; RI, ratio of uncertainty interval to mean concentration.

292 The uncertainty intervals between the median and lower bounds (UI) were
 293 significant, with some of them even accounted for more than half of the mean
 294 concentrations from field observations (MC). Therefore, uncertainty resulting from
 295 these parameters could not be ignored. The ratio of uncertainty to mean concentration
 296 (RI) increased basically with decreased concentration of observations, although the UI
 297 decreased at the same time. For example, the RI of Chlorophyll-a simulation in
 298 Southwest Zone was 45.1%, higher than that of Meiliang Bay (37.3%, Table 2),
 299 although UI decreased from 15.59 to 13.00 $\mu\text{g/L}$. The UI of different indicators were
 300 also variable in simulation of nitrogen. The UI of nitrate nitrogen was greater than
 301 that of ammonia nitrogen, especially in the Southwest Zone which showed that the
 302 accuracy of nitrate nitrogen simulation was highly important in the simulation of total
 303 nitrogen.



304 **Fig.3** Uncertainty interval related to nitrogen in three subareas. (a), (b), and (c) are the simulations for ammonia nitrogen; (d), (e), and (f) are the simulations for
 305 nitrate nitrogen; (g), (h), and (i) are the simulations of total nitrogen.



306 **Fig. 4** Uncertainty interval related to phosphorus and chlorophyll-a in three subareas. (a), (b), and (c) are the simulations for phosphate; (d), (e), and (f) are the
 307 simulations for total phosphorus; (g), (h), and (i) are the simulations of chlorophyll-a.

308 In simulation of nitrogen and chlorophyll-a, the cumulative differences between
309 the lower and upper bounds (CD) increased slowly at the beginning, but more rapidly
310 after half of the simulation time. This indicated that the uncertainty of some
311 parameters was strongly related to model simulation time. For example, the CD of
312 ammonia nitrogen in the Central Zone (Fig. 3(b)) increased slowly before 150 days,
313 but more rapidly after that time. In simulation of phosphorus, the CD were founded to
314 be highly related to chlorophyll-a. Especially for phosphate, for example, the
315 uncertainties in Central Zone were lowest when simulation time was about 120 and
316 300 days, with highest concentrations of chlorophyll-a (Fig. 4(b) (h)).

317 Some observations were found not to be within the confidence intervals. For
318 example, the simulation of nitrate nitrogen in Meiliang Bay (Fig. 3(d)) did not
319 conform to field observations, and the median of the simulated results underestimated
320 the concentration. In this case, only 58.33% of the monitoring data was within the
321 confidence interval. The model appears to be missing several important nutrients
322 peaks, as it can be easily in Figs. 3 & 4. This result most likely stems from some
323 other uncertainty factors such as inflow rivers, monitoring data and so on, which
324 could also be significant factors and not be ignored when the water quality model is
325 modified.

326 **3.2 Sensitive parameters in the simulation**

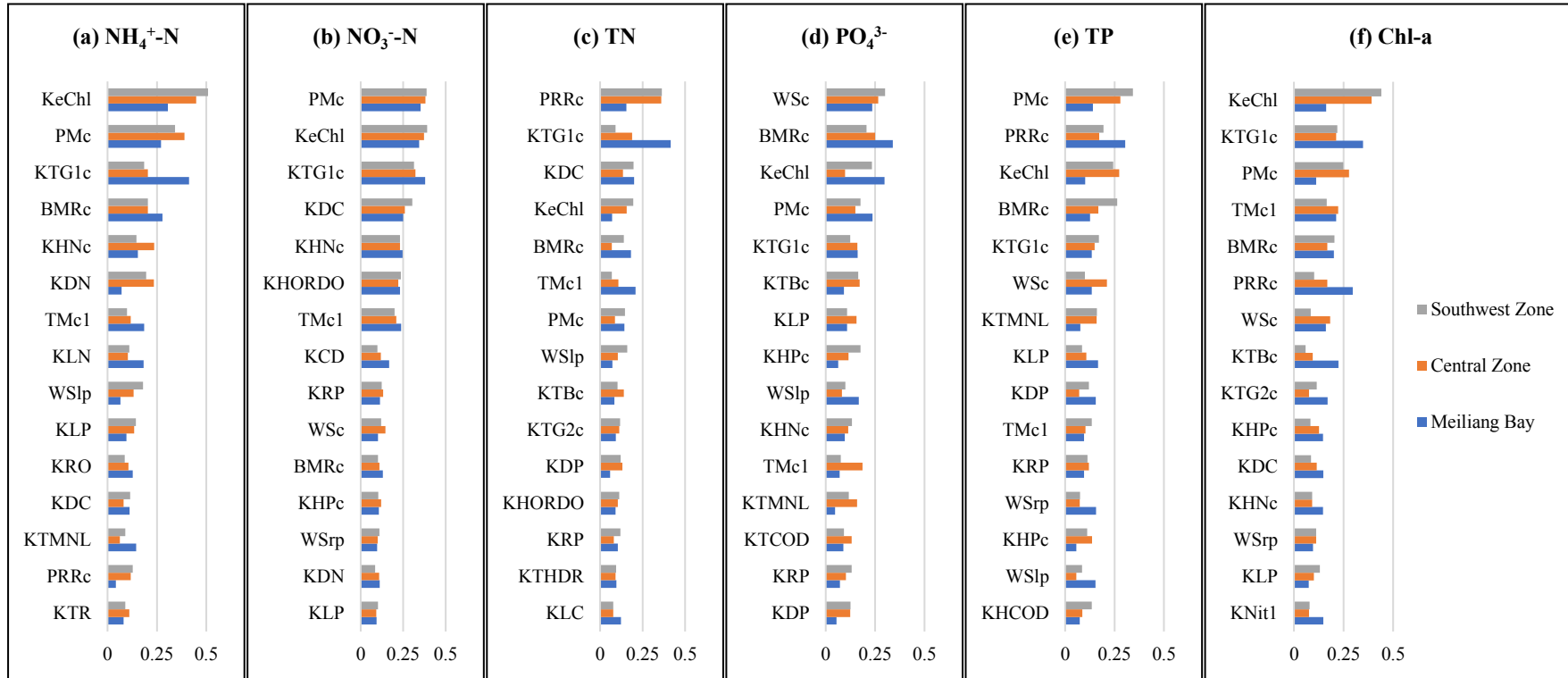
327 The maximum vertical distance (MVD), calculated by using the
328 Kolmogorov-Smirnov test (Eq.5), was used to represent sensitivity indices (SI) of
329 parameters. Sensitive parameters with an SI greater than 0.1 are shown in Fig. 5.

330 The maximum growth rate (PMc), basal metabolism rate (BMRC), predation rate
331 (PRRC), light extinction due to Chlorophyll A (KeChl), and suboptimal temperature
332 effect coefficient for growth (KTG1c) were all found to be sensitive parameters in
333 simulations of all indicators. All of these sensitive parameters are connected with
334 algal growth kinetics which indicated that water quality simulations were influenced
335 by algae.

336 Sensitive parameters distinguished between different indicators. In the
337 simulation of ammonia nitrogen and nitrate nitrogen, PMc, KeChl and KTG1c were
338 very sensitive parameters. PRRc was found to be the most sensitive parameter in the
339 simulation of total nitrogen but it was not a sensitive parameter in the simulation of
340 ammonia nitrogen and nitrate nitrogen. This may indicate that PRRc is a significant
341 parameter in the simulation of organic nitrogen. KDC, a parameter representing the
342 minimum dissolution rate of DOC, was also a sensitive parameter in the simulation of
343 nitrate nitrogen and total nitrogen which influenced simulations through
344 denitrification. The settling velocity of cyanobacteria (WSc) was the most sensitive
345 parameter in the simulation of phosphate since settling of algae with absorbed
346 phosphate is one way for soluble phosphate to be removed from the aquatic system
347 (Fig. 5(d)). WSc was also a sensitive parameter in the simulation of phosphorus and
348 algae although the sensitivity was lower than that of other parameters such as three
349 important parameters related to algal kinetics (i.e. PMc, PRRc and BMRC). Two
350 parameters related to light and temperature (i.e. KeChl and KTG1c, respectively)
351 were the most important parameters in simulation of algae. TMc1, optimal
352 temperature for algal growth, was also a significant parameter for simulating algae.

353 Sensitive parameters also varied spatially and were influenced primarily by
354 concentration. The bar charts (Fig. 5), showing six indicators, indicated that some
355 parameters are clearly distinguished between the three subareas such as KTG1c,
356 KeChl and PMc. In the simulation of nitrate nitrogen and algae, the SI of KTG1c in
357 Meiliang Bay was higher than that of the Central Zone and Southwest Zone. For
358 ammonia nitrogen and total nitrogen, the SI of KTG1c in Meiliang Bay was almost
359 two times higher than that of the other two subareas. In simulation of almost all
360 indicators except for phosphate, the SI of KeChl in Meiliang Bay were lower than
361 that of the other two subareas, which demonstrated KeChl was a more sensitive
362 parameter in the Central Zone and Southwest Zone. In the simulation of phosphate,
363 the SI of KeChl and PMc in Meiliang Bay was obviously higher than that of the

364 Central Zone and Southwest Zone, which became lowest in the simulation of total
365 phosphorus and algae. It indicated that the sensitivities of these two parameters were
366 influenced by both indicators and locations. The SI of other indicators in the three
367 subareas was almost identical which means the parametric sensitivity of these
368 indicators was less affected by location. Although sensitive parameters were
369 distinguished in the three subareas, the situations in the Central Zone and Southwest
370 Zone were similar probably due to the close concentrations in these two subareas. We
371 suggest that sensitivities of these parameters are highly influenced by concentrations
372 of indicators (Fig. 5).



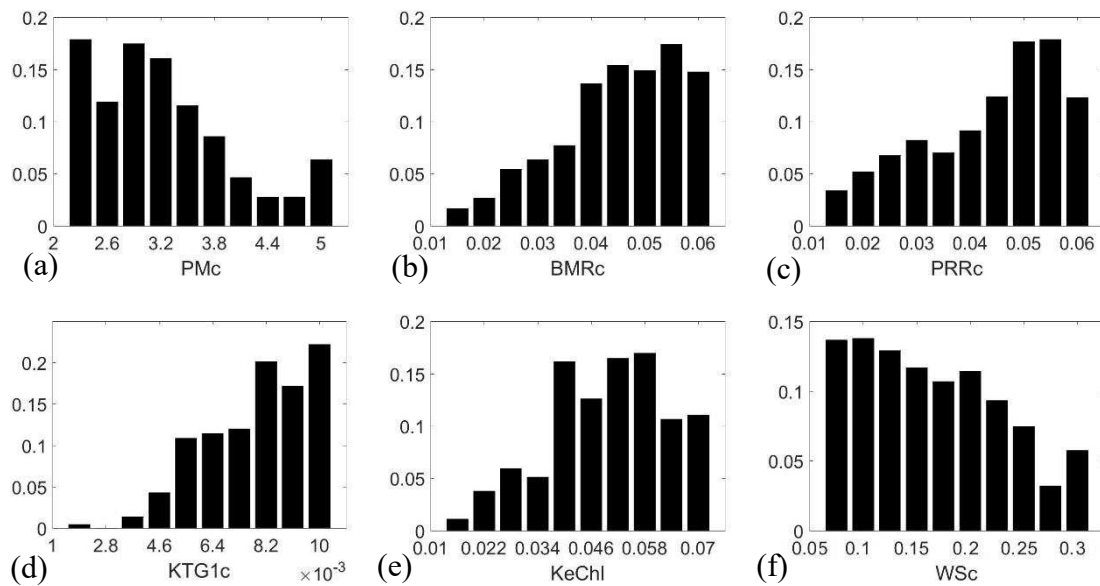
374

375 **Fig. 5** Sensitive indices in the simulation of water quality.

376

377 The cumulative distribution functions (CDFs) of likelihood measures within each
 378 group were calculated to be the posterior distributions of parameters (Fig. 6). The
 379 sensitivity and the proper range of parameters can be found directly by the deviation
 380 of the posterior distribution.

381 For example, the probability of cumulative distribution functions increased
 382 obviously when $\text{BMRC} > 0.04$, which mean that the simulation with $\text{BMRC} > 0.04$ are
 383 more likely to have high likelihood measures. Therefore, the probably suitable range
 384 of BMRC was from 0.04 to 0.06/day. Other speculative ranges of sensitive parameters
 385 are also shown in Table 3. The CDFs were useful not only for setting parameter
 386 ranges, but also for specifying more informative distributions than the uniform or
 387 normal distributions used in this analysis. PMc fits a normal or gamma distribution
 388 well, which PRRc should probably use a triangle distribution, with suitable values at
 389 0.05.



390 **Fig. 6** Posterior distributions of sensitive parameters. X axis is the range of parameters and Y axis
 391 is the probability of cumulative distribution functions.

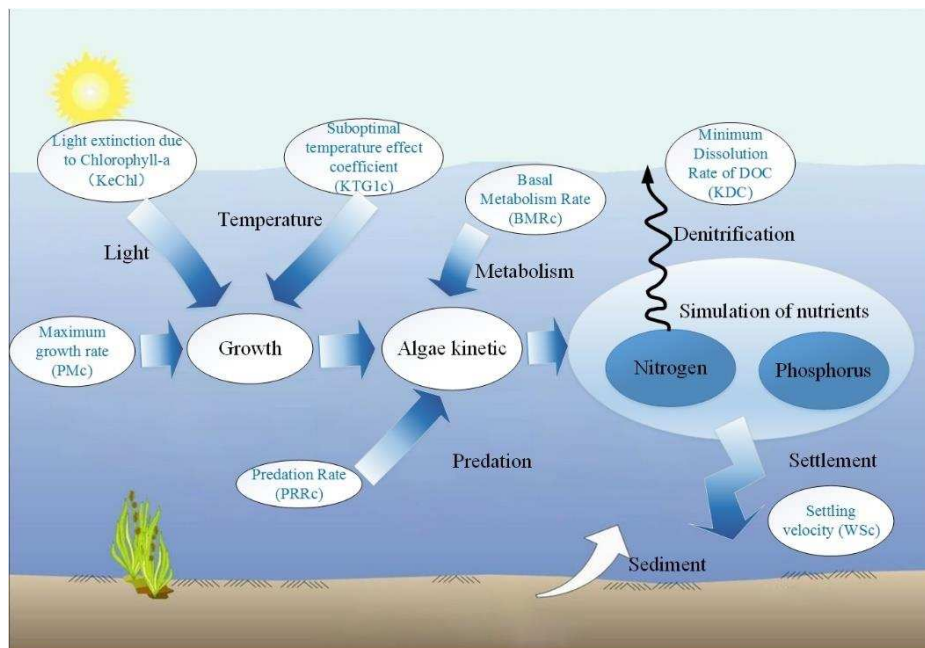
392 **Table 3** Possible range of sensitive parameters.

Parameters	PMc (1/day)	BMRC (1/day)	PRRc (1/day)	KTG1c (-l)	KeChl (1/m per mg/l)	WSc (m/day)
Min	2	0.04	0.04	0.0046	0.034	0.05
Max	3.8	0.06	0.06	0.01	0.058	0.2

393 4 Discussion

394 4.1 Influence of algae on parameter sensitivity

395 Biological activity was found to be an important mechanism in influencing the
396 simulation of water quality, particularly in lakes with higher concentrations of algae.
397 As shown in Fig. 7, most of the sensitive parameters were found to be related to algal
398 growth kinetics, such as PMc, BMRC and PRRc. In the three-dimensional
399 nutrients-algal dynamic model built using EFDC in Lake Dianchi, which is a large
400 shallow lake similar to Lake Taihu and also suffers from algae blooms, the global
401 sensitivity analysis also showed the maximum growth rate and basal metabolism rate
402 were sensitive parameters in the simulation of TN and TP (Yi et al. 2016). In the
403 Venetian Lagoon, a large shallow lake with average depth of 1.1m, maximum growth
404 rate of phytoplankton and zooplankton, also had significant impacts on simulation
405 results (Pastres and Ciavatta 2005; Pastres et al. 1997). We suggest that parameters
406 related to algal growth kinetics are significant parameters for large shallow lakes with
407 high concentrations of algae.



408
409 **Fig. 7** Relation schema of sensitive parameters in the simulation of water quality. Sensitive
410 parameters in the study were marked in blue.

411 In this study, the minimum value for PMc was set to 2/day which may be a little

412 higher than the value in ever research (Hoogenhout and Amesz 1965; Edwards et al.
413 2015; Kruk et al. 2010). From measured values reported in literatures, a mean value
414 for *Microcystis* (which is common in Taihu) was 0.53/day (temperature-adjusted), or
415 0.7/day without temperature correction (Robson et al. 2018; Edwards et al. 2015).
416 However, we checked the real time growth rate in our model when PMc was set to
417 3/day and found the values varied from 0.15/day to 0.6/day which was close to the
418 range reported in literatures. We have conducted several pre-researches with a wider
419 range of PMc and the results showed that the concentration of algae will be quite low
420 if we set the PMc lower than 2. We attributed the difference to the overestimation of
421 settling of algae, which lead to a lower rate of algal increase. Cyanobacterial settling
422 (WSc) was found in this study to be a sensitive parameter, especially in the simulation
423 of phosphorus, in part because it is one of ways for soluble phosphate to be removed
424 from the aquatic system. Another P removal processes is adsorption to suspended or
425 benthic sediment surfaces and it may be compensated for in part by high
426 cyanobacterial settling. Therefore, a higher PMc used would then be needed to
427 compensate for the effect of high cyanobacterial settling on chlorophyll-a
428 concentration and the possible range of PMc would be lower than the speculative
429 range we provided.

430 Light and temperature impacts on algal growth also have significant influence on
431 models (Benke et al. 2008; Confalonieri 2010). In Meiliang Bay, parameters related to
432 energy such as light and temperature were found to be more sensitive than parameters
433 concerned with nutrients (Li and Chen et al. 2015). In marine biological models, the
434 result of sensitivity analysis also suggested that light limitation was a sensitive
435 parameter on phytoplankton growth (Chu et al. 2007). In our research, light extinction
436 due to Chlorophyll-A (KeChl) was a very sensitive parameter in simulations of all
437 water quality indicators and similar phenomenon was also found in Lake Dianchi (Yi
438 et al. 2016). In these eutrophic lakes, algae concentration is very high and play an
439 important role in light extinction, which in return lead to a great impact on algal

440 growth and then affect the simulation of nutrients. Temperature was also a significant
441 factor in algal growth, and the suboptimal temperature effect coefficient (KTG1c) was
442 a very sensitive parameter in the limitation of temperature in our research. Due to the
443 great change of temperature seasonally in Lake Taihu, temperature effect coefficient
444 was sensitive, which was not found in lakes with little difference in temperature over
445 time like Dianchi (Yi et al. 2016).

446 **4.2 Spatial variability of sensitivity and uncertainty**

447 Sensitive parameters were apparently related to concentrations of water quality
448 indicators in the three subareas. In the Central Zone and Southwest Zone with lower
449 concentrations, the rank of very sensitive parameters was almost identical, while they
450 changed significantly in Meiliang Bay (Table 4). In simulations of phosphorus, for
451 example, BMRC and PRRc were more sensitive in Meiliang Bay, while WSc and PMc
452 were very sensitive in other two subareas with lower nutrients concentrations. In
453 Meiliang Bay, KTG1c was the most sensitive parameter in simulations of most
454 indicators, which meant that temperature was the most significant factor in this
455 subarea. In subareas with lower concentrations (i.e. Central Zone and Southwest
456 Zone), KeChl were the most important parameters (Table 4). Thus, influence of light
457 should be given greater attention. We attribute the phenomenon to the difference in
458 limiting factors in three subareas. In subareas with lower algae concentration, algae
459 play an important role in light extinction, which in return lead to a great impact on
460 algal growth and then affect the simulation of nutrients. However, influence of light
461 decreases in subareas with too high algae concentration because algae on the water
462 surface has already intercepted most light. Temperature then became a limiting factor
463 in these subareas.

464 Not only light and temperature have great impact in simulation, but also other
465 boundary conditions could also be responsible for the spatial variability of sensitivity.
466 For example, wind speed was found to have the largest impact on simulation between
467 in/out flow, wind speed, wind direction and initial water level (Li et al. 2014). Thus,

468 some parameters concerned with wind like wind drag coefficient were found to be
 469 very sensitive in our previous research on hydrodynamic conditions (Li and Tang et al.
 470 2015). The effects of external nutrients reductions on algal blooms were investigated
 471 to evaluate the influence of boundary conditions on the model and results showed that
 472 Chlorophyll a (Chl-a) concentrations only decreased a little when implementing high
 473 nutrients reduction scenario (Tang et al. 2016). It is consistent with our results that
 474 little parameters related to nutrients were sensitive.

475 **Table 4** Sensitivity ranks of parameters in the three lake subareas.

Subarea	Rank	Ammonia nitrogen	Nitrate nitrogen	Total nitrogen	Phosphate	Total phosphorus	Chlorophyll -A
Meiliang Bay	1	KTG1c	KTG1c	KTG1c	BMRc	PRRc	KTG1c
	2	KeChl	PMc	-	KeChl	-	PRRc
	3	BMRc	KeChl	-	-	-	-
	4	PMc	-	-	-	-	-
Central Zone	1	KeChl	PMc	PRRc	WSc	PMc	KeChl
	2	PMc	KeChl	-	BMRc	KeChl	PMc
	3	-	KTG1c	-	-	-	-
	4	-	KDC	-	-	-	-
Southwest Zone	1	KeChl	KeChl	PRRc	WSc	PMc	KeChl
	2	PMc	PMc	-	-	BMRc	PMc
	3	-	KTG1c	-	-	-	-
	4	-	KDC	-	-	-	-

476 Uncertainty of simulation also had a close relationship with indicators'
 477 concentration in different subareas. Meiliang Bay is connected to some inflow rivers
 478 with high concentrations of nutrients and greater benthic fluxes due to thick sediment
 479 deposits (Luo et al. 2004). The simulation in this subareas was therefore less
 480 influenced by model parameters, and lower concentration subareas should be given
 481 much attention when modifying parameters. In addition, currents and waves were
 482 weak in this bay area where the impact of wind is expected to be less than other two
 483 subareas. The calculation of water quality variables was based on hydrodynamic
 484 conditions, strong currents and waves will accelerate transportation and
 485 transformation of nutrients, which results in higher relative uncertainty in the Central
 486 Zone and Southwest Zone.

487 Uncertainty of simulation was related to the simulation time as well. According

488 to the results, the uncertainty in the three subareas increased rapidly when the
489 simulation time was over 150 days, while the concentration of algae began to rise and
490 algae blooms frequently occurred at the same time. With increasing temperature and
491 light intensity, algal growth, basal metabolism and some other algal kinetic processes
492 became more active. From the results of the sensitivity analysis that most sensitivity
493 parameters were related to algal kinetics, we infer that the increased uncertainty over
494 time mostly resulted from enhanced algal kinetic processes.

495 Finally, it was hard to simulate all water quality indicators through modification
496 of model parameters since other uncertain factors also showed significant impact on
497 simulation results. Several important nutrients peaks were missed in Figs. 3 & 4.
498 Almost all of the missed peaks were located in offshore areas (i.e. Meiliang Bay and
499 Southwest Zone) which were highly influenced by boundary conditions. We attributed
500 the result to the uncertainty of nutrients loading data, especially for the non-point
501 source pollution. We checked the rainfall data and found that there is a strong
502 relationship between missed peaks and the intensity of rainfall. We suggested that the
503 non-point source pollution resulted from rainfall was underestimated which caused
504 reduce in nutrients loading.

505 **4.3 Generalization for a larger modelling community and future work**

506 Except external input from rivers and internal input from sediment beds,
507 biological activity is a significant part for nutrients simulation in these models, with
508 more sensitive parameters than that in hydrolysis, mineralization and settlement.
509 Since net algal production can be divided into five phases: algal growth, metabolism,
510 predation, settling, and external sources (Ji 2007), maximum growth rate, basal
511 metabolism rate and predation rate were sensitive apparently, which was found both
512 in our study and other places like Lake Kinneret (based on a DYRESM–CAEDYM
513 model) (Bruce et al. 2006). Light was an important limitation on algae growth and
514 light extinction due to Chlorophyll-A was a very sensitive parameter in this study.
515 However, for some deep lakes like Lake Washington, background light extinction was

516 more sensitive (Arhonditsis and Brett 2005). Thus, light extinction due to
517 Chlorophyll-A in shallow lakes with serious algal blooms were more sensitive than
518 that in deep lakes where background light extinction was more sensitive. Temperature
519 was also a significant factor in algal growth and the optimal temperature effect
520 coefficient was a very sensitive parameter in the limitation of temperature in our
521 research. Seasonal temperature, varying widely in Lake Taihu, was mostly lower than
522 the optimal temperature for cyanobacterial growth. In contrast, the temperature of
523 Lake Dianchi was higher than that of Lake Taihu, and temperature effect coefficient
524 was not a sensitive parameter in the Dianchi Model (Yi et al. 2016). Hence, we infer
525 that the temperature effect coefficient might turn out to be a sensitive parameter in
526 lakes with an obvious seasonal temperature variation. Some water quality models
527 used widely are based on similar theory which contains dissolved oxygen, algae,
528 nutrients and so on. Some modern models are only subtle variations on model
529 structures established in the 1970s or earlier (Franks 2009). The governing equations
530 in these models such as EFDC, WASP and DYRESM are similar as well (Park et al.
531 2005; Cerco and Cole 1993), which encourage us to extend the results in this study to
532 a larger modelling community.

533 Producing a believable output requires not only a realistic growth rate response
534 to limiting nutrients but also a realistic consumption of non- or lesser limiting
535 nutrients (Flynn 2003; Flynn 2005). For the future work, variable stoichiometry
536 phytoplankton models like Caperon-Meyer quota model need to be considered for
537 non-steady state applications rather than some traditional models like
538 Michaelis-Menten nutrient kinetics (Flynn 2008, 2005; Flynn and Mitra 2016).
539 Though this requires better statistical comparisons of models and data, it can make
540 planktonic ecosystem models much more powerful tools (Franks 2009). Redfield-
541 Monod models often use nutrient limitation as a significant factor controlling
542 phytoplankton growth, and yet biologically such nutrient limitation is associated with
543 significant variation in elemental stoichiometry (Flynn 2010) such as the variable

544 stoichiometry (C:N:P and in some models C:Chl) of phytoplankton cells (Jackson et
545 al. 2017; Butenschön et al. 2016; Robson 2014; Baird et al. 2013; Flynn 2001; Droop
546 1975). It can demonstrate the behavior of the dynamic Chl parameterization over a
547 range of light- and nutrient-limiting environments for phytoplankton of different sizes
548 and growth rates (Baird et al. 2013). The appropriate description of the control of the
549 transport of the non-limiting nutrient is also important and a fixed algal N:P should
550 not be assumed (Flynn 2008).

551 Including zooplankton explicitly rather than a fixed predation rate leads to much
552 more realistic plankton dynamics. Due to the complexity of zooplankton model, there
553 are no advanced module in EFDC currently. Current knowledge of plankton ecology
554 ascribes a large proportion of zooplankton losses to zooplankton cannibalism and
555 carnivory, rather than via the activity of higher trophic levels beyond the plankton.
556 Planktonic ecosystem models typically represent all zooplankton losses by
557 mathematically (rather than biologically) justified closure functions. Even these
558 closure functions include zooplanktonic cannibalism and carnivory, these processes
559 are not explicitly implemented within the grazing function. While the biomass outputs
560 may appear similar, the fate of annual primary production and f-ratios vary widely
561 (Mitra 2009).

562 **5 Conclusions**

563 In this research, nutrients were chosen as output indicators and 40 parameters
564 were sampled. GLUE and RSA methods were applied to analyze the parametric
565 uncertainty and sensitivity of the EFDC model in Lake Taihu, a typical large shallow
566 lake. Three parameters related to algal kinetics (i.e. PMc, BMRC and PRRc) were
567 sensitive parameters in the simulation of water quality in the eutrophic waterbody. For
568 shallow lakes with frequent algal blooms light extinction due to Chlorophyll-a is also
569 a sensitive parameter, while background light extinction has also been shown to be
570 sensitive for deep lakes. For lakes with seasonal temperature variation, the
571 temperature effect coefficient for algal growth is sensitive. Sensitive parameters also

572 varied in different lake subareas. For high nutrients and algae concentration subareas,
573 temperature was more likely to be a limiting factor, whereas sensitive factors could be
574 light in lower concentration subareas. Since most sensitive parameters were related to
575 algae, uncertainty of simulation results increased with increase in algal kinetic
576 processes over time. It also varied in different subareas. Lower nutrients and algae
577 concentration subareas were more easily influenced by model parameters and
578 nearshore areas were highly influenced by boundary conditions. For the future work,
579 variable stoichiometry phytoplankton models will be considered and zooplankton will
580 be integrated into the model explicitly rather than a fixed predation rate.

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