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# Identification of watershed priority management areas under water quality constraints: A simulation-optimization approach with ideal load reduction



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# ABSTRACT

Targeting nonpoint source (NPS) pollution hot spots is of vital importance for placement of best management practices (BMPs). Although physically-based watershed models have been widely used to estimate nutrient emissions, connections between nutrient abatement and compliance of water quality standards have been rarely considered in NPS hotspot ranking, which may lead to ineffective decision-making. It's critical to develop a strategy to identify priority management areas (PMAs) based on water quality response to nutrient load mitigation. A water quality constrained PMA identification framework was thereby proposed in this study, based on the simulation-optimization approach with ideal load reduction (ILR-SO). It integrates the physically-based Soil and Water Assessment Tool (SWAT) model and an optimization model under constraints of site-specific water quality standards. To our knowledge, it was the first effort to identify PMAs with simulation-based optimization. The SWAT model was established to simulate temporal and spatial nutrient loading and evaluate effectiveness of pollution mitigation. A metamodel was trained to establish a quantitative relationship between sources and water quality. Ranking of priority areas is based on required nutrient load reduction in each sub-watershed targeting to satisfy water quality standards in waterbodies, which was calculated with genetic algorithm (GA). The proposed approach was used for identification of PMAs on the basis of diffuse total phosphorus (TP) in Lake Dianchi Watershed, one of the three most eutrophic large lakes in China. The modeling results demonstrated that 85% of diffuse TP came from 30% of the watershed area. Compared with the two conventional targeting strategies based on overland nutrient loss and instream nutrient loading, the ILR-SO model identified distinct PMAs and narrowed down the coverage of management areas. This study addressed the urgent need to incorporate water quality response into PMA identification and showed that the ILR-SO approach is effective to guide watershed management for aquatic ecosystem restoration.

#### 1. Introduction

Nonpoint Source (NPS) pollution, resulted from agricultural activities and urban runoff, has caused water quality deterioration and eutrophication in waterbodies across the world (Conley et al., 2009). Since significant achievement has been made to deal with point source pollution in recent years, excess NPS nutrient loss has increasingly become a threat for water quality improvement and aquatic ecosystem restoration (Sharpley and Wang, 2014). The NPS pollution presents significant spatial heterogeneity due to diverse soil types, topographical properties, climatic conditions, and human activities, which is difficult to identify and control (Schoumans et al., 2014; Xu et al., 2016). To improve water quality affected by excess NPS nutrient loss, best management practices (BMPs) are effective and widely implemented to control transport and delivery of nutrients to waterbodies (Chaubey et al., 2010; Laik et al., 2014).

For large-scale watersheds, it's costly and technically difficult to implement BMPs throughout the watersheds. Spatial heterogeneity of NPS should be recognized as an important consideration for BMP placement at the watershed scale. It's reported that some sub-watersheds contribute significantly more nutrient loads than others (Schilling and Wolter, 2009; Strauss et al., 2007; White et al., 2009). Confining BMPs to high polluted areas is usually more cost-effective than implementing universal controls or random placement (Giri et al., 2012; Strauss et al.,

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Abbreviations: BMPs, best management practices; CSA, critical source areas; GA, genetic algorithm; HRUs, hydrologic response units; ILR, ideal load reduction; ILR-SO, simulationoptimization approach with ideal load reduction; LII, load impact index; LMBP, Levenberge Marquardt back propagation; LUAI, load per unit area index; NPS, nonpoint source; NSE, Nash-Sutcliffe efficiency; PMAs, priority management areas; SWAT, Soil Water Assessment Tool; TP, total phosphorus

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2007). Consequently, identification of vulnerable areas that pose greater risk of NPS pollution is crucial for more practical and efficient management strategies, taking into account both time and financial resource constraints. The concept of critical source areas (CSAs) has thereby been widely adopted for cost-effective watershed management decision-making, which are defined as relatively small portions of watersheds contributing a large quantity of pollutant loads to nearby water bodies (Renkenberger et al., 2016; Wei et al., 2017).

Identification of CSAs can be conducted through field monitoring or numerical model simulation (Sharpley et al., 2002). Field-specific measurement of pollutant loads at the watershed scale is time consuming and expensive, which can only represent the local characteristics (Giri et al., 2012). The physically-based watershed models are effective tools to support CSA identification by tracking the complicated hydrologic, soil erosion, plant growing and nutrient transport processes and estimating nutrient spatial distributions based on monitored discharges and nutrient concentrations (Baginska et al., 2003; Niraula et al., 2013; Yang et al., 2016). Improvement in watershed modelling and targeting approaches in recent decades has enabled reliable identifications of CSAs. Niraula et al. (2013) analyzed the effect of model choice on identification of CSAs. Hughes et al. (2005) used multi-criteria analysis considering factors that influence overall potential for nutrient loss. Shen et al. (2015) presented a stepwise approach to identify CSAs based on specific uses of particular water bodies, defined as water functional zones. Huang et al. (2015) identified CSAs based on the relationship between precipitation and nutrient yields, which could provide a better coverage through accommodating spatial precipitation characteristics.

In previous studies, targeting CSAs with watershed simulation models is usually based on the total source pollutant loads from land units (Loads per Unit Area Index, LUAI) (Giri et al., 2012; Levi et al., 2018). However, LUAI overlooks pollutant transport and transformation processes in channels, and thus could not represent distinct water quality responses to spatially diverse nutrient abatement, which is of vital importance to guide BMP placement. Although the impacts of NPS pollution on water quality have triggered worldwide attention (Wall et al., 2011), responses of rivers and lakes to nutrient load abatement have been rarely incorporated in targeting CSAs. Sharpley et al. (2003) stated that targeting CSAs should explicitly demonstrate that (a) these areas are the main sources of pollution; and (b) implementing mitigation practices at these areas will significantly reduce pollutant concentration in receiving waterbodies. Hydrological connectivity between overland pollution sources and waterbodies has received limited attention (Yu et al., 2015; Thomas et al., 2016). Only some preliminary attempts have been made to weight land units according to their distance to the water bodies (Johnes and Heathwaite, 1997; Lane et al., 2009). Superior to the distance index, physically-based models are able to serve as more sophisticated and reliable tools by representing complicated channel transport processes. Some studies targeted CSAs based on total pollutant loads across the river segments (Load Impact Index, LII) (Tuppad and Srinivasan, 2008; Giri et al., 2014). The LII incorporates contributions of the entire upstream areas. It cannot eliminate impacts of the pollutant loads from the upstream, and consequently, the downstream areas have a great chance to be identified as CSAs if the upstream areas are seriously polluted.

The CSAs identified with the LUAI and LII methods focus on seriously polluted overland areas and river segments, respectively. However, the ultimate management goal is to improve water quality in receiving waterbodies. In this regard, the CSAs identified based on current pollutant loading might not provide sufficient support to guide BMP implementation without connecting nutrient abatement with sitespecific water quality goal compliance. That might result in inefficient BMP placement or failing to reach the water quality targets. There is a critical need for providing deep insights into water quality response to pollution mitigation, which has been rarely considered when targeting CSAs. To overcome the limitations of the conventional methods for

CSAs identification, we developed a water quality constrained targeting framework. The concept of priority management areas (PMAs) is adopted (Chen et al., 2014; Heck et al., 2017). Instead of merely focusing on pollutant loading, PMAs are defined as the areas where diffuse pollution mitigation can achieve relatively better water quality improvement in the present study. PMAs represent the areas with a high priority for BMP implementation. A Simulation-Optimization approach based on Ideal Load Reduction (ILR-SO) was developed to identify PMAs, integrating an optimization model with the physicallybased Soil and Water Assessment Tool (SWAT) watershed model. In this study, ideal load reduction (ILR) was defined as the required nutrient load abatement in each land unit to meet site-specific water quality standards in particular waterbodies. The SWAT model was used to simulate nutrient fate and transport at the watershed scale, including both overland and instream processes. A Levenberge Marquardt back propagation (LMBP) network was established to quantify water quality response to nutrient load reduction. The ILR was calculated with an optimization model incorporating constraints of water quality standards. The optimization approach has been widely used for optimal decision making in nutrient load allocation or abatement estimation (Destouni et al., 2006; Gren and Destouni, 2012; Zhang et al., 2017). However, simulation-based optimization, to the best of our knowledge, has not been used for CSA/PMA ranking. The ILR-SO approach has advantages over the LUAI and LII methods as it integrates NPS pollution with water quality goal compliance, and in the meanwhile, mitigates interference of the upstream areas. The main objectives of this study are to (a) establish the connections between nutrient load abatement and compliance of site-specific water quality standards; and (b) prioritize areas to implement BMPs for NPS pollution mitigation with the new ILR criterion. The ILR-SO was used to identify PMAs in the Lake Dianchi Watershed, which incorporates multiple tributaries with distinct water uses and water quality standards. The detailed modelling procedure and results are presented in the following sections.

# 2. Material and methodology

#### 2.1. Study area

Lake Dianchi, located in the southwestern China, is the sixth largest lake in China and the largest one in Yunnan Province, with a capacity of  $15.8 \times 10^8 \,\text{m}^3$  and an average water depth of 5 m. It is among the three most eutrophic shallow large lakes in China. The watershed (102°29'-103°01'E and 24°29'-25°28'N) covers a drainage area of 2920 km<sup>2</sup>. The main tributaries (Fig. 1) draining into Lake Dianchi include the Panlong (PL) River, Baoxiang (BX) River and Luolong (LL) River, etc. The Panlong River, with a length of 108 km and drainage area of 847 km<sup>2</sup>, is the longest river in the study area. The elevation of the watershed ranges from 1880.6 m to 2837.6 m above the mean sea level. The prevailing climate in the watershed is humid and mild. The mean annual air temperature and precipitation are about 15 °C and 1075 mm, respectively. Land covers of the watershed mainly consist of forest (about 55% of the watershed area), cropland (20%), urban area (17%), water (5%), and pasture (3%). Most of the croplands are located around the Baoxiang River and southwestern Lake Dianchi Watershed. Slopes of nearly half area of the watershed are larger than 20%. The main soil type is the red soil, which is easy to weather and hydrolyze. Since red soil covers more than 60% of the basin area, the region is vulnerable to suffer from soil erosion. Lake Dianchi is now facing a serious eutrophication problem, resulting from a mass of nutrient inputs from fertilizer application, urban storm runoff, and domestic sewage, etc. Water quality restoration for Lake Dianchi has raised considerable attention and become a great challenge along with booming population and urbanization. In this study, PMAs were identified based on diffuse total phosphorus (TP) loading, which is regarded as the main culprit that leads to eutrophication of Lake Dianchi (Liu et al., 2006; Wu et al., 2017).



Fig. 1. The location, monitoring stations, rivers, and land use of Lake Dianchi Watershed.

# 2.2. Methodological framework

The proposed modelling framework for targeting PMAs at the watershed scale integrates watershed simulation and nutrient abatement optimization (Fig. 2). In this study, SWAT was used for spatial delineation and simulation of terrestrial and instream processes at the watershed scale. The ideal nutrient load reduction, defined as ILR, was calculated with an optimization model constrained by water quality standards. The PMAs for Lake Dianchi Watershed were identified by ranking sub-watersheds with the ILR criterion. The decision procedure is elucidated as follows.

# 2.2.1. Step 1: Watershed delineation and simulation with SWAT

The watershed was delineated into sub-watersheds based on spatial properties including Digital Elevation Model (DEM) and river networks. Each sub-watershed was partitioned into smaller hydrologic response units (HRUs), the basic computational units. A SWAT model was established and run to simulate hydrological and nutrient cycles in each HRU, and subsequently the instream transport processes. To improve prediction performance, sensitive SWAT parameters were calibrated based on the observations in the discharge and water quality monitoring stations. Watershed simulation with SWAT provides the estimation of present-day spatial diffuse TP load contributions, which is the basis of PMA identification.

# 2.2.2. Step2: ILR-SO model development and solution

The calibrated SWAT model quantifies relationship between overland diffuse TP reduction in sub-watersheds and water quality improvement in their connected river segments. The ILR-SO model, an integration of SWAT simulation and optimization algorithm, was developed to calculate the ILR ratio, which represents the relative TP load reduction to the present-day total TP loads in each sub-watershed. It was formulated with the objective to minimize TP reduction amounts in the entire watershed, which is constrained to satisfy the water quality standards. The ILR-SO model integrates SWAT, which involves complicated processes and therefore cannot be solved directly with the conventional gradient-based algorithms (Chaparro et al., 2008). A metamodeling-based optimization approach, integrating LMBP with genetic algorithm (GA), was used to solve the ILR-SO model without the need to access detailed mechanistic equations of SWAT. By solving the



Fig. 2. PMA identification framework with the ILR-SO method.

ILR-SO model, the ILR ratios of sub-watersheds were calculated.

#### 2.2.3. Step 3: Identification of PMAs

Instead of TP loading per unit area or across a river segment, ILR was used as the criterion to identify PMAs. To eliminate interference of different sub-watershed sizes on PMA identification, ILR amounts per unit area were calculated for each sub-watershed, based on the ILR ratios optimized with the ILR-SO model. For the rivers meeting water quality standards, their adjacent sub-watersheds were regarded as '*Very Low*' level priority areas. The other sub-watershed with a higher rank indicated a greater priority to implement management practices.

# 2.3. Watershed simulation with SWAT

#### 2.3.1. SWAT model development

SWAT was employed to develop a simulation model for Lake Dianchi Watershed. Developed by the United States Department of Agriculture (USDA), SWAT is a semi-distributed and physically-based watershed modelling tool computing at daily time steps. SWAT consists of computation modules including hydrology, plant growth, soil erosion, nutrients, pesticides and agricultural management practices, etc. Watershed simulation with SWAT is divided into overland and channelized portions (Meaurio et al., 2015). The overland portion calculates flow, sediment and other constituents (e.g. nutrients and pesticides) transported into the channel from all HRUs for each sub-watershed. The channelized portion simulates water movement and nutrient cycling through the channel network towards the watershed outlet with physically-based methods. Instream water routing and nutrient transport are simulated with the modified kinematic wave model and QUAL2E model, respectively. Surface runoff is predicted with the modified Soil Conservation Service curve number (SCS-CN) method based on daily rainfall (US SCS, 1972). Soil erosion is computed with the modified universal soil loss equation (MUSLE) in each HRU (Williams, 1975). The simplified version of the erosion productivity impact calculator (EPIC) model is used to simulate plant growth (Krysanova and Arnold, 2008).

The input data required for SWAT modelling consist of the DEM,

land use types, soil properties, meteorological data, land management strategies and point pollution sources. In this study, DEM with a resolution of 30 m from United States Geological Survey (USGS) was used to identify the boundary of the watershed and delineate sub-watersheds. The Lake Dianchi Watershed was delineated into 64 sub-watersheds, and further divided into 319 HRUs by overlapping land cover, soil and slope layers. The buffer areas (Fig. 1) were eliminated for not contributing TP loading directly to the tributaries. Soils were characterized with the soil datasets with the scale of 1:1.000.000 from the Yunnan Institute of Environmental Science. Land cover is developed from Landsat TM data in 2008 with a spatial resolution of 30 m. Tillage and fertilizer application information derives from the farm survey in 2008 across the watershed. Daily precipitation records from 15 weather stations were used to drive the SWAT model (Fig. 1). The other meteorological data, including daily air temperatures, solar radiation, relative humidity, and wind speed, were monitored in the Kunming weather station. Monitored daily effluent flow and TP concentration of wastewater treatment plants (WWTPs) were inputted into the SWAT model as point sources. Outflows of WWTPs directly discharge into the nearby streams. Daily flow data were monitored at two stations (Ganhaizi Station in the Baoxiang River and Kunming Station in the Panlong River). Monthly observed TP concentration data were gathered from 2004 to 2010 at the outlet of the Baoxiang River (Baoxiang Station).

#### 2.3.2. Model calibration and validation

Some parameters have significant influence on the SWAT model results but cannot be directly determined by field investigation (Lelis et al., 2012). To identify the sensitive parameters for calibration, a manual one-at-a-time (OAT) sensitivity analysis was conducted (Giri et al., 2015). Seventeen sensitive parameters associated with runoff and TP simulation were detected. Calibration and validation were carried out to improve predictive performance for the SWAT model. The overall simulation period is from 2001 to 2010. The first two years (2001-2002) were taken as warm-up years to minimize the impact of uncertain initial system conditions. The USGS load estimator (LOADEST) regression model (Park and Engel, 2016) was used to convert the observed TP concentration samples into continuous loading data. The instream flow data from 2003 to 2010 were used to calibrate and validate the SWAT model. The parameters relevant to flow were calibrated from 2003 to 2006 and validated from 2007 to 2010 by comparing simulated discharges with observations. Afterwards, the other TP-related parameters were calibrated during 2004-2007 and validated during 2008-2010 based on monthly TP loading data. Model calibration and validation were conducted with the method of the sequential uncertainty fitting algorithm (SUFI-2) at the monthly step. SUFI-2 is a sequential procedure which samples the parameters with the Latin hypercube method and determines pentameter uncertain domains with global search (Abbaspour et al., 1997). In this study, the SWAT model for Lake Dianchi Watershed was calibrated with two iterations, and each with 1000 runs. The Nash-Sutcliffe efficiency (NSE) coefficient was adopted to quantitatively describe predictive accuracy for the SWAT model (Nash and Sutcliffe, 1970).

# 2.4. ILR-SO model development for PMA identification

An ILR-SO model integrating SWAT with optimal decision-making was developed to target PMAs for Lake Dianchi Watershed based on ILR. HRUs, the basic SWAT computational units, are decentralized blocks and thus not appropriate to be used for integrated management. Therefore, PMAs were identified at the sub-watershed scale. The TP reduction ratios of each sub-watershed were defined as decision variables for optimization. Our study aims to guide BMP placement for NPS pollution mitigation, and therefore, abatement of point source pollution was not taken into account. The optimization model is based on the hypothesis that BMP cost is positively correlated with TP load abatement. In this regard, minimizing TP load reduction under constraints of water quality standards indicates achieving the management goal with minimum conservation efforts. The ILR-SO model is formulated as follows:

**Objective function:** minimizing TP load reduction for Lake Dianchi Watershed.

$$Min\sum_{k=1}^{K} \lambda_k SL_k \tag{1}$$

Constraints:

(1) water quality standards constraints.

$$\frac{TP_m^0 - TP_m}{TP_m^0} \geqslant STA_m; \quad m = 1, 2, \dots, M$$
(2)

(2) watershed simulation equations.

$$TP_m^0 = SIM_m(SL_1, SL_2, \dots, SL_k)$$
(3)

$$TP_m = SIM_m(SL_1, SL_2, \dots, SL_k, \lambda_1, \lambda_2, \dots, \lambda_k)$$
(4)

(3) technical constraints.

$$0 \leq \lambda_k \leq 1; k = 1, 2, \dots, K \tag{5}$$

where *k* represents the sub-watershed, with k = 1,2,...,K; *K* is the total number of sub-watersheds (K = 64); *m* represents the river, with m = 1,2,...,M, *M* is the number of rivers (M = 15);  $\lambda_k$  is the TP reduction ratio for the sub-watershed *k*;  $SL_k$  is the background overland TP loading of the sub-watershed *k*;  $TP_m^0$  is the background TP loading at the outlet of the river *m*;  $TP_m$  is the TP loading (ton) inputted into Lake Dianchi from the river *m* after reducing overland diffuse TP loss. The  $SIM_m$  represents the SWAT simulation model for the river *m*, with outputs of TP loading at the river outlet. The  $STA_m$  is the expected TP load reduction ratio to reach the water quality standard of the river *m*, which is defined as follows:

$$STA_{m} = \begin{cases} 0 & C_{a,m} \leq C_{s,m} \\ \frac{C_{a,m} - C_{s,m}}{C_{a,m}} & C_{a,m} > C_{s,m} \end{cases}$$
(6)

where  $C_{a,m}$  and  $C_{s,m}$  are the monitored and standard TP concentration for river *m* respectively (mg/L).  $C_{s,m}$  is quantified according to water use of the river *m* (Table 1) based on Environmental Quality Standards for Surface Water of China (GB3838-2002), which divides surface water

Water quality goals and current conditions of 15 main tributaries in Lake Dianchi Watershed.

Abbr.	River Name	Water quality goal	Monitored TP (mg/L)	Goal compliance
DG	Daguan River	IV	1.19	N
YL	Yunliang River	IV	2.64	Ν
PL	Panlong River	III	1.06	Ν
HH	Haihe River	III	3.48	Ν
BX	Baoxiang River	III	0.87	Ν
ML	Maliao River	III	0.38	Ν
LL	Luolong River	III	0.07	Y
LY	Laoyu River	III	0.07	Y
NC	Nanchong River	III	0.13	Y
YN	Yuni River	III	0.47	Ν
GC	Gucheng River	III	0.51	N
ZH	Zhonghe River	III	0.67	Ν
CH	Chai River	III	0.42	Ν
BY	Baiyu River	III	0.16	Y
DD	Dongda River	III	0.07	Y

*Note*: Monitored TP represents the average TP concentration from 2004 to 2010; Y and N represent meeting the water quality target (Y) and not (N), respectively.

Table 1

quality conditions into five categories (Classes I-V which limit TP concentrations to 0.02, 0.1, 0.2, 0.3, and 0.4 mg/L, respectively). The  $STA_m$  is set to 0 when  $C_{a,m}$  is less than  $C_{s,m}$ , which indicates the river m has reached its water quality standard, and thus it's not necessary to implement TP mitigation measures in its adjacent sub-watershed. In the ILR-SO model formulated as Eqs. (1)-(6),  $SL_k$  were quantified by SWAT overland simulation. Reduced surface TP loading based on  $\lambda_k$  was fed back to SWAT to calculate the instream TP loading.  $\lambda_k$  is adjusted and optimized by the optimization algorithm. In this way, ILR-SO coupled the mechanistic SWAT model with the optimization model. Based on optimized  $\lambda_k$ , the ideal TP load reduction per unit area for each sub-watershed *ILR*<sub>k</sub> (kg/ha) was calculated as follows:

$$ILR_k = \frac{\lambda_k \cdot SL_k}{AR_k} \tag{7}$$

where  $AR_k$  is the area of the sub-watershed k (ha). A larger  $ILR_k$  value represents greater TP load reduction requirement, which indicates that taking TP mitigation measures in the corresponding sub-watershed could contribute to more significant water quality improvement. Therefore,  $ILR_k$  is regarded as the basic criterion for sub-watershed ranking and targeting. The sub-watersheds with larger  $ILR_k$  values were identified as higher level PMAs.

#### 2.5. ILP-SO model solution with metamodeling

The ILR-SO model, an integration of physically-based SWAT simulation and optimal decision-making, is a complicated non-linear simulation-optimization problem. GA is a promising global-search technology to deal with complicated problems (Holland, 1992). It can be easily coupled with simulation models without accessing the detailed mechanistic functions and the computer codes (McKinney and Lin, 1994). As a global random search method, GA represents possible solutions in the feasible region as individuals of the population and encodes them as chromosomes with genes. Fitness of each individual is evaluated based on objective functions of the optimization model. Individuals with greater fitness values are more likely to survive and generate a new population by crossover and mutation for the next generation. SWAT should be run numerous times during the iterative process of GA to calculate the fitness value for each individual, which results in time-consuming global search. In this study, metamodeling is used to reduce computation and improve decision making efficiency. Metamodeling is an approach to approximate the complicated model with an efficient mathematical surrogate model (Broad et al., 2015). It has been proven effective to speed up process-based optimization significantly (Broad et al., 2015; Heuvelmans, 2010). The LMBP network, a back propagation artificial neural network (ANN) incorporating the Levenberge Marquardt algorithm (Hagan and Menhaj, 1994), was used for metamodeling in the present study. Compared with the conventional back propagation (BP) algorithm, LMBP could improve speed of convergence significantly (Saini and Soni, 2002). The procedure to solve the ILR-SO model integrating GA and metamodeling consists of the following steps:

#### 2.5.1. Step1: Design of experiments

The Monte Carlo method (Binder, 1986) was used to simulate decision variables  $\lambda_k$  within the range [0,1] repetitively with a simulation number N = 20000. The simulated values of  $\lambda_k$  are represented with  $\lambda_k^i (i = 1, 2, ..., N; k = 1, 2, ..., K)$ .

#### 2.5.2. Step 2: Dataset construction

Reduction ratio samples  $\lambda_k^i$  were converted into TP loading:

 $Load_k^i = (1 - \lambda_k^i)SL_k$ 

where  $Load_k^i$  is the overland TP loading for the kth sub-watershed and *i*th sample.  $Load_k^i$  was inputted into SWAT and the TP loading at the outlet of each river  $TP_m^i$  was thus obtained:

$$TP_m^i = SIM_m(Load_1^i, Load_2^i, ..., Load_K^i)$$
(9)

The reduction ratios and corresponding TP loading outputs are used as the sample dataset for *meta*-model training  $S_m^i = \langle (\lambda_1^i, \lambda_2^i, ..., \lambda_K^i), TP_m^i \rangle$ .

# 2.5.3. Step 3: Metamodeling with LMBP

The samples  $S_m^i$  were divided into three datasets randomly for LMBP training, among which 60% were the training set, 20% were the validation set and the remaining 20% were the test set. The network weights were adjusted based on the training set. The validation set was synchronously monitored, and the training process would be interrupted when the validation error increased during 6 continuous iterations. Network training would also terminate when reaching the error threshold of  $1.0 \times 10^{-4}$  or the maximum iteration number of 100. The predictive performance was evaluated with the test set. The metamodel for the *mth* river trained with LMBP was represented with  $NET_m$ , which was used to substitute for  $SIM_m$  if reaching the precision threshold, otherwise the simulation number N was required to be increased and the above steps should be repeated to train new networks. The SWAT model was replaced with  $NET_m$ , and thus  $TP_m$ , the TP loading of the *mth* river, was estimated with Eq. (10).

$$TP_m = NET_m(\lambda_1, \lambda_2, \dots, \lambda_k)$$
<sup>(10)</sup>

# 2.5.4. Step 4: Optimization with GA

The ILR-SO model was solved with GA by adopting Eq. (1) as the fitness function for individual evaluation and selection. During the iterative process of GA, the individuals violating the constraints formulated as Eq. (10) were eliminated. After some trial runs, GA with a population number of 100, crossover probability of 0.8 and mutation probability of 0.1 was used to explore optimal solutions. The search process would be terminated when exceeding the maximum generation number 500 or the average variation of fitness values less than  $1.0 \times 10^{-4}$ . By solving the ILR-SO model with GA, the optimal TP load reduction ratio  $\lambda_k$  for each sub-watershed could be obtained. All the sub-watersheds were subsequently ranked based on *ILR<sub>k</sub>*, which was calculated with Eq. (7).

#### 3. Results and discussions

#### 3.1. SWAT calibration and validation

The parameters were automatically optimized within their predefined allowable value ranges during the calibration period. The calibrated values of selected parameters were presented in Table 2. The values of CN2, SOL AWC, and SOL K varied spatially among different HRUs, and thus they were calibrated relatively to their initial reference values. USLE P and USLE K are two important parameters for sediment simulation. Although sediment was not calibrated in this study for lack of observed data, the parameters related to sediment were still taken into consideration as most P losses moves with sediment (Kronvang et al., 1997). Performance of the SWAT model with the optimized parameters was calibrated and validated by comparing simulated flow and TP loading results with observations (Fig. 3). The model performance was evaluated with NSE. The NSE value greater than 0.5 is commonly considered to be 'satisfactory', 'good' for the value above 0.65, and 'very good' for the value larger than 0.75 (Moriasi et al., 2007). Model performance for flow simulation at the two stations is similar. NSE reached to 0.76 and 0.81 during the calibration period in the Kunming (Fig. 3a) and Ganhaizi (Fig. 3b) stations, respectively. A

(8)

#### Table 2

The SWAT parameters calibrated for Lake Dianchi Watershed.

Model process	Parameter	Description	Range	Calibrated value
Surface runoff	CN2 <sup>a</sup>	Moisture condition II curve number	-0.5,0.5	0.02
Groundwater	ALPHA_BF	Base flow alpha factor (days)	0,1	0.45
Evapotranspiration	ESCO	Soil evaporation compensation factor	0,1	0.87
Soil water	SOL_AWC <sup>a</sup>	Available water capacity of the soil layer	-0.5, 0.5	0.11
Surface runoff	SURLAG	Surface runoff lag time (days)	0,24	8.19
Soil water	SOL_K <sup>a</sup>	Saturated hydraulic conductivity	-1,1	0.8
Groundwater	REVAPMN	Threshold depth of water in the shallow aquifer for revap to occur (mm)	0,500	58.7
Groundwater	GWQMN	Threshold depth of water in the shallow aquifer required for return flow to occur (mm)	0,5000	4556
Channel	CH_N2	Manning's "n" value for the main channel.	0,0.3	0.12
Channel	CH_K2	Effective hydraulic conductivity (mm/hr)	0,150	9.5
Sediment	USLE_P	USLE equation support practice factor	0,0.3	0.09
Sediment	USLE_K	USLE equation soil erodibility factor	0,0.3	0.03
Phosphorus	ERORGP	Phosphorus enrichment ratio	0,5	1.53
Phosphorus	PSP	Phosphorus availability index	0.01,0.7	0.67
Phosphorus	PHOSKD	Phosphorus soil partitioning coefficient	100,200	189

<sup>a</sup> The parameter was changed relatively to the initial value.

good performance was also achieved during the validation period. The NSE values for flow validation in at the Kunming and Ganhaizi stations are 0.86 and 0.78, respectively.

There is no obvious drop in performance from calibration to validation, which indicates that the SWAT model is reliable for flow prediction in Lake Dianchi Watershed. The model could capture both the baseflow and peak flow in the two stations. Most areas in the downstream Panlong watershed are urbanized, where surface runoff demonstrates more significant inter-annual fluctuation caused by anthropic activities. By contrast, the Baoxiang watershed is dominated by cropland, and instream flow shows relatively regular seasonal variation. Model performance for TP loading predictions is not as good as flow, but could still be considered 'satisfactory' (Fig. 3c). NSE for the validation period (0.74) is higher than that of the calibration period (0.64). The reason is that there are more loading peaks during the calibration period (2004-2007), some of which could not be well captured with the model, whereas TP loading is much lower during the validation period, which might be a result of implementation of management practices in the watershed during the last decade (e.g. buffer strips and wetlands). The peaks of TP loads and stream flow are synchronously, which usually occur in summer (June to August) driven by rainfall events.

# 3.2. Identification of PMAs

The calibrated SWAT model for the Lake Dianchi Watershed was run over the period of 2001-2010, and TP losses in each sub-watershed were estimated. The results of TP yields were analyzed in a typical wet year (2007). Spatial distribution of diffuse TP loading demonstrates significant spatial heterogeneity (Fig. 4). The upstream Baoxiang River watershed and southeastern Dianchi Watershed are the main source areas of TP losses, which results from fertilizer application in cropland. Diffuse TP loads in the upstream watershed of the Panlong River are less than 0.1 kg/ha, where the dominated landcover is forest. All the 64 sub-watersheds were prioritized according to their diffuse TP contributions, which is quantified with corresponding TP loading per unit area (Fig. 4c). The sub-watersheds around the outlets of the Chai River (CH) and the Yuni River (YN) are significantly more seriously polluted by diffuse P (3.25 kg/ha and 3.20 kg/ha for sub-watershed 48 and 43, respectively) than other areas. The TP loads and areas of the ranked sub-watersheds were cumulated, respectively. The TP and area cumulative ratio curves (Fig. 4a-b) demonstrate that 85% of the total diffuse

TP loads derive from a small fraction of the watershed area (30%). The TP cumulative ratio curve increases sharply with the higher-ranked subwatersheds, and then levels up gently. Most sub-watersheds contribute merely a small percentage of TP losses for the entire watershed. Spatial distributions of TP loading in Lake Dianchi Watershed indicate that PMA identification is critical for diffuse TP abatement and BMP placement.

According to the GB3838-2002 standards, most rivers in the watershed are far from reaching the water quality standards, except the Luolong (LL), Laoyu (LY), Nanchong (NC), Baiyu (BY), and Dongda (DD) rivers. For the Panlong River and Baoxiang River, the two largest rivers in the watershed, it was estimated that nearly 75% and 77% of the instream diffuse TP loading should be reduced to meet the water quality standards, respectively. The ILR of each sub-watershed was calculated with the ILR-SO model. There are 20 out of 64 sub-watersheds not taken into account for TP load reduction since water quality standards were satisfied in their adjacent rivers (Fig. 5). After being ranked with the ILR criterion, the sub-watersheds were classified into four categories: high, medium, low and very low priority levels, based on cumulative TP reduction relative to the total TP reduction requirement (Table 3). Cumulative TP reduction ratios with 60%, 90%, and 100% were used to classify sub-watersheds with TP loading reduction requirement into high, medium and low level PMAs. The sub-watersheds without TP reduction requirement were identified at 'very low' levels, including the 20 sub-watersheds connected to the rivers reaching water quality standards, and 12 sub-watersheds where the ILR was equal to zero. The ILR varied from 0.87 to 3.25 kg/ha, 0.26 to 0.60 kg/ ha and 0.01 to 0.15 kg/ha for high, medium and low level PMAs, respectively. Six sub-watersheds were regarded as PMAs with a high-level priority, located in the watersheds of Baoxiang, Chai, and Yuni rivers where the dominated land use type was cropland (Fig. 5). The downstream watershed of the Panlong River was identified as medium-level PMAs, where NPS pollution derives from urban storm water predominantly.

With the ILR-SO method, sub-watershed management priority is determined based on optimized TP load reduction, which is regarded as "ideal" because load reduction potentials are not taken into account. However, TP mitigation capacity might vary spatially with applicable conservation practices and local landscapes. The ILR optimized by the ILR-SO approach could not be regarded as predicted or expected BMP efficiency. It is merely used for spatial comparison and ranking in this study.



Fig. 3. Flow calibration and validation results in the (a) Kunming station, (b) Ganhaizi station, and (c) TP results in the Baoxiang station. The lines represent the simulation results and the dots for observed values.

# 3.3. Comparison with other targeting methods

The proposed ILR-SO targeting method was compared with the conventional LUAI (Fig. 6a) and LII methods (Fig. 6b), which are based on overland pollutant losses per unit area and pollutant loading for each reach segment, respectively. Point sources were omitted when estimating instream loading for the LII method to eliminate interference of point sources on PMA identification and make the its results

comparable with LUAI and ILR-SO. The thresholds of cumulative TP ratios 60%, 90%, and 100% were used to divide sub-watersheds into high, medium and low level PMAs with the LUAI and LII methods, consistently with PMAs identification with the ILR-SO method. The 'very low' level priority areas without TP abatement requirements were not identified for the LUAI and LII methods, since water quality standards were not taken into account with these conventional methods. Despite that the southwestern sub-watersheds suffer from large diffuse



(c) Diffuse TP spatial distribution.

Fig. 4. Spatial distributions of annual diffuse TP loads simulated with SWAT in Lake Dianchi Watershed.

agricultural TP losses, some rivers have reached water quality standards (e.g. the average TP concentrations are 0.07 and 0.13, respectively, in contrast with Class III limiting TP concentration to 0.2 mg/L). The reason is that the southwestern sub-watersheds are not interfered by domestic pollution as much as the other areas (e.g. the northern subwatersheds). For instance, 85.0% of the sub-watershed 26, located in downstream of the Panlong River, is occupied by residential areas, whereas for the sub-watershed 42 in the Nanchong River, the proportion is only 1.8% (Fig. 1). The LUAI and LII methods identified most area of the southwestern sub-watersheds as high-level PMAs regardless of the fact that water quality standards were already satisfied, which resulted in a waste of time and resources. PMAs identified with the LUAI method are consistent with diffuse TP spatial distributions (Fig. 4c). Compared with LUAI, more sub-watersheds adjacent to the watershed outlets were regarded as higher priority areas with the ILR-SO method (e.g. sub-watersheds 21 and 26 around the outlets of the Yunliang River and the Baoxiang River, respectively). It makes sense because the ILR-SO method incorporated connectivity between pollution sources and instream loading, and it's commonly recognized that nutrient abatement at watershed outlets are more efficient (Arabi et al.,

2006). The LUAI method is more applicable for local concerns at the sub-watershed or field scale. LII-targeted PMAs are mostly located in the near-shore areas, reflecting effects of TP accumulation in channels. For instance, the downstream sub-watersheds of the Baoxiang River were identified as high-level PMAs (sub-watersheds 22 and 31) with the LII method (Fig. 5), whereas they were low-level PMAs with the ILR-SO method. Contrary to LUAI and LII, the ILR-SO method presents modest PMA identification results by taking both overland nutrient losses and instream transport processes into consideration.

# 3.4. Implications of uncertainty

Evaluation of uncertainty associated with watershed management has triggered worldwide attentions. The designed implementation strategies of BMPs might not be able to achieve the expected water quality goals due to uncertainty in watershed simulation. Considerable uncertainty sources for nutrient estimation at the watershed scale have been addressed. There is evidence that parameters of watershed models would affect nutrient fate and transport significantly (Arabi et al., 2007). Parameter uncertainty could be mitigated by conducting



Fig. 5. PMA identification with the ILR-SO method.

 Table 3

 Sub-watershed ranking and classification with the ILR-SO method.

calibration based on observed data to some extent, but it still remains one of the major uncertainty sources (Benaman and Shoemaker, 2004). Different projections of future climate change and landuse scenarios are also important factors influencing watershed hydrology and nutrient loading (Wu et al., 2012). Destouni et al. (2017) concluded that temporal nutrient loads were primarily dominated by hydro-climatically driven water discharge across Sweden. Spatial resolution of input data (e.g. DEM, land cover and soil properties) could have significant impacts on watershed model predictions (Zhang et al., 2014). A thorough uncertainty analysis was not conducted so far in our study because for hotspot identification with complicated watershed modelling, there is a tendency to adopt best-fit parameters and overlook randomness of climate change and hydrologic conditions (Niraula et al., 2013; Winchell et al., 2015). In addition, uncertainty-based simulation-optimization is extremely time-consuming. The physically-based model should be run numerous times during the globally searching process. The times of simulation run could increase exponentially with the number of uncertainty factors. Although tremendous progress has been made for uncertainty-based optimization in recent decades (Lee and Labadie, 2007; Cheng et al., 2017; Huang et al., 2017), complicated simulationoptimization based on uncertainty analysis is still limited by large computational demands. Development of advanced and efficient approaches are thus required for more robust BMP decision-making by enabling rigorous uncertainty analysis.

#### 4. Conclusion

A simulation-optimization approach with ideal load reduction (ILR-SO) was proposed to identify the watershed priority management areas under water quality constraints. It could support decision making in identification of hot spots and BMP placement at the watershed scale. The modelling framework was used for PMA identification in Lake Dianchi Watershed, which is a large watershed with significant spatial heterogeneity and comprising multiple tributaries:

(1) The watershed simulation results demonstrated that TP spatial distribution had significant heterogeneity. About 30% of the watershed area contributed 75% of TP loading; therefore, it's essential

No.	ILR (kg/ha)	TLR (ton)	CRR (%)	Rank/Level	No.	ILR (kg/ha)	TLR (ton)	CRR (%)	Rank/Level
43	3.25	0.51	1	1/high	27	0.15	0.45	91	17/low
48	1.74	1.67	6	2/high	22	0.13	0.05	92	18/low
46	1.70	6.97	27	3/high	31	0.13	0.55	93	19/low
14	1.00	7.33	48	4/high	11	0.13	0.43	94	20/low
29	0.97	0.11	49	5/high	10	0.09	0.54	96	21/low
20	0.87	1.55	53	6/high	9	0.08	0.31	97	22/low
50	0.60	1.93	60	7/medium	28	0.08	0.4	98	23/low
53	0.59	1.18	62	8/medium	16	0.06	0.15	99	24/low
32	0.58	2.41	69	9/medium	30	0.05	0.16	99	25/low
47	0.54	1.37	73	10/medium	12	0.04	0.09	99	26/low
17	0.40	2.05	79	11/medium	7	0.04	0.09	100	27/low
21	0.39	0.21	80	12/medium	45	0.03	0.08	100	28/low
13	0.37	1.14	83	13/medium	49	0.01	0.02	100	29/low
18	0.35	0.45	84	14/medium	23	0.01	0.01	100	30/low
44	0.30	1.42	89	15/medium	19	0.01	0.04	100	31/low
26	0.26	0.53	90	16/medium	15	0.01	0.02	100	32/low

*Note*: (a) No. represents the sub-watershed number; (b) the sub-watersheds without TP load reduction requirements are not presented; (c) ILR is the ideal TP load reduction amount per unit area calculated with Eq. (8); TLR is the total TP load reduction for each sub-watershed,  $TLR_r = \lambda_r SL_r, r = 1, 2, ...R$ , where *r* represents the priority rank; CRR is the cumulative reduction ratio by adding up the reduction ratios of all the sub-watersheds with higher priority ranks,  $CRR_r = \sum_{i=1}^r TLR_i / \sum_{i=1}^R TLR_i$ ; (d) ILR is used to rank sub-watersheds; CRR is used to determine thresholds of priority levels.



Fig. 6. PMA identification with the conventional targeting methods.

to identify PMAs at the watershed scale. Seven out of 64 sub-watersheds, where cropland is the dominated land use type, were identified as high-level PMAs.

- (2) PMAs identification with the proposed ILR-SO method was compared with the overland nutrient loss based LUAI and the instream nutrient loading based LII methods. The results indicate ILR-SO is a rational method by taking into account both pollution sources and instream processes. By incorporating water quality standards of multiple rivers draining into Lake Dianchi, ILR-SO identified less PMA areas than the conventional strategies for excluding areas without nutrient reduction requirement, which could contribute to more efficient watershed management.
- (3) The 15 major rivers draining into Lake Dianchi are distinct in location, length, pathway, and water use. That shows the ILR-SO approach's advantages in supporting decision-making in the complex watershed system and serving various conservation objectives. The approach is especially appropriate for, but not limited to, the watersheds with long hydrologic residence time in channel networks. The ILR-SO approach could also be extended to cases where

a river has hierarchical water quality standards from headwater to downstream.

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