- Landscape position units are universal PMA identification units finer than subbasins.
- A Markov chain-based surrogate model of SWAT+ is developed to identify PMAs.
- SWAT+ is qualified to provide the flow distribution matrix among LSUs and channels.
- LSU-based PMAs are more effective in distribution and cumulative load contribution.
- LSU-based PMAs have general applicability for diverse geographic environments.

1	Identification of watershed priority management areas based on
2	landscape positions: an- <u>An</u> implementation using SWAT <sup>+</sup>
3	
4	Highlights
5	• Landscape position units (LSU) are adopted <u>universal</u> to identify priority
6	management areas(PMAs)PMA identification units finer than subbasins.
7	• A Markov chain-based surrogate model of SWAT+ is proposed-developed to
8	identify PMAs.
9	• SWAT+ is qualified to provide <u>the</u> flow distribution matrix among LSUs and
10	channels.
11	• LSU-based PMAs are more effective in distribution and cumulative load
12	contribution.
13	• LSU-based PMAs have general applicability for various diverse geographic
14	environments.
15	
16	Abstract
17	Priority The priority management areas (PMAs) of a watershed are areas with high

18 contributions to the pollutant load toof the assessment outlet, such as the watershed 19 outlet, and, thus, have high priority in the decision\_-making forof comprehensive 20 watershed management. Existing spatial units used to identify PMAs are commonly 21 based on three concepts including subbasins, artificial geographic entities, and grid cells. However, these identification units cannot balance the general applicability to diverse 22 geographic environments and the representation degree of spatial heterogeneity, which 23 impacts the effectiveness of the PMAs. This study proposes adopting utilizing 24 landscape positions along the hillslope as identification units of PMAs, which can be 25

26	represented by slope position units (e.g., upland, backslope, and valley). Landscape
27	position units inherently have upstream-downstream relationships with each other and
28	with channels. Therefore, their contributions to the assessment outlet can be quantified
29	based on the propagation effects of hillslope and channel routing processes. The
30	proposed method was implemented using a restructured and enhanced version of the
31	Soil and Water Assessment Tool (SWAT <sup>+</sup> ) to quantify the pollutants released, and an
32	improved-Markov chain-based surrogate model to distinguish the source contribution
33	with the improvement of the transition matrix in representing both landscape position
34	and channel units. Two watersheds, one in China and one in the USA, with different
35	geographic characteristics were selected to separately conduct the comparative
36	experiments to identify PMAs at the landscape position and the subbasin levels. The
37	results showed that PMAs based on landscape positions have more accurate spatial
38	distribution and require less area for the future configuration of management practices
39	to achieve the same management goal as PMAs based on subbasins. The better
40	effectiveness of landscape position units in identifying PMAs is mainly due to their
41	better ability to represent hillslope processes and the spatial heterogeneity of underlying
42	surface environments within subbasins. The proposed method can be implemented by
43	using other watershed models that support landscape position units or different types of
44	spatial units with explicit upstream-downstream relationships within subbasins.
45	Keywords: Priority management areas; Landscape positions; Spatial units;

46 Pollutant load contribution; Best Management Practices; SWAT<sup>+</sup>

# 1 **1. Introduction**

2 The pPriority management areas (PMAs) areis a prioritizing prioritized areas for 3 pollution management in the a watershed, which has a high pollutant production, and more importantly, with a high contribution to the pollutant load of its direct or indirect 4 downstream water bodies (Chen et al., 2014). This concept is similar to the-a critical 5 source area (CSA), which is more commonly used to identify highly polluted areas 6 7 (Pionke et al., 2000; White et al., 2009) but usually does not emphasize propagation 8 effects from upstream to downstream in the watershed, which is essential in the for 9 decision-making of for comprehensive watershed management. Priority management 10 areas are ideal spatial locations for implementing suitable best management practices 11 (BMPs) to effectively control ecological and environmental problems, such as soil erosion and non-point source pollution (Shen et al., 2015; Tian et al., 2020; Guo et al., 12 13 2022). The identification of PMAs can be regarded as the first step in the spatial 14 configuration of BMPs for comprehensive watershed management, where factors 15 affecting actual management decisions, such as investment plans, stakeholders<sup>2</sup> 16 willingness, environmental goals, and BMP effectiveness, could can be considered. The spatial distribution of PMAs considerably affects the locations, areas, and effectiveness 17 18 of the configured BMPs, affecting the cost\_effectiveness of the BMP scenario (i.e., the spatial configuration of multiple BMPs in the watershed) (Chiang et al., 2014; Qin et 19 20 al., 2018; Wang et al., 2016; Zhu et al., 2021). Therefore, the accurate identification of 21 PMAs is a key issue for comprehensive watershed management (Chen et al., 2022).

The foremost important step in identifying PMAs is to determine an appropriate type of spatial units as a computing unit for pollutant production and contribution to the assessment outlet, such as the watershed outlet (hereafter referred to as the identification units) (Dong et al., 2018; White et al., 2009). The identification units adopted-utilized in existing research are mainly based on three concepts: subbasins (Shang et al., 2012; Chen et al., 2014; Shen et al., 2015; Dong et al., 2018), artificial geographic entities (Tian et al., 2020), and grid cells (Kovacs et al., 2012).

29 The <u>A</u> subbasin represents a relatively closed and independent geographic unit that 30 is linked to other subbasins through channels. Subbasin units are the most straightforward and most frequently used identification units because they are 31 32 delineated and modeled in most watershed modeling. In addition to directly utilizing 33 subbasin units, researchers also use the combination of subbasins as identification units according to administrative regions (such as villages; Shang et al., 2012), for the benefit 34 35 of making and implementing watershed management policies, especially in large study 36 areas (Liu et al., 2019; Shang et al., 2012). However, a subbasin can be recognized and 37 modeled as an integral of one or more levels of finer spatial units to better represent 38 spatial heterogeneity within it subbasin, such as hillslopes, slope position units, landuse fields, and even grid cells. Therefore, it may be too coarse to use these subbasin-39 40 based identification units because the heterogeneity of pollutant sources and transportation processes within the subbasins should be considered (Qin et al., 2018; 41 42 Wang et al., 2016).

43

Artificial geographic entities refer to artificially constructed and hydrologically

connected geographic entities based on the characteristics of a specific geographic 44 environment (Ghebremichael et al., 2013), such as polders that developed in lowland 45 46 plains with densely distributed rivers and lakes (Tian et al., 2020). Such spatial units have relatively homogeneous features from the perspectives of physical geographic 47 processes and/or anthropogenic activities. For example, a polder may contain 48 agricultural land, irrigation channels, ponds, and even villages, that are enclosed by 49 artificial dams to serve as conservation areas for flood management and waterlogging. 50 Although artificial geographic entities are appropriate for use as identification units 51 52 than subbasins in the corresponding geographic environments, they are not easy to beily generalized as generally applicable universal identification units and, thus, are cannot 53 54 be widely applied toin most diverse geographic environments.

Grid cells are commonly used spatial units with regular shapes in geographic modeling, and their underlying surface characteristics are homogeneous. <u>Grid cells are</u> <u>universal units to identify PMAs accurately u</u>Using <u>those</u> watershed models that explicitly represent flow routings among grid cells, <u>PMAs can be identified accurately</u> (Kovacs et al., 2012). However, using grid cells may cause more fragmentized distributions of PMAs, which reduces the implementation efficiency and limits further application (e.g., <u>the-for</u> PMA-based spatial optimization of BMPs).

Therefore, the existing spatial units used for identifying PMAs cannot balance the general applicability to diverse geographic environments and the representation degree of spatial heterogeneity. According to the <u>previous\_foregoing\_analysis</u>, proper identification units should (1) be broadly available and not be limited to a specific geographic environment; (2) be capable of representing the spatial heterogeneity of
underlying surface characteristics, physical geographic processes, and/or
anthropogenic activities inside the study area by a small number of units; and (3) have
hydrologic connections among each other.

70 This study proposes the use of landscape positions along hillslopes within each 71 subbasin to identify PMAs. In this study, Landscape positions refer to the geographic 72 objects - can be delineated by landform units (also referred to as slope position units) 73 that reflect the integrated effects of hillslope processes on topography and affect 74 geographic processes on the surface (Volk et al., 2007; Arnold et al., 2010; Miller and Schaetzl, 2015; Qin et al., 2018). Landscape position units are universality in most 75 76 geographic environments that can be delineated by slope position units (Wolock et al., 77 2004; Volk et al., 2007; Qin et al., 2009). Based on commonly used classification 78 systems of slope positions (e.g., the divide, backslope, and valley units adopted utilized 79 by Arnold et al. (2010)), each subbasin needs only a few spatial units (e.g., three) to 80 represent the spatial homogeneity from the perspective of hillslope processes (Qin et al., 2018; Rathjens et al., 2016). In addition, landscape position units have inherent 81 82 upstream-downstream relationships among each other, which have been considered in watershed modeling (Arnold et al., 2010; Bieger et al., 2019; Rathjens et al., 2015; Yang 83 et al., 2002) and spatial optimization of BMPs (Qin et al., 2018; Zhu et al., 2019; Zhu 84 et al., 2021). Thus, landscape position units meet the requirements for use as the 85 86 aforementioned identification units mentioned above.

87

This study proposes a PMA identification method based on landscape position

units exemplified by SWAT<sup>+</sup> (i.e., the restructured and enhanced version of the Soil and 88 Water Assessment Tool) and evaluates the effectiveness of the proposed method by 89 90 comparing it to widely used subbasin units. The remainder of this paper is organized as follows: Section 2 introduces the proposed method; and Section 3 presents a 91 92 comparative experimental design of using landscape position and subbasin units to 93 identify PMAs of total nitrogen in two watersheds with different geographic characteristics. The experimental results and discussion are presented in Section 4, and 94 95 the conclusions are presented in Section 5.

# 96 2. Method design

To identify PMAs at the landscape position unit level, two key issues must be addressed. The first is the quantification of pollutants released <u>at-from the</u> landscape position units. The second is how to distinguish the pollutant load contribution of each landscape position unit to the assessment outlet, that is, the residual amount of pollutant after being transported to its direct downstream channel and then transitioning in hierarchical channels before reaching the assessment outlet (Chen et al., 2014).

Generally, the contribution of the pollutant load cannot be directly determined from the results of most watershed models. Instead, watershed models output the pollutant released from each simulation unit (e.g., the hydrologic response unit [HRU] in SWAT) or lumped unit (e.g., subbasin), as well as the flow of substances in and out of each channel. To fill this gap, Grimvall and Stålnacke (1996) proposed a Markov chain-based surrogate model to simulate pollutant transitions from upstream channels

(one channel for each subbasin) to the assessment outlet in a statistical manner. Their 109 basic idea is to use analog pollutant transformation and transfer processes in 110 111 hierarchical channels as a Markov process, in which, the transition matrix is determined 112 by the upstream-downstream relationships among channels and the retention effects of 113 the channel routing process. After a finite number of transitions (equal to the length of 114 the longest branch in hierarchical channels), all pollutants from upstream subbasins reach the assessment outlet, thus, the corresponding pollutant load contributions can be 115 116 derived (Grimvall and Stålnacke, 1996).

117 Follow-up studies continued to adopt apply the subbasin unit in the Markov chainbased model (Chen et al., 2014; Rankinen et al., 2016), which includes pollutant 118 119 production onat hillslopes and pollutant routing in the channel. The transition matrix of 120 the Markov chain-based model can be improved to represent both landscape position and channel units. Therefore, if we can separate these two processes can be separated 121 122 in the landscape position units and channels, the improved Markov chain-based model 123 will be able to distinguish the pollutant contribution of each landscape position unit to 124 the assessment outlet. Based on this basic idea, the proposed method aims to incorporate a watershed model that supports landscape position units as simulation or lumped units, 125 to improve the Markov chain-based PMA identification method from the subbasin level 126 127 to the landscape position unit level. Therefore, the Markov chain-based PMA identification method can be generalized as a method framework that supports one or 128 129 more types of hierarchical spatial units with explicit hydrological connections (i.e., upstream-downstream relationships), such as subbasins and landscape position units 130

131 (Fig. 1).

132	2.1 Delineation and modeling of landscape position units in SWAT $^+$
133	As a restructured and enhanced version of the SWAT model, SWAT <sup>+</sup> (Bieger et al.,
134	2017, 2019) introduced a new type of spatial unit between the subbasin unit and HRU
135	named the landscape position unit (LSU), which includes the uplands and floodplains
136	(Fig. 2). <u>SWAT<sup>+</sup> uses the relative position index (RPI) of each cell in a gridded digital</u>
137	elevation model (DEM) to delineate LSUs (Rathjens et al., 2016). The RPI of each cell
138	is the ratio of the drop length to its downstream valley (i.e., the stream cell) and the
139	length from its upstream ridge cell to the same valley cell. The RPI ranges from 0 to 1.
140	The cell with a RPI less than the user-specific threshold is classified as the floodplain.
141	This means that the basic spatial discretization of a watershed in SWAT <sup>+</sup> contains three
142	types of nested spatial units as a hierarchy: subbasin, LSU, and HRU. The HRU, as the
143	basic simulation unit of SWAT+, is delineated as the unique combination of soil, land
144	use, and slope class within the LSU, which is spatially discrete (Fig. 2a) and even lacks
145	explicit spatial locations according to different delineation parameters. Therefore,
146	HRUs are unsuitable for PMA identification units since there are no hydrologic
147	connections between HRUs, although the HRU is finer than the LSU. In addition,
148	SWAT <sup>+</sup> also abstracts specific types of geographic entities as spatial units with locations
149	and properties to participate in watershed modeling. For example, reservoirs or ponds
150	within a subbasin are first generalized as one point in the channel that divides the
151	channel into two parts, and then defined by the upstream part with additional properties
152	such as storage capacity (Fig. 2 <u>a</u> ). The hillslopes, LSUs, and HRUs <u>also</u> are also

delineated accordingly, while the two aquifer units remain unchanged (Fig. 2b). These
spatial units can enrich the flow routing network of SWAT<sup>+</sup> and play important roles in
the simulation of study areas with specific geographic environments, such as,
agricultural ecosystems with densely distributed ponds.

With the new spatial discretization scheme, SWAT<sup>+</sup> improved improves the 157 representation of realistic hydrologic processes from hillslopes to channels (Bieger et 158 159 al., 2019). Instead of directly adding all released substances of from HRUs (including water, sediment, and pollutants) to the channel, SWAT<sup>+</sup> first lumps HRUs' outputs at 160 161 the LSU level and then routes these outputs to other spatial units using two different methods. The first method involves completely draining from the upland to the 162 163 floodplain and from the floodplain to the channel, which is applicable for lateral flow 164 in soils and groundwater recharge in aquifers (Fig. 2b). The second method distributes water from the upland to the channel/pond/reservoir by a constant ratio (e.g., 0.30 from 165 166 LSU2 to the pond and 0.66 from LSU4 to the channel, as shown in Fig. 2b; hereafter 167 'channel/pond/reservoir' is referred to as channel collectively) and the rest to the 168 floodplain as additional net precipitation to participate in the hydrologic simulation. 169 The output from the floodplain drains entirely into the channel (Fig. 2b). SWAT<sup>+</sup> provides two ways to determine this ratio: the user-specified global value for all upland 170 171 units in the watershed and the area ratio of each upland to its floodplain. The area ratio method has been proven to be more realistic in representing the connectivity than the 172 173 fixed ratio for the entire watershed (Bieger et al., 2019) and is, therefore, adopted 174 applied in this study.

With the flow routing network primarily constructed by <u>chain of HRU</u>, LSU, and channel (Fig. 2<u>b</u>), SWAT<sup>+</sup> is <u>qualified suitable</u> to quantify pollutants released at <u>the</u> landscape position units and the corresponding transportation amounts to their direct channels.

# 179 2.2 Pollutant load contribution of landscape position units derived 180 from a Markov chain-based surrogate model of SWAT<sup>+</sup>

Based on the flow routing network and simulation results of SWAT<sup>+</sup>, the key part of the Markov chain-based surrogate model can be determined, that is, the transition matrix of pollutants through LSUs and channels. Subsequently, using the lumped simulation results at LSUs as inputs, the Markov chain-based model can determine the pollutant load contribution of each landscape position unit.

## 186 2.2.1 Transition matrix of pollutants based on flow routing network and retention

## 187 effects of <u>the</u> channel routing process

The transition matrix is constructed using flow distribution relationships from upstream to downstream units and the retention coefficients of channel routing processes (Chen et al., 2014). According to the spatial discretization scheme of SWAT<sup>+</sup> (see Section 2.1), the flow distribution relationships among the LSUs and channels can be represented by an  $n \times n$  matrix H (Eq. 1). Fig. 3 shows an example of the matrix H.  $H(i,j) = \begin{cases} s, & \text{if LSU(floodplain)} j \text{ is adjacent downstream of LSU(upland)} i \\ 1, & \text{if CHA}(channel) j \text{ is directly downstream of LSU(upland)} i \end{cases}$  (1)

194 where *n* is the total number of LSUs and channels in the watershed, and *s* is the flow

11

distribution ratio from upland to floodplain. For surface runoff, s is initially set by the 195 area ratio of upland and hillslope, while for lateral flow and groundwater recharge, s =196 197 1 (Fig. 2b). Each row represents the flow distribution relationships of a spatial unit with its downstream units. The sum of all elements in one row equals 1, except for the 198 channel row where the assessment outlet is located (e.g., the 7<sup>th</sup> row in Fig. 3, when the 199 outlet of channel 7 is the assessment outlet). For a given assessment outlet of channel 200 k, there exists a smallest integer  $N_k$  to make  $H^{N_k} = 0$ , which means that after  $N_k$ 201 transitions, pollutants from all upstream spatial units of channel k will reach the outlet. 202 203 The physical meaning of  $N_k$  is the longest routing length from the uppermost spatial units to the outlet of channel k, for example,  $N_7 = 4$  in Fig. 3. 204

205 The complicated channel routing process of pollutants accountsing for the 206 chemical pollutant transformation or retardation of the interested substances. For example, a stepwise transformation from organic nitrogen to ammonia, then to nitrite, 207 and finally to nitrate is simulated in SWAT (Neitsch et al., 2011). For each channel of 208 209 the study area, the difference between the output substance and the input can be 210 explained by the retention effect of the channel, which is time-varying and affected by 211 pollutant concentration, water temperature, and other factors. The yearly average retention of each channel and transfer processes can be regarded as its stable removal 212 capacity of pollutants calculated as simplified by using a the retention coefficient (Eq. 213 2) (i.e., removal capacity of pollutants) as a surrogate calculation method (Chen et al., 214 215 2014; Grimvall and Stålnacke, 1996; Hejzlar et al., 2009). The landscape position unit 216 is a lumped unit of pollutant sources calculated at HRUs, thus, it has no retention effect.

217 
$$r = (\text{Load}_{in} - \text{Load}_{out})/\text{Load}_{in} \frac{r_r}{r_r} = (\text{Load}_{ur} - \text{Load}_{ur})/\text{Load}_{ur}$$
(23)  
218 where *r* denotes the retention coefficient of the channel to a specific pollutant; Load<sub>in</sub>  
219 is the pollutant input to the channel-*i* that includes pollutant outputs of adjacent  
220 upstream channels and pollutant released from upstream LSUs; and Load<sub>out</sub> is the  
221 pollutant output at the outlet of the channel-*i*.  
222 The retention coefficient of spatial units, *R*, also is also-represented by an *n* × *n*  
223 matrix, as follows:  
224 
$$R = \begin{pmatrix} r_1 & 0 & \cdots & 0 \\ 0 & r_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & r_n \end{pmatrix}$$
225 Where where the *i*th diagonal element *r<sub>i</sub>* can be calculated using Eq. 2 the simulation  
226 *r<sub>i</sub>* = (Load<sub>in</sub> - Load<sub>out</sub>)/Load<sub>in</sub> (3)  
227 results of for the channels, *r<sub>i</sub>* can be calculated using Eq. 2 the simulation  
228 *r<sub>i</sub>* = (Load<sub>in</sub> - Load<sub>out</sub>)/Load<sub>in</sub> (3)  
229 where Load<sub>in</sub> is the pollutant input to channel *j* that includes pollutant outputs of  
230 adjacent upstream channels and pollutant released from upstream LSUs; and Load<sub>out</sub> is  
231 the pollutant output at the outlet of channel *j*.  
232 The transition matrix,  $\hat{H}_i$  of the Markov chain-based model can be represented  
233 as follows and used to simulate the flow transitions of substances (e.g., water and  
234 pollutants) through the hierarchy of landscape position units and channels:  
235  $\hat{H} = H (I - R)$  (4)

236 where I is an identity matrix.

#### 237 2.2.2 Calculation of pollutant load contribution

Except for the transition matrix, the pollutant released from each LSU is the primary input data for the Markov chain-based model as the initial states. Because the channel acts as a receptor for pollutants, it contains no self-generated pollutants. An n $\times 1$  matrix,  $L_{a}$  is used to organize the input of the pollutant sources:

242 
$$L = (e_1, e_2, \cdots, e_i, \cdots, e_n)^{\mathrm{T}}$$
 (5)

where  $e_i$  is the pollutant released from spatial units *i* based on the simulation results of SWAT<sup>+</sup>. Specifically,  $e_i = 0$ , if *i* is a channel.

The pollutant load contribution of each spatial unit to a specific assessment outlet can be calculated using simple matrix calculations (Grimvall and Stålnacke, 1996):

247 
$$E = \left(\tilde{H}_k\right)^{N_k} V_k * L \tag{6}$$

248 
$$\tilde{H}_{k}(i, j) = \begin{cases} H(i, j), \text{ if } i \neq k \\ 1, & \text{ if } i = j = k \\ 0, & \text{ if } i = k \text{ and } j \neq k \end{cases}$$
(7)

249 
$$V_k(i) = \begin{cases} 1, & \text{if } i = k \\ 0, & \text{otherwise} \end{cases}$$
(8)

where *k* represents the assessment outlet located channel, and the corresponding modification from  $\tilde{H}$  to  $\tilde{H}_k$  implies that the *k*th state is transformed to an absorbing state  $\tilde{I}_{a^{-}} V_k$  is an  $n \times 1$  matrix for extracting the *k*th column of the  $(\tilde{H}_k)^{N_k}$ , resulting in the contribution rate of each unit  $\tilde{I}_{a^{-}}$  and the The asterisk\* denotes element-wise multiplication.

255 Considering that <u>the pollutants of interest may have various states that are modeled</u> 256 in different watershed processes, the calculation of <u>the pollutant load contribution</u>

should be combined with all components calculated by different transition matrixes, 
$$H_{\perp}$$
  
and pollutant source matrixes,  $L$ . For example, the total nitrogen consists of organic and  
inorganic nitrogen. In SWAT/SWAT<sup>+</sup>, the inorganic nitrogen output in the channel  
includes ammonia, nitrite, and nitrate nitrogen. The considered in this study mainly  
includes nitrate nitrogen (*NO*<sub>3</sub>) and the organic nitrogen (*ORGN*) are relatively stable  
forms of nitrogen in the soil that are routed from HRUs into the channel with water and  
sediment (Neitsch et al., 2011). Since the nitrogen output at the LSU level is the sum of  
its internal HRUs' output, the nitrogen released from LSUs considered in this study also  
comprises *NO*<sub>3</sub> and *ORGN*. For the sake of simplicity, we use the term of total nitrogen  
(TN) in this study. Tehe TN total nitrogen load contribution can be calculated as follows:  
 $E_{TN} = E_{NO3-SURF} + E_{NO3-TAT} + E_{NO3-GW} + E_{ORGN}$  (9)

268 
$$E_{\text{MOD}} = (H_{\text{SUPP}} (I - R_{\text{MOD}})_{*})^{N_{k}} V_{*} * L_{\text{MOD}} \text{SUPP}$$
(10)

$$\sum_{NO3-SURF} - (\prod_{SURF} (\prod_{NO3})_k) \cdot V_k \cdot \sum_{NO3-SURF} (10)$$

269 
$$E_{NO3-LAT} = \left(H_{LAT}(I - R_{NO3})_k\right)^{N_k} V_k * L_{NO3-LAT}$$
(11)

270 
$$E_{NO3-GW} = \left(H_{GW}\left(I - R_{NO3}\right)_{k}\right)^{N_{k}} V_{k} * L_{NO3-GW}$$
(12)

271 
$$E_{ORGN} = \left(H_{SURF} \left(I - R_{ORGN}\right)_{k}\right)^{N_{k}} V_{k} * L_{ORGN-SURF}$$
(13)

where *SURF* denotes the surface runoff, *LAT* denotes the lateral flow, *GW* denotes the groundwater recharge;  $H_{SURF}$ ,  $H_{LAT}$ , and  $H_{GW}$  describe the flow distribution relationships among the spatial units of surface runoff, lateral flow, and groundwater recharge, respectively;  $L_{NO3-SURF}$ ,  $L_{NO3-LAT}$ , and  $L_{NO3-GW}$  are the amounts of *NO*<sub>3</sub> released in surface runoff, lateral flow, and groundwater recharge, respectively; and  $L_{ORGN-SURF}$ is the amount of *ORGN* released in surface runoff. 278

#### 2.2.3 PMA identification based on classification of pollution degrees

279 Once the pollutant load contribution of each landscape position unit is 280 distinguished, a classification of pollution degrees can be adopted determined to 281 identify different levels of PMAs, such as high-, medium-, and low-contribution PMAs. 282 The classification methods in existing studies include the natural breaks method, standard deviation method, and water quality control targets method (Chen et al., 2014; 283 Giri et al., 2016). In this study, we adopted the natural breaks method, a commonly used 284 classification method (De Smith et al., 2018; Giri et al., 2016), to classify the pollutant 285 load contribution. The natural breaks method classifies the data into different classes 286 with the statistical groupings and pattern characteristics inherent in the data to minimize 287 the data difference within a class and maximize the difference between classes. 288

# 289 **3. Experimental design**

To illustrate the effectiveness of the proposed method, a comparative experimental 290 study was designed to identify the PMAs of for total nitrogen at the landscape position 291 292 and subbasin levels based on the same calibrated SWAT<sup>+</sup> model. The source of total nitrogen considered in this study is summed by nitrate nitrogen and organic nitrogen on 293 the LSU. Since the improvement of the Markov-based surrogate model in this study 294 does not change the calculation principle of the original model, the differences in 295 identifying PMAs can be attributed to the identification units adopted (i.e., the LSU and 296 the subbasin unit). The same experimental design was used in two watersheds to 297 evaluate the applicability of the method under different geographic characteristics (e.g., 298

topographical, climatic, hydrological, and ecological conditions), that is, the
Zhongtianshe Watershed (~42 km<sup>2</sup>) in southern China and the Willow River Watershed
(~212 km<sup>2</sup>) in western Wisconsin, USA (Fig. 4).

302

# 3.1 Study areas and data

303 The Zhongtianshe Watershed, located in the south of Liyang-City, Jiangsu Province, China, is a typical hilly area situated in the upstream region of Lake Tai. The 304 study area is characterized by a subtropical monsoon climate. The average annual 305 temperature is 15.5°C and the average annual precipitation is 1160 mm. The main soil 306 type is yellow-red soil, which is a type of acidic soil that is easily weathered. The main 307 308 land use types were are forests (77%), croplands (10%, primarily rice paddy fields), orchards (3%), residential areas (8%), and water areas (2%). The watershed experiences 309 310 frequent agricultural activities, and the cultivation of rice and wheat is the primary 311 contributor to local non-point source pollution. Because the study area is on-in the drinking water source of Liyang, knowing the details of the pollution situation and 312 313 taking reasonable measures to control <u>pollution</u> is a vital issue for the local government (Shi et al., 2021). 314

The Willow River, located in western Wisconsin, USA, is a tributary of the St. Croix River. It is classified as <u>part of</u> the Central Wisconsin Undulating Till Plain based on a report by the <u>U.S. environmental Environmental protection Protection agency</u> <u>Agency (EPA, 2020)</u>, and is characterized as relatively flat compared to the Zhongtianshe watershed. The area has a continental climate with high evapotranspiration, an average annual temperature of 11.8°C, and an average annual

precipitation of 788 mm. The soils are predominantly silt loams with moderately well-321 322 drained characteristics. The main land use types were-are grasslands (45%), forests 323 (27%), croplands (18%), residential areas (6%), and wetlands (3%). Watershed crops are dominated by corn-silage, soybeans, and alfalfa, resulting in non-point source 324 pollution and relatively poor water quality. As the headwater of the popular Willow 325 River State Park and attractive trout fishing destinations, the watershed has been the 326 focus of non-point source pollution control for decades (Almendinger and Murphy, 327 328 2007).

The input data of the study areas for <u>the</u> SWAT<sup>+</sup> modeling consisted of a <del>digital</del> elevation model (DEM), land use types, soil types and properties, meteorological data, agricultural management practices, and observed data at the watershed outlet. Detailed descriptions of the data for the two watersheds are <u>presented-listed</u> in Table 1.

#### 333

## **3.2 Modeling and calibration of the SWAT<sup>+</sup> model**

Two SWAT<sup>+</sup> models (version 59.3) were built by QSWAT<sup>+</sup> version 1.2.2 and 334 335 SWAT<sup>+</sup> version 59.3 -to simulate the total nitrogen pollution in each study area. A total of 15 subbasins, 41 LSUs, and 1260 HRUs were generated in the Zhongtianshe 336 Watershed, while 19 subbasins, 131 LSUs, and 7245 HRUs were generated in the 337 Willow River Watershed (Fig. 5). The RPI thresholds for delineating uplands and 338 floodplains were manually determined by visual interpretation of contour lines, which 339 340 are 0.14 and 0.3 for the Zhongtianshe Watershed and the Willow River Watershed, 341 respectively. In most situations, each subbasin has one upland and one floodplain. There 342 may be an additional floodplain due to the very short channel generated after the setting 343 of a pond or reservoir-.

Limited by the available observed data of for the Zhongtianshe Watershed, we set the year 2011 was set as a warm-up period, and 2012–2013 and 2014–2015 were set as calibration and validation periods, respectively, for daily flow modeling. The model performance of for the total nitrogen was calibrated using the only-5-day or 3-day monitoring data from 2014 to 2015 (a total of 181 values, of which 53 values during the rainy season were sampled in about three days interval from June to August in the two years), without validation.

For the Willow River watershedWatershed, the model had a 2-year warm-up period. The calibration period ranged from 1 January 2012 to 31 July 2014, and the validation period was from 1 October 2010 to 31 December 2011, respectively. The available daily ammonia and organic nitrogen were combined to calibrate and validate the nitrogen modeling.

Model performance was evaluated using the Nash-Sutcliffe efficiency (NSE, 356 357 Nash and Sutcliffe, 1970), percentage bias (PBIAS), root mean square error-standard deviation ratio (RSR), and coefficient of determination  $(R^2)$ , as listed in Table 2. 358 359 According to the criteria of monthly model performance proposed by Moriasi et al. (2007), a satisfactory model should generally have the NSE > 0.50, RSR < 0.70, and 360 PBIAS ±25% for flow, ±55% for sediment, ±70% for nutrients. calibrated SWAT<sup>+</sup> 361 models have approximately satisfactory performance for flow modeling in both study 362 363 areas. For nitrogen, considering that a shorter time step may Meanwhile, the daily model is more likely to cause have poorer model performance than the monthly model 364

(Engel et al. 2007)., and that the simulation trends represented by R<sup>2</sup> have good (shown 365  $\frac{1}{10}$  R<sup>2</sup>) was quite consistencyt with the observed data. Therefore, considering this study 366 367 mainly utilizes the relative rather than absolute reliable model results to verify the effectiveness of the proposed PMA identification method, both calibrated models can 368 369 be regarded as acceptableare applicable for the validation of the proposed PMA identification method in this study. Besides, considering the SWAT<sup>+</sup> is still in active 370 development, we created an open-source repository to store the modeling data and 371 372 update the modeling details and results routinely in our following study 373 (https://github.com/lreis2415/WatershedModelingData).

# **3.3 Identification and evaluation of PMAs at LSU level and subbasin**

375 **level** 

To evaluate the effectiveness of the PMAs at the LSU level, PMAs <u>also</u> were <u>also</u> identified at the subbasin level in the same study area based on the same calibrated SWAT<sup>+</sup> model and the <u>original</u> Markov chain-based surrogate model.

The average annual total nitrogen modeled during the calibration period was used <u>for the input data of the Markov chain to identify the PMAs, with the watershed outlet</u> set as the assessment outlet. The natural break<u>s</u> method was <u>adopted utilized</u> to classify the nitrogen load contribution of the spatial units into three classes, and highcontribution areas were identified as PMAs.

The comparison of <u>the PMAs</u> identified at the LSU and subbasin levels was <u>conducted\_done</u> from two perspectives, the spatial distribution and cumulative load contributions. The spatial distribution of PMAs is an intuitive way to qualitatively analyze the spatial consistency and differences between different units. The cumulative
load contributions were used to quantitatively compare the relationships between the
areas of PMAs and their total pollutant load contribution.

# 390 4. Experimental results and discussion

## 391 **4.1 Spatial distribution of PMAs**

In the Zhongtianshe Watershed, five LSUs and two subbasins, classified as high-392 contribution areas, were identified as PMAs (Fig. 6). There was a relatively consistent 393 394 spatial correlation between the two levels. For example, one subbasin was identified as 395 PMA at both levels, that is, subbasin S2 in Fig. 6b and its two LSUs, L2 and L3 in Fig. 396 6a. PMAs identified at the LSU level had have a more accurate spatial distribution 397 because of the inherent characteristics of the LSUs that can represent the spatial heterogeneity within subbasins. Considering the retention effect of ponds and reservoirs 398 in SWAT<sup>+</sup>, the upstream part of the subbasin may have a distinctive load contribution 399 400 compared to the downstream part. For example, in the subbasin S1 in Fig. 6b, the 401 upstream part constituted by composed of floodplain L10 and upland L12 in Fig. 6a 402 were identified as medium-contribution areas, while the downstream floodplain L1 was 403 the high-contribution area. In addition, most LSU-based PMAs were floodplains in the 404 Zhongtianshe Watershed. This may be because that the cropland in the study area is mostly distributed along the valley plain, which is a direct cause of local non-point 405 source pollution. These results also prove-indicate that SWAT<sup>+</sup> is well suited for 406 characterizing pollutants released at the LSU level and their transitions in the 407

408 reconstructed routing network by LSUs and channels (including ponds).

In the Willow River Watershed, two LSUs and two subbasins, classified as high-409 410 contribution areas, were identified as PMAs (Fig. 7). It was similar that at both the LSU 411 and subbasin levels where the northeast areas of the watershed were identified as low 412 contribution areas, owing to the upstream pollution predominantly reduced by the ponds and wetlands along the main channel. Although the results identified at the two 413 levels had similar spatial distributions, the subbasin-based PMAs covered larger areas 414 415 than the LSU-based PMAs, which may result in additional screening work or more 416 investment in watershed management decision- making. In contrast, the LSU-based PMAs were the upland areas within the subbasins, that is, uplands L1 and L2 (Fig. 7a) 417 418 within two subbasins (Fig. 7b). The medium-contribution areas identified at the LSU 419 level were also more specific and detailed than the areas identified at the subbasin level. Therefore, it is clear that LSU-based results can provide a finer identification than 420 421 subbasin-based results in the Willow River Watershed.

In addition, for the Willow River Watershed, LSUs belonging to subbasin L2 in Fig. 7b were not identified as PMAs but as contribution areas <u>below\_classified as</u> medium-contribution areas. This shows that the application of detailed spatial units could decompose the aggregation of the pollutant load within a subbasin in a relatively realistic representation, although subbasin S2 contributed a high pollutant load as the result of <u>being</u> the largest subbasin in the watershed.

428 Overall, LSU-based PMAs have improved the accuracy of identification from the 429 perspective of spatial distribution compared with subbasin-based PMAs. It is also 430 proven shown that the proposed PMA identification method at landscape position units
431 using SWAT<sup>+</sup> is effective and applicable to different watersheds.

432

## 4.2 Cumulative load contribution

To quantitatively evaluate the difference in PMAs identified at the LSU and subbasin levels for each case study, each type of spatial unit was ranked by load contribution in descending order and plotted in Figs. 8 and 9, with the cumulative area and load contribution calculated.

In the Zhongtianshe Watershed, LSU-based PMAs contributed 48.6% of the total nitrogen in 23.3% of the watershed area, whereas subbasin-based PMAs only contributed 44.7% in as much as 30.1% of the area (Fig. 8a). This means that landscape position units are more effective in identifying the PMAs. Moreover, the cumulative area-contribution line of the LSU-based method in Fig. 8a was always higher than that of the subbasin-based method, proving its better effectiveness, although based on different types of identification units.

444 In the Willow River Watershed, LSU-based PMAs contributed 31.7% of the total nitrogen in 5.9% of the watershed area, whereas subbasin-based PMAs contributed 54.9% 445 of the total nitrogen in 21.5% of the area (Fig. 9a). It is not convincing to simply use 446 447 these numbers to compare the effectiveness of the two levels in this watershed. However, the line in Fig. 9a shows that the LSU-based PMAs almost always covered 448 449 less area than the subbasin-based PMAs under the same cumulative contribution. In 450 general, the results revealed that there would be less work on the reduction of pollution at the LSU level if the local government wanted to control the pollution to a certain 451

452 extent.

Furthermore, there was no deterministic relationship between the area of the spatial unit and its pollutant load contribution. For example, LSU L1 in the Zhongtianshe Watershed contributed 12.0% of the total nitrogen but ranked 17 in area, while subbasin S1 contributed 24.3% of the total nitrogen with the 2<sup>nd</sup> largest area (Fig. 8). In the Willow River Watershed, LSU L1 contributed 16.8% of the total nitrogen with the 2<sup>nd</sup> largest area, and subbasin S1 contributed 31.7% of total nitrogen which haswith the 2<sup>nd</sup> largest area of all subbasins (Fig. 9).

460 Although absolute differences exist in the results of the two watersheds due to different geographic characteristics, the comparison between them is less important for 461 462 the scope of this study (which is to evaluate the effectiveness of the PMAs at the LSU 463 level). Instead, the similar appearance depicted by the relations between the area of PMAs and their total load contribution at the two levels in different watersheds can also 464 show the universality and effectiveness of LSUs. In summary, identifying PMAs based 465 466 on landscape positions performs better than subbasins from the perspectives of both the 467 spatial distribution and cumulative load contribution in both test watersheds. Thus, LSU-based PMAs have the merit of accounting for more pollutant load contributions 468 with smaller areas, and can effectively be utilized in the spatial configuration of BMPs 469 for integrated watershed management. 470

# 471 **5. Conclusions**

472

This study proposes the use of landscape position units (LSUs), derived from a

universal type of spatial unit for most geographic environments, as identification units 473 474 for priority management areas (PMAs). An improved-Markov chain-based surrogate 475 model of the SWAT<sup>+</sup> model was implemented with the improvement of the transition 476 matrix in representing both landscape position and channel units to distinguish the 477 pollutant load contribution of each LSU to the assessment outlet and then identify the 478 PMAs according to a classification method. Experimental The experimental results show that landscape position units are more effective than widely used subbasins in 479 480 identifying PMAs because of their superior ability to represent hillslope processes and 481 the spatial heterogeneity of underlying surface environments within subbasins. Therefore, LSU-based PMAs are much more valuable for providing accurate locations 482 483 for implementing suitable BMPs for integrated watershed management.

484 The improved Markov chain-based PMA identification method can be regarded as a method framework. More types of spatial units with explicit upstream-downstream 485 486 relationships may be proposed and validated to identify PMAs with the support of 487 proper watershed models. In addition, several issues may be worth attention in future 488 research such as 1) how to consider various climate scenarios to determine the retention effects of channel routing processes; 2) how to better quantify the hydrological 489 connectivity among landscape positions and channels and its effects on PMA 490 491 identification; 3) how a specific type of identification unit affects the PMA identification of PMAs under different delineation methods; 4) how the modeling accuracy and 492 493 precision of the same or different watershed models affects PMA identification; and 5) how PMAs derived from different identification units impact the effectiveness and 494

495 efficiency of the spatial optimization of BMPs.

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# Table

	Zhongtianshe Watershed	Willow River Watershed			
DEM	DEM with a resolution of 25 m from	DEM with a resolution of 30 m from National			
	Provincial Geomatics Centre of Jiangsu	Elevation Data, USGS			
Land use	Manually interpreted from a_Google Earth	Land use map from National Land Cover Data			
	image derived in 2015	(NLCD, 2011 Edition), USGS			
Soil	Soil type map obtained from Soil Science	Soil dataset from the Soil Survey Geographic			
	Database of China and soil properties from	database (SSURGO), U.S. Department of			
	field sampling	Agriculture-Natural Resource Conservatio			
		Service			
Meteorological	Daily meteorological data (such as	Daily meteorological data from 2008 to 2014			
data	precipitation, temperature, humidity, wind	provided by Climate Forecast System			
	speed, and solar radiation) from 2011 to 2015 Reanalysis dataset Dataset, U.S. N				
	provided by China Meteorological Data	Centers for Environmental Prediction			
	Service Centre and Liyang meteorological				
	Meteorological stationStation				
Agricultural	Cropping and irrigation schedule including	Crop rotations, tillage practices, and fertilizer			
management	crop types and fertilizer usage from field	usage collated from Almendinger and			
practices	survey	Murphy (2007)			
Observed data	Daily measured flow (2011–2015) and 5-day	Daily flow and ammonia plus organic			
at the outlet	or 3-day* measured total nitrogen data (2014-	nitrogen data (from 1 October 2010 to 31 July			
	2015) from the site-monitoring station at the	2014) measured at the monitoring station by			
	watershed outlet <u>of the USGS</u> (no. 05341687)				

Table 1. Data description of the study areas for building <u>a</u> SWAT<sup>+</sup> <u>model.</u>

\* A total of 181 values were monitored in the Zhongtianshe watershed. During the rainy season (i.e., June to August), the sampling interval is about three days.

			NSE	PBIAS	RSR	$\mathbb{R}^2$
	Calibration	Flow	0.48	13.36%	0.72	0.52
71		Nitrogen	0.27	-16.57%	0.86	0.40
Znongtiansne watersned	Validation	Flow	0.52	12.55%	0.69	0.59
		Nitrogen	_	_	_	_
	Calibration	Flow	0.48	-28.82%	0.72	0.51
Willow Divor Wotorshod		Nitrogen	0.37	3.97%	0.79	0.39
willow Kiver Watersned	Validation	Flow	0.34	-58.16%	0.81	0.47
		Nitrogen	0.25	-128.73%	0.87	0.54

Table 2. The SWAT<sup>+</sup> model performance <u>of-for</u> the two <u>study</u> watersheds.

# Figure



Fig. 1. Generalized framework of the Markov chain-based PMA identification method using a hierarchy of one or more types of hydrologically connected spatial units.





Fig. 2. Schematic of the spatial discretization scheme (a) and hydrologic connections between spatial units\_
(b) implemented in SWAT<sup>+</sup>. AQU, aquifer; CHA, channel; HRU, hydrologic response unit; LSU, landscape position unit; LAT, lateral flow; PND, pond; RES, reservoir; RHG, groundwater recharge; SUR, surface runoff; TOT, total outflow (specifically, for LSU, it equals to surface runoff plus lateral flow); and numbers represent flow distribution ratio (values less than 1.0 are presented for example) from source unit to receiving unit (adapted from Bieger et al., 2017, 2019, and the source code of SWAT<sup>+</sup> version 59.3).



Fig. 3. Example of <u>constructing construction of the</u> flow distribution matrix,  $H_3$  based on upstreamdownstream relationships among landscape position units (LSUs) and channels and flow distribution ratios from upland to floodplain (e.g.,  $s_1$  and  $s_2$  in different subbasins).



Fig. 4. Overview of the Zhongtianshe and Willow River <u>Watershedswatersheds</u>.



Fig. 5. Delineation of three types of spatial units in the SWAT<sup>+</sup> model of the Zhongtianshe Watershed: (a) subbasin, (b) LSU, <u>and</u> (c) HRU (<u>take-taking</u> one subbasin as an example); and the Willow River
Watershed: (d) subbasin, (e) LSU, <u>and</u> (f) HRU (<u>take-taking</u> one subbasin as an example). Each color within the same subbasin in the HRU map represents one unit, i.e., a particular combination of land use, soil type, and slope classification.



Fig. 6. Ranking and classification of nitrogen load contribution at the (a) LSU (landscape position unit) and(b) subbasin levels in the Zhongtianshe Watershed. The labelled number is the ranked sequence of load contribution in descending order. High-contribution areas are identified as PMAs.



Fig. 7. Ranking and classification of total nitrogen load contribution at the (a) LSU (landscape position unit) and (b) subbasin levels in the Willow River Watershed. High-contribution areas are identified as PMAs, which are ranked and labelled by load contribution.



Fig. 8. Relationships between cumulative areas of spatial units and corresponding load contributions in the Zhongtianshe Watershed. (a) each point represents a spatial unit arranged in the descending order of load contribution. Detailed load contribution of landscape position units (LSUs) and subbasins are presented in (b) and (c), respectively.



Fig. 9. Relationships between cumulative areas of spatial units and corresponding load contributions in the Willow River Watershed. (a) each point represents a spatial unit arranged in the descending order of load contribution. Detailed load contribution of landscape position units (LSUs) and subbasins are presented in (b) and (c), respectively.