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Research article

Refined water security assessment for sustainable water management: A case study of 15 key cities in the Yangtze River Delta, China

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ABSTRACT

Water security represents ecological security and a policy priority for sustainable development; however, ungridded assessment results cannot be used to support urban environmental management decisions. This study proposes a systematic framework to obtain a gridded regional water security assessment, which reflects the regional natural resource, based on the index system derived from the Pressure-State-Response (PSR) model and the Integrated Valuation of Ecosystem Services and Tradeoffs (InVEST) model. The results were applied to sustainable water management. Using 15 key cities in the Yangtze River Delta (YRD) region as a case study to apply the methodology, we found that the comprehensive water security was relatively high and high-value areas were widely distributed, accounting for about two-thirds of the study area. Low-value areas were mainly distributed in central and eastern regions, such as Shanghai, Suzhou, and Nanjing. There was evidence of a water resource shortage during the twelve-month period studied, particularly in August. The proportions of comprehensive water security in each administrative unit and the differences between simulated and target water quality could be used in the spatial planning and the exploration of payments for ecosystem services (PES) mechanism in county-level or smaller administrative units. Despite the premise requirement and the grid resolution problems of the InVEST model, it can be concluded that our assessment method proves capable of matching spatial and temporal differences in water supply and demand at a fine scale, and results can be used to supply useful information for urban management decision making.

1. Introduction

Under the background of global change, ecological security issues have become increasingly serious and have become a hot area of concern for international environmentalists and ecologists (Peng et al., 2018; Lu et al., 2020; Huang et al., 2020). Water is an important natural ecological element, and its security pattern is also an important part of watershed and regional ecological security pattern optimization (Veettil and Mishra, 2018; Sen and Kansal, 2019; Chawla et al., 2020). Water security is a dynamic concept that evolves with stakeholder interests and may involve freshwater supply, water scarcity, water management, flood risk, and national security (Damkjaer and Taylor, 2017; Howlett and Cuenca, 2017). Interests range from "broad" to "narrow" and "academic" to "applied" (Bakker, 2012), though the core endeavor is to improve knowledge in order to guide environmental planning and management. Integrating the concepts related to water security, we defined it as: In a certain basin or region, based on the current situation of social development, predictable technology and the principle of sustainable development, the state that water resources and water environment can sustain economic development and maintain the ecosystem health. Basin and regional water security always been the focus of attention worldwide (Bakker, 2012; Mekonnen and Hoekstra, 2016; Veettil and Mishra, 2020). Because the large population lives in the alluvial plains on both sides of the river, estuarine delta, and the coastal

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plain. For example, the Yangtze River Delta is the most developed region in China with 358,000 km^2 area and 227 million population. Freshwater supply is crucial to sustainable development of regional economies and ecosystems (Lang et al., 2017). However, increasing anthropogenic demand for freshwater resources, coupled with pollution and wastage of water, has exacerbated water scarcity, causing a water security crisis in many areas (Shomar and Dare, 2015). It has a significant impact on ecological security, food security and even national security.

Water security is an urgent policy priority, appropriate indicators are needed to assess current conditions and guide action (Jensen and Wu, 2018). The index tracks imbalances between supply and demand, such as the Falkenmark water stress index (Falkenmark, 1989) or the water poverty index (Sullivan, 2002). Traditional hydrological models have long been used in water management to evaluate water security (Lüke and Hack, 2018). However, the regional feedback between the ecosystem and human activities have become important (Hoekstra et al., 2018; Reyers et al., 2013), which leads to the evolvement of the watershed management strategy. More recently, ecosystem services evaluation models providing detailed information on temporal and spatial variability of water-related ecosystem service provision at the watershed or hydrological resource unit (HRU) level. For instance, the Integrated Valuation of Ecosystem Services and Tradeoffs (InVEST) model is suitable to assess the impact of land use/land cover (LULC) change on ecosystem services (Vigerstol et al., 2011), which is widely used in China (Zheng et al., 2016; Hu et al., 2020; Cong and Sun, 2020) and internationally (Wang et al., 2017; Redhead et al., 2018). The InVEST model has the advantage of the easy access of the input data for large areas and the consideration of non-point source pollution. This model is good at simulating the total nitrogen (TN) and total phosphorus (TP), which are important indicators of surface water pollution in regions under anthropogenic pressure (e.g. industrial and urban land use) (Zheng et al., 2016).

Because water security is often a policy issue, the administrative boundary of policy-makers usually determines the scale of analysis. Studies have included risk analysis, water resource allocation, pollution alleviation, and national security strategies (Ouyang et al., 2004). Sun et al. (2016) reported that about 80% of water security assessments in China are at the level of administrative regions due to data availability and the nature of the methodology. However, multi-faceted and broad scale analysis cannot support urban environmental management decisions. Firstly, assessment results based on statistical yearbook or HRU scales can only be strategic targets. Moreover, the spatial development plan demands heterogeneous standards and targets for specific districts, counties, and towns. However, the boundary of traditional HRU analysis does not always align with administrative boundaries, creating a need for cross-regional management. Water security assessment at the grid scale is a prerequisite for the refined resource and environment management, and is also the direction of future development (Mekonnen and Hoekstra, 2016). Secondly, managers must identify the appropriate decisions to take to reach strategic water security targets, for example if a payment for ecosystem services (PES) mechanism is selected, the area in which it will be implemented and the beneficiaries (and payers) of subsidies must be identified. This is especially difficult in areas where monitoring data are lacking. PES has been widely applied worldwide, and there are plenty cooperation networks to implement the mechanism with the basis of the identification of the PES achievements and distribute compensation. The water managers need the simpler input parameters and finer scale assessment results.

To address the above-mentioned issue, we proposed the gridded water security map based on the InVEST model and the potential management applications. The main objectives of this study are to: (1) propose a method for constructing a regional water security assessment index at the grid scale; (2) verify the method by applying to 15 key cities in the Yangtze River Delta (YRD) region and analyzing water security patterns in the study area; and (3) demonstrate how to apply the assessment results for environmental management purposes, such as future development orientation of county-level administrative units, and PES fund allocation for surface water.

2. Materials and methods

2.1. Study area

The study area (116.68°–122.27°E, 28.85°–33.42° N) is 118,192.33 km^2 (Fig. 1), includes Shanghai and the 14 key cities. The definition of city in this study is refers to administrative units, including built-up areas and suburbs. The boundary of YRD urban agglomeration varied according to the different official documents launched by the national government. Therefore, we selected these 15 key cities with highly developed economy, industrialization, urbanization and intense human activities. They are very relevant to carry out water security assessment and sustainable water. Furthermore, the 15 selected cities disclosed the official and accurate pollution data which could be used for the InVEST model.

The region has the subtropical monsoon climate, with the average annual precipitation 1826.9 mm and the evapotranspiration 664.9 mm in 2015. Industrial and domestic use water are taken from adjacent drinking water sources, and agricultural irrigation draws water directly from nearby rivers. Therefore, there are few requirements for the long-distance water transfers. The elevation of the region decreases from the southwest to the northeast, mainly in plains and hilly terrain.

The YRD region is the most developed coastal region in China, and includes large cities in Jiangsu, Anhui, and Zhejiang provinces as well as Shanghai municipality. Environmental management of the YRD region is becoming increasingly integrated, where the water security is the key environmental problem restricting regional economic development. Water resources mainly stem from surface water, groundwater use accounting for less than 1% of total water consumption is negligible (Jiangsu Water Resources Bulletin, 2015; Anhui Water Resources Bulletin, 2015; Zhejiang Water Resources Bulletin, 2015; Shanghai Water Resources Bulletin, 2015). However, the natural water in this area is seriously polluted. According to the Surface Water Quality Standard in China (GB 3838-2002), there are 5 classes of surface waters. The proportion of surface water quality of the national monitoring station reaching Class III (TN $\leq$ 1.0 mg/L, TP $\leq$ 0.2 mg/L) in 2015 was only 45.27% (the national average rate was 64.5%).

2.2. Methodology

We proposed a refined and systematic technical framework to assess the regional water security in water resources, water environment, exploitation and utilization potential, as presented in Fig. 2.

2.2.1. Index of water security assessment

Water resources, water environment, development and utilization potential are connected and interacted with each other to form the unified and complex water security system. We followed the logic of Pressure-State-Response (PSR) model to select indicators that can be spatialized at the grid scale. The indicator layer comprises eight indicators covering the basic characteristics of water security (Table 1). We selected eight indicators to build a water security index system for three main reasons: (1) The eight indicators cover the basic characteristics of water security according to the three subsystems of water security; (2) The eight indicators comprehensively consider the characteristics of the study area. There are studies that use a lot of indicators to build an index system, which can fully characterize water security, but most indicators do not take into account the regional characteristics and may not be applicable to our study area; (3) The eight indicators can be spatialized at the grid scale. The spatialization of the indicators is also the main problem we consider when selecting the indicators. For instance, the two indicators representing the water environment can be well simulated with the InVEST model to obtain spatial

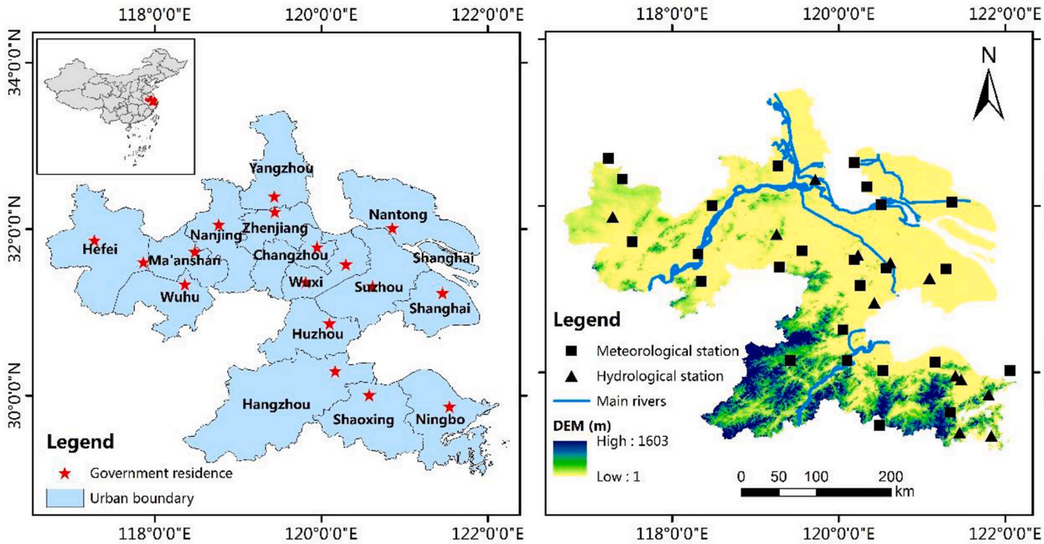

Fig. 1. Location of 15 key cities in the Yangtze River Delta region, China.

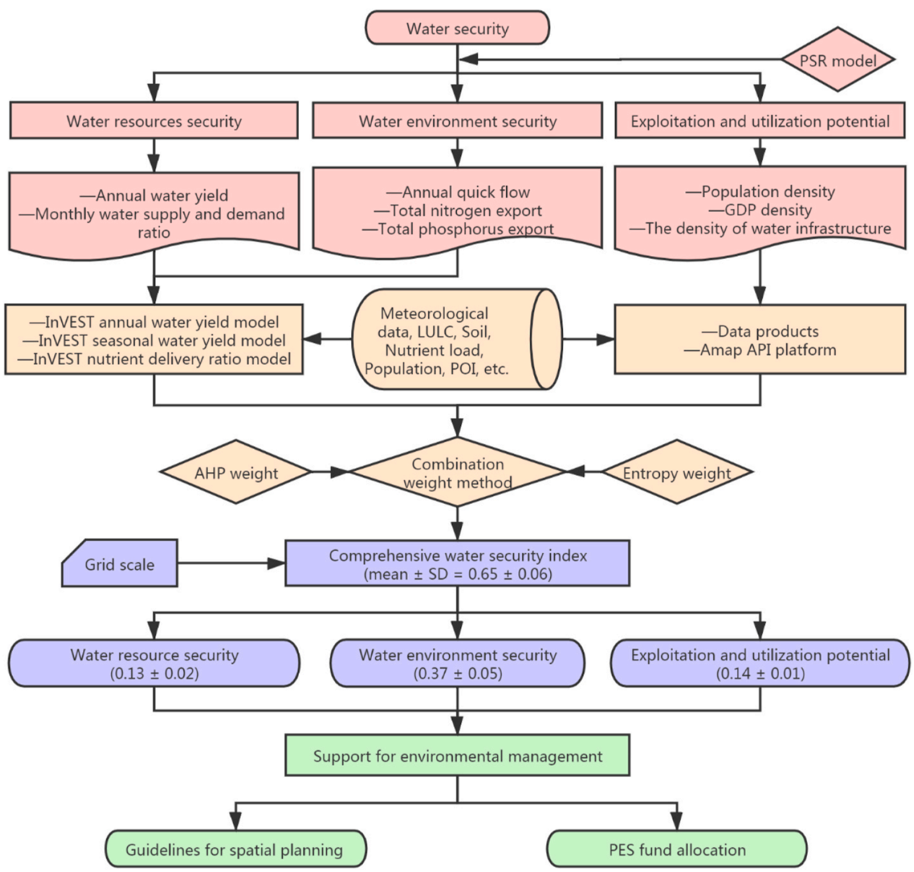

Fig. 2. Technical framework for the water security assessment at the grid scale and the application for the environmental management. The red part described the index system of water security. The carnation part described the combination of the data and the sources of the index. The purple part was the assessment result. The green part was the application. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

results.

Weighting of indicators is important in water security assessment. The analytic hierarchy process (AHP) uses expert scoring, combining quantitative and qualitative analysis, to determine the relative importance of each indicator (Saaty, 2008). However, this scoring is subjective. The entropy weight method is an objective fixed weight method. The weight of each indicator is calculated according to the degree of variation of each indicator by using information entropy (Pan et al., 2015). The entropy weight avoids subjectivity to a certain extent but does not consider the priorities of decision-makers. Combination weight method combining subjective and objective can effectively solve the shortcomings of single weight method. Weighting of each index was

Table 1
Index system and weight of water security assessment at the grid scale.

Target Layer	Criterion layer	Indicator layer (±)	PSR category	Units	AHP weight	Entropy weight	Combination weight
Water security	Water resources security	Annual water yield (+)	State	m^3/km^2	0.0427	0.1308	0.0868
		Monthly water supply and demand ratio (R) (+)	State	N/A	0.2133	0.1396	0.1765
	Water environment security	Annual quick flow (+)	State	mm/km^2	0.1342	0.1220	0.1281
		Total nitrogen export (−)	Pressure	kg/km^2	0.2683	0.1197	0.1940
		Total phosphorus export (−)	Pressure	kg/km^2	0.2683	0.1193	0.1938
	Exploitation and utilization potential	Population density (−)	Pressure	$person/km^2$	0.0183	0.1286	0.0735
		GDP density (−)	Pressure	$Yuan/km^2$	0.0183	0.1275	0.0729
		The density of water infrastructure (+)	Response	per/km^2	0.0366	0.1125	0.0746

PS: +/− represents the positive or negative indicator for the Min-max normalization method. The positive indicator means the more the better, vice versa. The formula of R could be seen in the supplementary materials.

obtained by combination weight method, which is the arithmetic average of AHP and the entropy weight method.

2.2.2. *Support for environmental management*

Spatial planning guidelines are based on the results of the water security assessment. Comprehensive water security was divided into five levels using Jenks Natural Breaks (Jenks, 1967). The first two levels have higher values of water security and stronger resource and environmental carrying capacity. The Jenks Natural Breaks method was also used to divide the total area of levels I and II (comprehensive water security index > 0.64) in each county unit into four levels. Finally, the study area was classified into restricted, optimized, prioritized, and prohibited development zones corresponding with the low, moderate, high water security assessment and the natural reserves defined by the national government.

Buyer and provider of PES were identified by examining the difference between current and target water qualities in the study area and ranking these differences. Target water quality was defined as Class III (TN $\leq$ 1.0 mg/L, TP $\leq$ 0.2 mg/L).

2.3. *Data source and processing*

The detail descriptions of all the data and their sources are reported in the table S1. The meteorological data include daily precipitation, temperature, relative humidity, wind speed and sunshine time, etc. The study area with 26 meteorological stations was divided into 26 climate zones through the Tyson polygons created by the stations. The rain events of 26 climate zones were derived from precipitation data at each meteorological station. The production of LULC data was identified based on Landsat TM/ETM remote sensing image as the main data source. The LULC was divided into 6 primary types, including cultivated land, woodland, grassland, water area, construction land and unused land, and 25 sub-types. Root restricting layer depth was replaced by soil depth according to the recommendation of the model manual (Sharp et al., 2016). Data from 12 hydrological stations were used for the validation of the InVEST nutrient delivery ratio (NDR) module. Water infrastructure included reservoirs, dams, sewage treatment plants, etc. The density of water infrastructure was calculated by the point of information (POI) number per km of water infrastructure. All data of model input, output and results with a resolution of 1 km.

2.4. *Water resource security*

2.4.1. *Annual and seasonal water yield modules*

The InVEST annual water yield module is based on the Budyko hydrothermal coupling equilibrium hypothesis, which assumes that all the water (excepting evapotranspiration) reaches the basin outlet. The module which requires 9 input parameters is calculated in units of grid cell (Sharp et al., 2016). The formula could be seen in the supplementary materials.

The seasonal water yield module can quantify the monthly water supply helps to understand the hydrological processes in a watershed, in particular the partitioning between quick flow (occurring during or shortly after rain events) and baseflow (occurring during dry weather) (Sharp et al., 2016).

2.4.2. *Sensitivity analysis and model calibration*

We verified the accuracy of kriging, inverse distance weighted (IDW), radial basis functions (RBF), global polynomial interpolation (GPI), and interpolation with barriers (IWB) methods, which were used to interpolate precipitation and evapotranspiration by "leave-one-out cross-validation" (Kohavi, 1995). This validation removes the data at one location and then predicts it based on the remaining data. For example, with 26 observation points, the value of each point is calculated using the remaining 25 data points, and predicted and observed values are compared. The root mean square error (RMSE) was used to measure the deviation between predicted and observed values (Wu et al., 2019).

The input parameter Z, in the annual water yield module is an empirical constant that captures local precipitation patterns and hydrogeological features, typically between 1 and 30 (Sharp et al., 2016). The Budyko dryness index theory shows that the higher the Z value, the smaller the effect of seasonal constant Z on model results (Zhang et al., 2004). Therefore, we selected the optimal Z value by comparing simulated water yields and observed data from the Water Resources Bulletin.

2.4.3. *Water demand*

Annual water demand data for 15 cities is reported in the Water Resources Bulletins of the Jiangsu (Jiangsu Water Resources Bulletin, 2015), Zhejiang (Zhejiang Water Resources Bulletin, 2015), and Anhui (Anhui Water Resources Bulletin, 2015) Provinces, and Shanghai (Shanghai Water Resources Bulletin, 2015). To maintain consistency, water demand was split into three categories: agricultural, industrial, and domestic. Agricultural irrigation and forestry, and animal husbandry and livestock water use were combined into agricultural water demand, and urban public water, residential water, and ecological environment water (only urban greening water) were combined into domestic water demand.

Water demand was converted to monthly values. Annual agricultural water demand was converted into monthly demand using the proportion of monthly evapotranspiration (Drastig et al., 2016; Sun et al., 2018). Regional differences are mainly related to variations in the spatial distribution of vegetation so monthly agricultural water demand was rasterized according to the Normalized Difference Vegetation Index (NDVI) (Jiang et al., 2003). Industrial and domestic water supply is centralized, so the proportion of monthly urban water consumption reported in the literature was used to convert annual industrial and domestic water demands to monthly values (Pesic et al., 2013; Chang et al., 2015). Industrial and domestic water demands are mainly related to Gross

Domestic Product (GDP) and population density, respectively. Therefore, monthly industrial and domestic water demands were rasterized using GDP and population distribution data.

2.5. Water environment security

2.5.1. Nutrient delivery ratio module

The NDR module aims to evaluate the water purification services of vegetation and soil in ecosystems based on the mechanism that the vegetation and soil remove or reduce nutrients in runoff through the storage and conversion. The main algorithm is:

$$ALV_x = HSS_x \times pol_x \tag{1}$$

where, ALV_x is the adjusted nutrient (TN, TP) load value of the grid x, HSS_x is the hydrological sensitivity score of the grid x, and pol_x is the export coefficient of the grid x.

2.5.2. Sensitivity analysis and model calibration

Calibration of the InVEST NDR module included three steps. Firstly, the model manual recommends to use the "quick flow" as the "Nutrient runoff proxy" input parameter. We followed the suggestion to use the output of the validated water yield module in order to guarantee model accuracy. Secondly, we calibrated threshold flow accumulation (TFA) by comparing the real regional river map with the modelled stream map. Lastly, the optimal Borselli k value was selected by comparing simulated results with observed values at 12 hydrological monitoring stations in the study area. The effect of Borselli k on the magnitude and direction of change in nitrogen and phosphorus export is region-specific, driven by topography (Redhead et al., 2018).

2.6. Calculation of water security index

Indicators in the index of water security assessment have different dimensions and orders of magnitude. Therefore, original indicator data were normalized using min-max normalization (Wang et al., 2019a). The calculation formulas of the positive and the negative index are (2) and (3):

$$Y = \frac{X - X_{min}}{X_{max} - X_{min}} \tag{2}$$

$$Y = \frac{X_{max} - X}{X_{max} - X_{min}} \tag{3}$$

where Y is the standardized value, X is the original value, X_{max} and X_{min} are the maximum and the minimum values of the indicators respectively.

To calculate the combination weight:

$$W_c = \frac{W_a + W_e}{2} \tag{4}$$

where, W_c is the combination weight, W_a is the weight of the AHP, and W_e is the weight of the entropy weight.

3. Results

3.1. Model calibration and sensitivity analysis

Kriging was used to spatially interpolate precipitation and potential evapotranspiration (ET_0) (Table S2 and S3); although the Kriging RMSE for precipitation in June and July was greater than that of IWB, it was smallest in other months and for the whole year. Similarly, the Kriging RMSE for evapotranspiration in November was equal to that of RBF but was the smallest of all methods in other months and for the whole year.

Comparison of observed and simulated water resources in the basin provided a Z value of 30 (Table S4). The modelled steam map most closely resembles observed values when TFA = 200. A default value of 2 was selected for Borselli k. When k = 2, the error between simulated and observed values of TN is 8.93%, and of TP is 3.56%, and the model error is the smallest (Fig. S1). For the details, please see the supplementary materials.

3.2. Indicator spatialization and analysis

3.2.1. Indicators of water resource security

Areas with high water yield are mainly distributed along the main stream of the Yangtze River. Areas with low water yield are mainly distributed in the central, northwest, and southeast regions (Fig. 3). The top three cities in terms of average water yield are Wuhu (average water yield = 152.31 × 10^4 m^3/km^2), Nantong (140.83 × 10^4 m^3/km^2), and Changzhou (137.12 × 10^4 m^3/km^2), and the bottom three cities are Suzhou (100.64 × 10^4 m^3/km^2), Yangzhou (107.40 × 10^4 m^3/km^2), and Shaoxing (113.12 × 10^4 m^3/km^2).

Water supply and demand match at the seasonal scale. However, there are small unmatched regions at the monthly scale (Fig. S2 and S3). Generally, high water supply occurs mainly in June (mean ± SD = 13.65 ± 5.93 × 10^4 m^3/km^2) and July (14.16 ± 6.63 × 10^4 m^3/km^2), and the low values are in January (10.17 ± 2.25 × 10^4 m^3/km^2) and February (9.63 ± 3.22 × 10^4 m^3/km^2). The high-water demands are in July (4.43 ± 6.37 × 10^4 m^3/km^2) and August (4.93 ± 6.44 × 10^4 m^3/km^2), and the low values were in December (2.28 ± 5.96 × 10^4 m^3/km^2) and January (2.12 ± 5.91 × 10^4 m^3/km^2). However, the water shortage problem always occurred at some areas ($R < 0$), especially in August (Fig. 4). Previous assessments have struggled to identify water shortage at the grid scale. In terms of average ratio (R), the best three months are January (R = 0.72), October (0.68), and November (0.66), and the worst are August (0.30), May (0.52), and March (0.53).

There is a spatial mismatch between water supply and demand. High values of water supply are distributed mainly in the mainstream of the Yangtze River. Low value areas are distributed mainly in the southern part of the YRD (Zhejiang Province). Water demand is centered mainly on urban built-up areas and declines in urban suburbs. R values increase from the coast inland, showing a pattern of high in the west and low in the east. High R value areas are mainly distributed in Wuhu (R = 0.79), Ma'anshan (0.78), and Hangzhou (0.70), whereas low-value areas are mainly found in Shanghai (0.15), Suzhou (0.41), and Wuxi (0.42).

3.2.2. Indicators of water environment security

The top three cities in terms of average quick flow are Wuxi (average quick flow = 385.12 mm/km^2), Shanghai (375.18 mm/km^2) and Wuhu (349.98 mm/km^2), and the bottom three cities are Shaoxing (130.51 mm/km^2), Yangzhou (152.70 mm/km^2) and Nantong (160.66 mm/km^2) (Fig. 3). Nutrients (TN and TP) were the main pollutants in the region. The average TN and TP exports are 2463.62 ± 3441.95 (mean ± SD) kg/km^2 and 151.18 ± 198.16 kg/km^2 respectively (Fig. 5). High-value areas of TN and TP exports are similar, distributed mainly in Shanghai, Nanjing and Hangzhou, forming a spatial pattern of "one center, two sub-centers".

3.2.3. Indicators of exploitation and utilization potential

The average population and GDP density are 901 ± 1975 (mean ± SD) person/km^2 and 9914 ± 29,294 RMB/km^2 respectively. The highest density of water infrastructure is 24 per/km^2 (Fig. 6). The spatial distribution of population, GDP, and water infrastructure density are similar, with the high values in the urban built-up areas and the decline in surrounding suburbs. As to the entire study area, the high-value areas decreased from the coast to the inland, showing the pattern of high in the east and low in the west.

3.3. Water security

Average comprehensive water security is 0.65 ± 0.06 (mean ± SD),

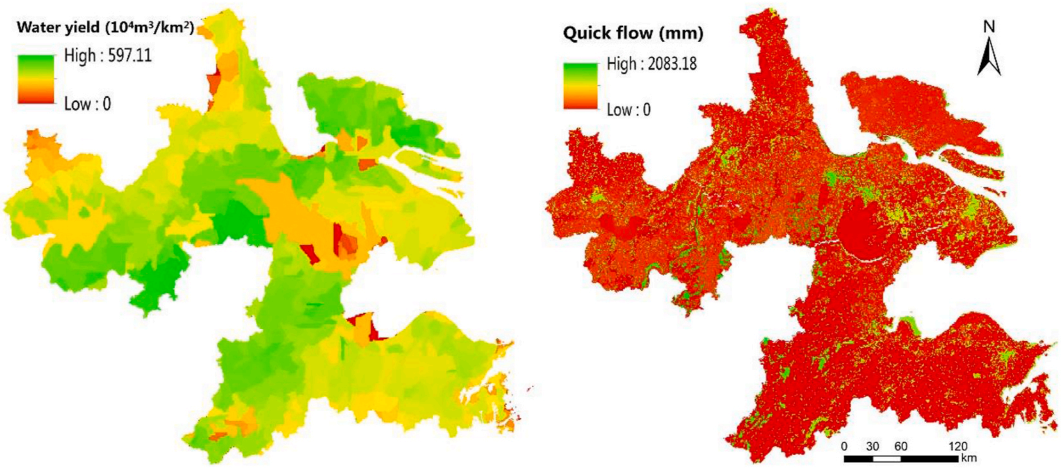

Fig. 3. Annual water yield and quick flow of 15 key cities in the Yangtze River Delta region.

which relatively high (Fig. 7). High-value areas are widely distributed. Low-value areas are concentrated in central and eastern regions. The highest ranked cities for average comprehensive water security are Wuhu (average comprehensive water security index = 0.685), Ma'anshan (0.673), and Changzhou (0.672), which represent strong water resources and environmental carrying capacity. The lowest ranked cities are Shanghai (0.519), Suzhou (0.620), and Nanjing (0.623), which face water security problems. Comprehensive water security level I and II combined account for 65.67% (Table 2).

Average of water resources security is 0.13 ± 0.02 (mean ± SD). High-value areas are in the western region. Low-value areas are in central and eastern regions. The highest ranked cities for average water resources security are Wuhu (average water resources security index = 0.147), Ma'anshan (0.139), and Huzhou (0.138). The lowest ranked cities are Shanghai (0.107), Suzhou (0.120), and Yangzhou (0.121). The water resources security level I and II combined account for 65.67% (Table 2).

Average water environment security is 0.37 ± 0.05 (mean ± SD). High-value areas are in the western region, while low-value areas are in the central and eastern regions as well. The highest ranked cities for average water environment security are Changzhou (average water environment security index = 0.396), Wuhu (0.393) and Huzhou (0.388). The lowest ranked cities are Shanghai (0.277), Nanjing (0.352) and Suzhou (0.356). The water environment security level I and II reached 67.57% (Table 2).

Average exploitation and utilization potential is 0.14 ± 0.01 (mean ± SD). High-value areas are in urban suburbs. Low-value areas are in urban built-up areas. The highest ranked cities for average exploitation and utilization potential are Ma'anshan (average exploitation and utilization potential index = 0.146), Huzhou (0.145) and Hangzhou (0.145). The lowest ranked cities are Shanghai (0.138), Wuxi (0.144) and Suzhou (0.144). The exploitation and utilization potential level I and II reached 95.85% (Table 2).

3.4. Guidelines for spatial planning based on water security

Comprehensive water security classification across administrative units is shown in Fig. 8. The sum of the proportions of comprehensive water security levels I and II in 130 county-level administrative units in the 15 cities was divided using the Jenks Natural Break method in ArcGIS 10.2 to identify management zones. The sum of the proportion of levels I and II ranges from 0 to 25.25% for restricted development zones, 25.25%–66.86% for the optimized development zone, and 66.86%–100% for the prioritized development zone. The prohibited development zone was identified based on nature reserves in the Yangtze River Basin. The detailed results and analysis of the development zone are in the supplementary materials and the table S5.

3.5. Exploration of PES mechanism

Current water quality was calculated using TN and TP emissions and water yield. The difference between current and target water quality is shown in Fig. 9. Areas of positive difference indicate that pollution is more severe than the water purifying capacity and those who are responsible for this pollution should be buyers of ecosystem services. Areas of negative difference are providers of ecosystem services and should be compensated by funds. The buyer can calculate the PES amount based on compensation standards (e.g., the cost of treating pollutants) and both buyer and provider can allocate PES based on the rank of differences between current and target water qualities.

There are 31 county-level administrative units, accounting for 23.85% area, with negative TN difference that should accept compensation funds. The top three of these are Rudong (difference between current and target water quality = −0.76 mg/L), Feidong (−0.51 mg/L), and Chun'an (−0.49 mg/L). There are 99 county-level administrative units, accounting for 76.15% area, with positive TN difference, the top three of which are Putuo (difference between current and target water quality = 14.78 mg/L), Yangpu (14.75 mg/L), and Minhang (14.71 mg/L). There are 88 county-level administrative units, accounting for 67.69% area, with negative TP difference, the top three of which are Rudong (difference between current and target water quality = −0.18 mg/L), Xiangyang (−0.17 mg/L), and Yixing (−0.16 mg/L). There are 42 county-level administrative units, accounting for 32.31% area, with positive TP difference, the top three of which are Shangcheng, (difference between current and target water quality = 0.74 mg/L), Binjiang (0.71 mg/L), and Xuanwu (0.60 mg/L).

Among the 130 county-level administrative units in the study area, most of the restricted development zone (accounting for 43.4% area) comprises urban municipal districts. The Shanghai municipal district has the strongest external influence, and is connected with Suzhou and Nantong. These areas overlap with areas of buyers of ecosystem services. The priority development zone (accounting for 28.9% area) is in the exurbs, which overlap with PES provider areas, except for three cities in Anhui Province.

4. Discussion

4.1. Model accuracy

Ecosystem services models can be used in areas where there is a lack of data and it is difficult to calibrate or validate model results (Pandeya et al., 2016; Villa et al., 2014). However, some factors of the InVEST

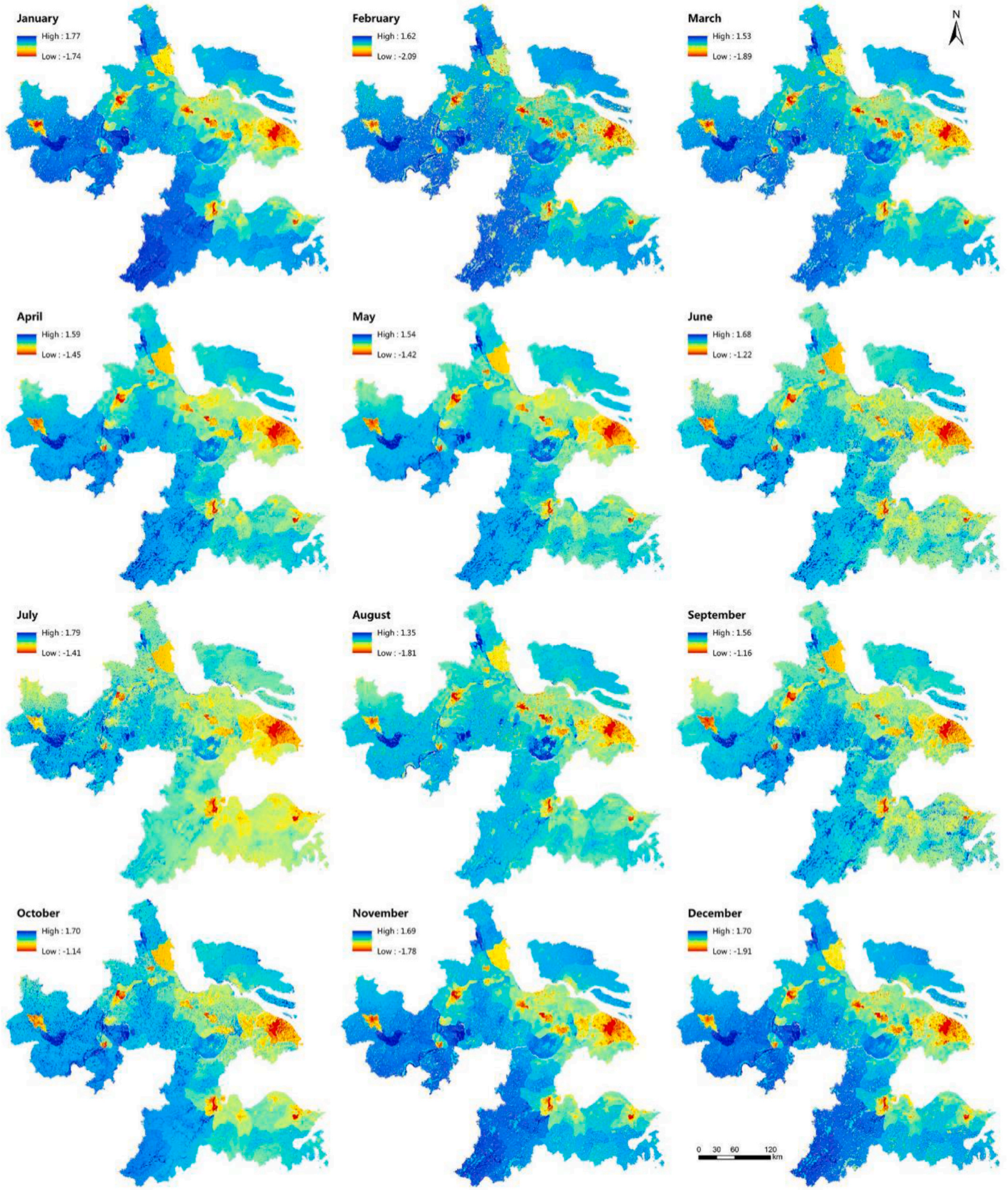

Fig. 4. Monthly water supply and demand ratios of 15 cities in the Yangtze River Delta region.

model affect its accuracy. For example, the input parameters of the annual and seasonal water yield modules, such as plant available water content (PAWC) and ET_0, are calculated based on empirical formulae. However, different empirical formulae provide different results (Dou et al., 2019). Moreover, meteorological parameters, especially precipitation, are sensitive to the simulation result (McMahon et al., 2013; Redhead et al., 2016). Observations of precipitation and ET_0 were interpolated and rasterized by different methods that produced certain

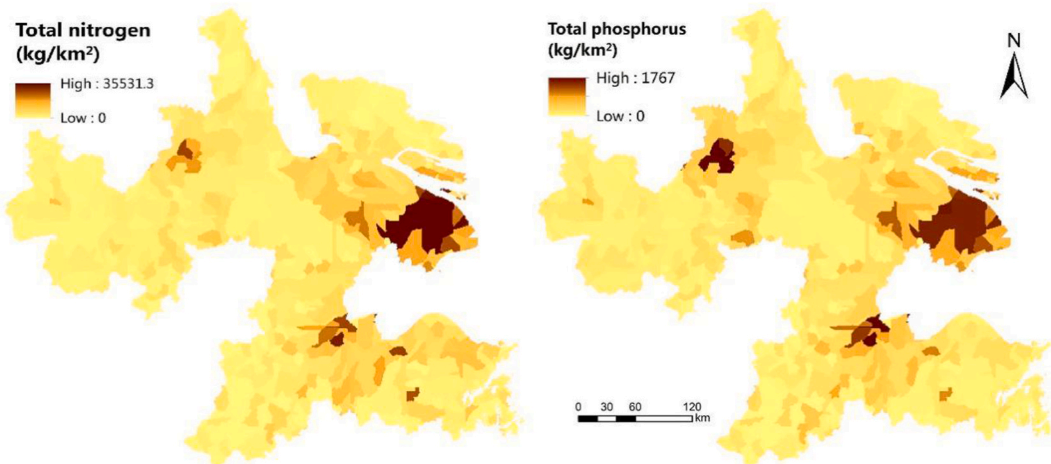

Fig. 5. Total nitrogen and total phosphorus exports of 15 key cities in the Yangtze River Delta region.

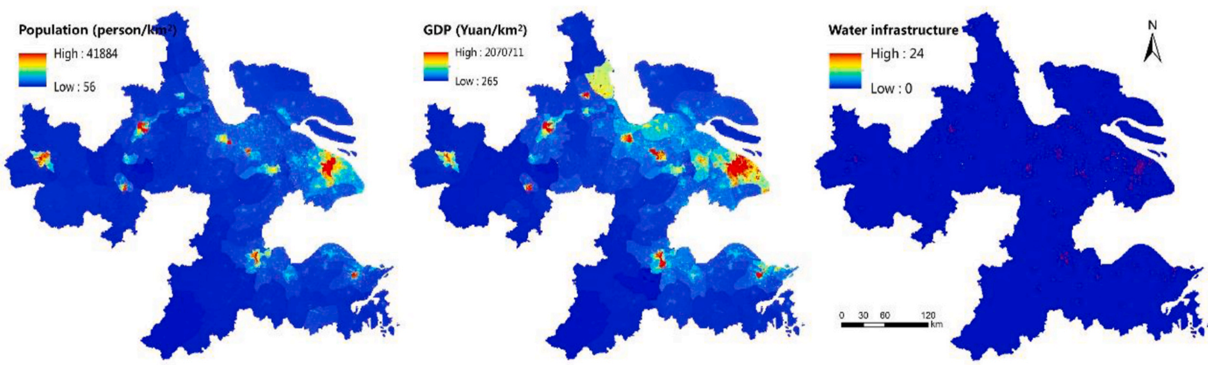

Fig. 6. Spatial distribution of population, GDP, and water infrastructure densities of 15 cities in the Yangtze River Delta region.

errors. The seasonal constant Z was adjusted by comparing simulated results with actual water resources. Optimal Z varies regionally. Simulation accuracy was improved by optimizing input parameters according to local conditions. Firstly, input parameters were calculated by empirical formulae recommended in literature from the study area. Secondly, five methods were examined to find the best interpolation for the spatial distribution of precipitation and ET_0. Finally, the relative error between simulation results and reported water resources was reduced to 1.65% by adjusting the Z value. Observations from a greater number of meteorological sites could further improve simulation.

The NDR module is sensitive to both nutrient load and purification efficiency (Redhead et al., 2018). The initial design of the module focused on diffuse (i.e. non-point) sources of nutrient only. Using LULC data, agricultural emissions were estimated for cultivated land, and industrial and domestic emissions on urban construction land, in order to account for point source pollution. Changes in TFA improve the representation of nutrient movement in some catchments, while reducing accuracy in others (Redhead et al., 2018). The grid resolution of digital elevation model (DEM) and LULC layers caused errors in simulations in different catchments. For example, simulated TN was less sensitive to resolution changes than TP Borselli k governs the relationship between the connectivity index–a function of topography–and NDR. Accuracy was ensured in this study by using quick flow data generated by the calibrated InVEST annual water yield model as an input. TFA was adjusted to obtain the best real stream network. Finally, Borselli k was adjusted in order to calibrate simulated nutrient export with observed values from key monitoring stations in the study area.

4.2. Water security assessment

The core definition of water security determines the construction and weighting of the evaluation system. In many water security and water environmental carrying capacity assessments, water resource and quality are the two most important aspects. Natural, socioeconomic, and cultural attributes are recurring elements of the agricultural water resources security concept (Malekian et al., 2017). Different assessments in the same place may have different research objectives, behaviors, and results. For research focusing on urban water safety assessment, social, economic, management, ecological, and engineering aspects should be included (Romero-Lankao and Gnatz, 2016). However, most studies only focus on certain aspects because of data availability and different stakeholder concerns (Hanjra and Qureshi, 2010). Since it is difficult to spatialize efficiency indicators that reflect exploration of the water environment, such as water consumption per GDP and water recycling rate. Although, we selected 8 indicators because of the complementary and comprehensive representation of the water security and the regional characteristics. Urban pipe network data and urban flood risk representing the regional water infrastructure conditions could be considered in future assessments.

To compared our results with the prior studies, Jia et al. (2018) assessed water resource carrying capacity based on annual water demand and resources, finding the greatest capacity in Zhejiang, followed by Anhui, Jiangsu, and Shanghai. Anhui and Jiangsu had more balanced water resources than Zhejiang (Wang et al., 2019b). This differs from the current study, in which Anhui was the most balanced, followed by Zhejiang, Jiangsu, and Shanghai. This difference may arise from consideration of monthly instead of annual supply and demand. In the

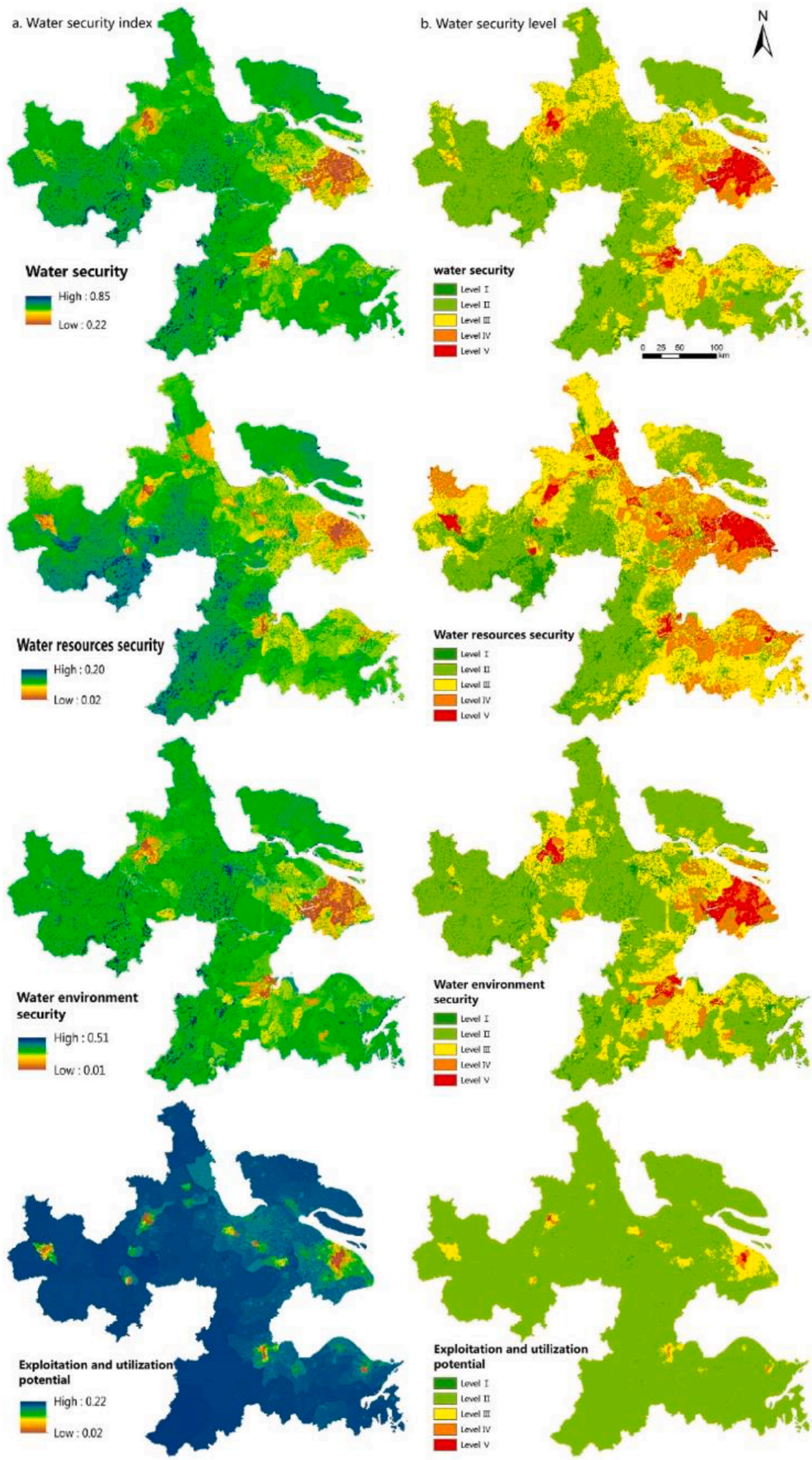

Fig. 7. Water security index in 15 key cities in the Yangtze River Delta region.

Table 2
The classifications and statistics of water security index of 15 cities in the Yangtze River Delta region.

	Comprehensive water security		Water resources security		Water environment security		Exploitation and utilization potential	
	Interval	Area proportion	Interval	Area proportion	Interval	Area proportion	Interval	Area proportion
Level I	(0.71,0.85]	8.64%	(0.15,0.20]	8.49%	(0.42,0.51]	9.83%	(0.15,0.22]	0.37%
Level II	(0.64,0.71]	57.03%	(0.13,0.15]	35.41%	(0.37,0.42]	57.74%	(0.14,0.15]	95.48%
Level III	(0.58,0.64]	25.89%	(0.12,0.13]	33.09%	(0.32,0.37]	24.01%	(0.12,0.14]	3.71%
Level IV	(0.49,0.58]	5.48%	(0.10,0.12]	17.56%	(0.25,0.32]	5.31%	(0.09,0.12]	0.36%
Level V	[0.22,0.49]	2.95%	[0.02,0.10]	5.46%	[0.01,0.25]	3.11%	[0.02,0.09]	0.08%

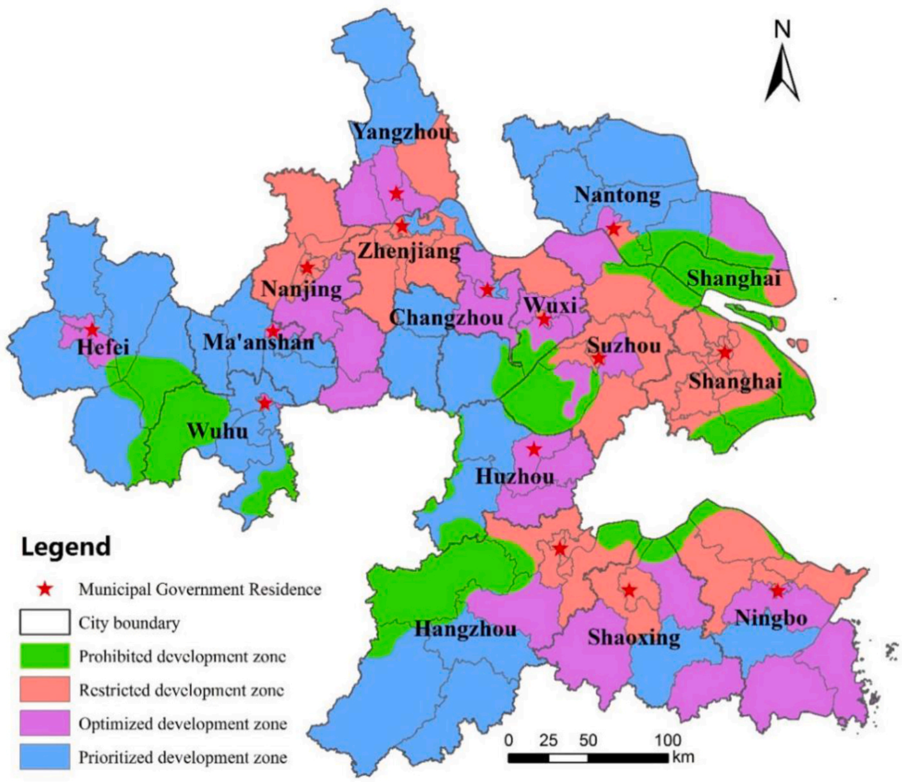

Fig. 8. Water security zoning of 130 county-level administrative units in the Yangtze River Delta region.

aspect of the water environmental assessment, although different indicators were used, the overall pattern of results is consistent between studies–Anhui is superior to Zhejiang, Jiangsu, and Shanghai.

4.3. Implications of assessment results

We assessed water security at the grid scale to refine the results of water security, and found water resources and water environment problems that were difficult to identify in the total assessment (at the city and the provincial scales). There is currently no way to formulate policy recommendations for each pixel, which is also unrealistic. Policymakers in China usually elaborate environmental policies and land use development plans based on the administrative level. Therefore, we gave the recommendations at the county-level. In addition, policymakers can identify future development orientations of county-level administrative units based on our water security assessment results. Environmental management measures should be carried out according to the spatial guideline identification, such as in low value areas of water resources and high value areas of nutrient emission.

The application of PES is mainly for (1) the division of buyers and providers of PES; (2) the allocation of PES amount. The PES mechanism has a wide range of applications in the region. The criteria used for management of the administrative department is the basin water quality accountability system. The fund is paid according to the proportion of the national control monitoring section that meets the standard. However, the funding available is far less than the construction and opportunity costs of local PES projects. For example, in 2012, the pilot plan for Xin'an River basin compensation was jointly carried out by the national government and two provincial governments. The upstream Huangshan municipality cancelled aquaculture, cleared up polluting enterprises, and constructed sewage treatment facilities. The local government spent a total of 10.9 billion RMB, of which 3.02 billion RMB of compensation funds were obtained from two rounds of PES pilot work. In China, PES is not comprehensive enough to compensate providers based on the water quality accountability system, due to the lack of consideration of water resources and efforts made. Therefore, PES performance evaluation is an important basis for allocation. Indicator choice involves a trade-off; easily evaluated indicators reduce transaction costs and facilitate communication but risk missing important information and may not actually meet protection goals. In contrast, more rigorous indicators may accurately capture service values, but will increase transaction costs. Therefore, simulations using ecosystem service models with lower data requirements are a simple and comprehensive way to evaluate PES performance.

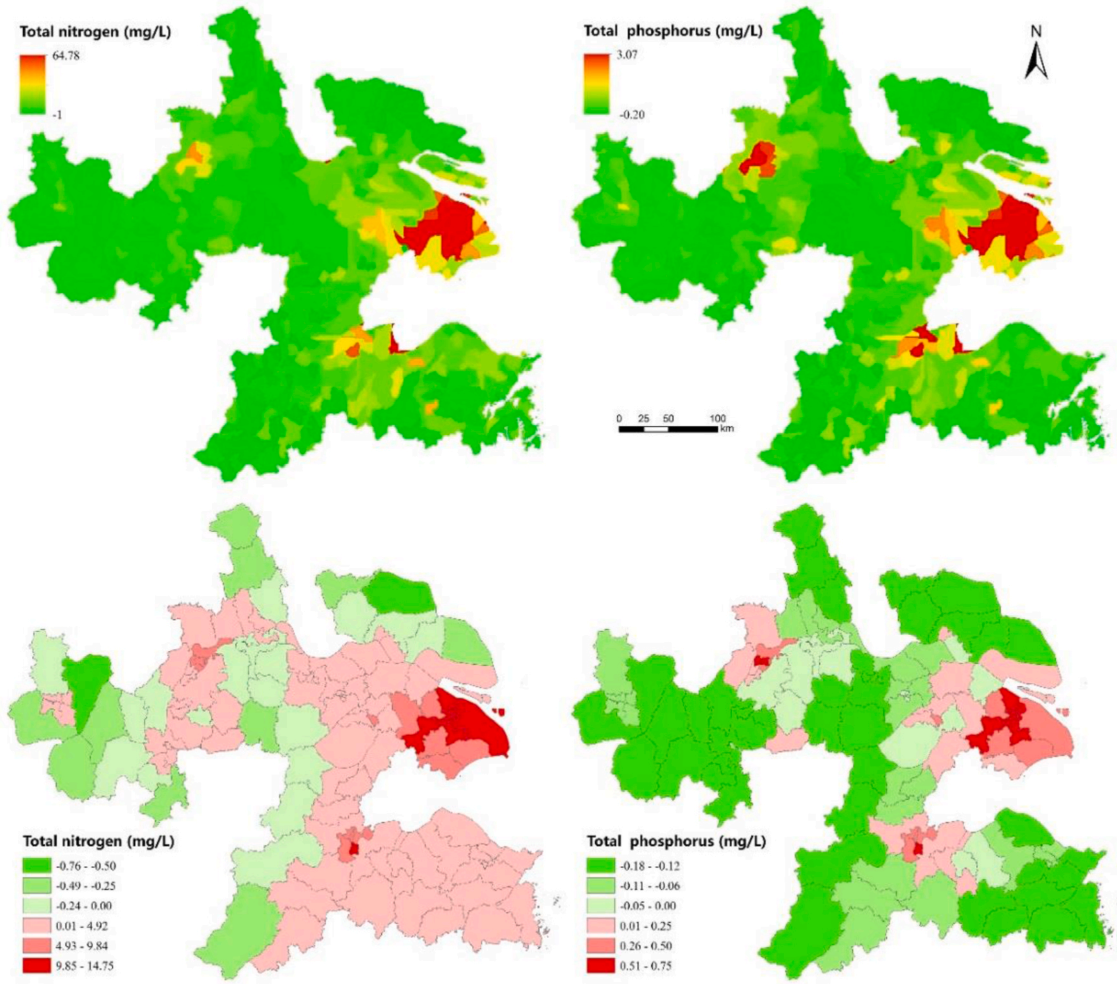

Fig. 9. Difference between current and target water quality in 130 county-level administrative units in the Yangtze River Delta region.

4.4. Strengths and limitations

This study demonstrates that water security assessment at the grid scale is practical. The strengths are as follows: (1) temporal and spatial differences between water supply and demand can be matched; (2) spatial distribution of point and non-point source pollutant discharges and the pattern of exploration and utilization potential can be understood; and (3) results can be used for regional spatial planning and coordinated management. On this basis, considering the needs of the evidence-based policymaker, assessments of the three target indicator layers could provide management guidance at certain administrative boundary levels and the grid level. Maps of the spatial distribution of 3 subsystems can help city managers to accurately locate areas that would benefit from interventions, allowing more targeted management. This study is one of few to assess both spatial and seasonal differences in water supply and demand. The ecosystem service model used in this study can be applied when monitoring data is lacking, providing managers with a regional overview and hierarchical management guidance based on simulation results. Regional water security was measured at a finer scale than in previous studies, allowing identification of areas for water regulation interventions.

This study also has a number of limitations. First, although the InVEST model could be used for the omitted data regions, the annual water yield module is based on a simplified equilibrium hypothesis which requires the study region should be large enough to fulfill the premise. Second, the outputs of the NDR module generally show high sensitivity to inputs, such as accurate nutrient load data and retention efficiency. Besides, the impact of grid resolution on the NDR simulation results has not been well studied. Third, the water security assessment in this study was based on the ecosystem service function, which reflects the regional natural resource endowment. The long-distance water withdrawal has not been considered.

5. Conclusions

In this study, we proposed a refined and systematic framework to assess the regional water security, analyzed water security patterns in 15 key cities in the YRD region, and applied assessment results to environmental management. Please find the abbreviations in the table S6.

(1) The comprehensive water security index in the study area is relatively high. High-value areas (Levels I and II) are widely distributed, accounting for 65.67% of the study area. Low-value areas (Levels III to V) are mainly distributed in the central and eastern regions, such as Shanghai, Suzhou, and Nanjing.
(2) The assessment method used in this study is capable of matching spatial and temporal differences in water supply and demand at the fine scale. Water supply and demand are seasonally matched, but there are small mismatches at the monthly scale. Supply and demand are spatially unmatched in the study area. There is a shortage of water resources at the grid scale during the 12 months period, with the worst water security in August.
(3) Regarding water environment security, the spatial distribution of high-value areas of TN and TP export are similar, mainly

distributed in Shanghai, Nanjing, and Hangzhou, forming a spatial pattern of "one center, two sub-centers", which are developed cities with high levels of urbanization and industrialization. The spatial distribution of point and non-point source pollutant discharges and the spatial configuration of development and utilization potential can be accurately delineated.

(4) Assessment results can provide support for spatial planning guidelines and the exploration of PES mechanisms for county-level or smaller administrative units. Based on differences between simulated and target water quality, PES providers and buyers can be determined and the performance of PES evaluated simply and comprehensively. The assessment method proposed in this study can guide policy-makers to carry out sustainable water management practices, identify areas that need intervention, and provide the basis and reference for PES implementation for regional water environment coordination. Moreover, ecosystem service model simulations have lower data requirements than other methods and are therefore useful to managers of areas where data are lacking.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data related to this article can be found at https://doi.org/10.1016/j.jenvman.2021.112588.

Credit author statement

P. Dou: interpreted the data and wrote the manuscript; S. Zuo and S. Dai: visualized the data and provided the data resources; Y. Ren and M.J. Rodriguezd: conceived the methodology and supervised the data analysis.

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