Modeling the integrated framework of complex water resources system considering economic development, ecological protection, and

food production: A practical tool for water management

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Supplement: Supplementary materials (Data availability)

S1. Description of pendulum dynamics

The external driver of the integrated modeling system is mainly socio-economic changes that are reflected by changing population and productivities. It can be outlined by the term of "pendulum model" that addressed by Van et al. (2014) and Kandasamy et al. (2014). According to Kandasamy et al. (2014), The social development is at the expense of sacrificing the environment, and the "pendulum model" is therefore addressed based on different development stages over the past years and adapted in Australia. Kandasamy et al., (2014) stressed that the term "pendulum swing" refers to the shift in the balance of water utilization between economic development and environmental protection. The pendulum "swing" periodically and can be divided into four stages.

The agricultural-based society is at the beginning of the evolution, and the environmental problems have not emerged in this stage. This stage is called "expansion of agriculture and associated irrigation infrastructure". In this stage, Europeans settled in Australia and displaced Aboriginals. The Europeans need to survive, and therefore, they introduced new grasses, cereal crops, cattle and sheep, and further built farm dams and introduced irrigation schemes for intensive cultivation and more productive use of lands on the floodplains. It reveals the enlargement of agricultural productivities, and the investment of the government facilitates the growth of the whole community and the agricultural industry. As a result, crop production has greatly increased.

In the second stage, as water resources benefit both agricultural and socio-economic development with massive government policy support and investment, the whole society's demand for resources has intensified due to the sharp growth of population due to increased irrigation area and agricultural productivity. This stage is called "onset of environmental degradation and ad hoc solutions". Some problem has emerged, including saltwater intrusion, salinization of lands due to irrigation, blooms of blue-green algae. Saltwater intrusion impacts landowners and farmers along the lower reaches of the river who strongly advocated for the construction of barrages to keep the water fresh in the lower reaches. Salinization decreases crop production and economic losses. The blooms of blue-green algae are also the main problem of water environment.

As productive activities still proceed, the environmental problem tends to deteriorate. This is the stage called "establishment of widespread environmental degradation". The environment will be significantly damaged, which can be regarded as the pendulum "swings" towards economic development. The characteristic of this stage is the rapid population growth accompanied by the accelerated consumption of water resources. It further reduces the river ecological streamflow and challenges the river ecological health, affecting the biodiversity of aquatics and coastal plants. It also challenges the biodiversity of wetlands. Fortunately, the government realized this problem and issued the relative laws to protect the environment, which is the beginning of the fourth stage.

The fourth stage is called "remediation and emergence of the environmental customer". When environmental awareness is on the rise, the government will invest more in ecology, resulting in a declining population. In this case, more water is used to protect the environment, reflecting that the pendulum has "swung" back to the environment. In this stage, the population growth rate will decrease.



Fig S1. Illustration of pendulum dynamics

The Municipal Government of Guilin City (MGGC) predicted the population and GDP size of 2020, 2030, and 2040 and therefore the time stage can be separated into three stages (2016~2020, 2021~2030, 2031~2040). To apply this theory in the current study, according to the characteristic of this model, the stage 2 and 3 can be merged because they both reveal the acceleration of economic growth and deterioration of the environment. The population size in 2030 is quite larger than that in 2020, which corresponds to the stage 2 & 3 in this pendulum model. Other stages addressed by MGGC is similar to the first and last stage in the pendulum model.

S2. Description of each agent

S2.1 Economic agent

This agent is used to determine the socio-economic and water interactions, including water withdrawal, usage, consumption, and drainage (Luo and Zuo, 2019). From the water supply perspective, it also supplies water for social (household) use. The household and industrial water demand are presented as follows:

$$WD_{hou} = \frac{q_{hou} \times N \times d}{1000} \tag{1a}$$

$$WD_{indus} = I_{GDP} \times q_{indus} \tag{1b}$$

$$\frac{dN}{dt} = rN \tag{1c}$$

where WD_{hou} and WD_{indus} are the annual household and industrial (including secondary and tertiary) water demand (m³), N is population size, d is the days of a certain year and r is the natural growth rate, I_{GDP} is the industrial added value (10⁴ Yuan), q_{hou} and q_{indus} are the domestic and industrial water usage quota, which means daily water consumption per person (L/person/day) and water consumption of the industrial added value per 10⁴ Yuan (m³/10⁴ Yuan), respectively. The population equation presented in Eq.(1c) is a simple linear differential model called Malthusian growth model (Jørgensen and Bendoricchio, 2001; Feng et al., 2016), and GDP size is also suitable for this model. For agricultural economy, the economic basis of farmer's response is reflected by average incomes that can be expressed by Eq.(4) of the main paper. The food production is a significant component of both primary industry value and can measure farmers' income, because farmers sell these foods to customers and get profits. The calculation of food production is shown in S2.3.

S2.2 Ecological agent

(1) Ecological water demand for vegetation

Ecological water demand of vegetation is used to maintain the physiological function of canopies, including photosynthesis, respiration, and evapotranspiration. The method of evaluating the amount of vegetation ecological demand is based on their evapotranspiration that can be treated as the water gap (Shi et al., 2016; Saxton et al., 1986):

$$WD_{veg} = K_s \cdot K_c \cdot ET_0 - P_e \tag{2a}$$

$$ET_{0} = \frac{0.408\Delta(H_{net} - G) + \gamma \frac{900}{T + 273}u_{2}(e_{0} - e_{z})}{\Delta + \gamma(1 + 0.34u_{2})}$$
(2b)

$$K_{s} = \frac{\ln\left[100 \times \frac{S - S_{w}}{S_{c} - S_{w}} + 1\right]}{\ln 101}$$
(2c)

where WD_{veg} is the vegetation water demand. P_e is the effective precipitation. ET_0 is potential evapotranspiration based on the Penman-Monteith equation, and the particular variables can be seen in Neitsch et al., (2011). K_s and K_c are soil moisture and canopy coefficients, respectively, which denotes the ratio of maximum water demand and potential evapotranspiration. S, S_c, and S_w are the coefficient of actual, wilting, and critical soil moisture, respectively.

(2) River ecological demand

River ecological demand is the instream water demand that is used to maintain river health and function. Its health degree can be reflected by the annual proportional flow deviation (APFD) that is used to assess the diversity of fish species (Gehrke et al., 1995). However, it is computationally

unstable when the monthly streamflow is near zero (Yin et al., 2010). In this study, we use the amended indicator, AAPFD, to assess the river ecological demand (Ladson and White, 1999):

$$AAPFD = \frac{1}{n} \sum_{j=1}^{n} \sqrt{\sum_{m=1}^{12} \left(\frac{Q_{mj} - QN_{mj}}{\overline{QN_j}} \right)^2}$$
(3)

where Q and QN are the actual and observed streamflow. The subscript n, m, and j are the total year number, mth month, and jth year. According to Ladson and White (1999), the smaller deviation suggests the better river ecology, which is reflected by smaller AAPFD, and the value of AAPFD ranges from zero to five. When the value is larger than five, the river ecosystem will be seriously damaged (Yin et al., 2010; Tan et al., 2019). Therefore, the goal of evaluating the river ecological demand is to find a suitable Q to make AAPFD a minimum.

S2.3 Food agent

The food agent is mostly related to agricultural water usage, including crop water requirements based on phenological stages and farm management, including livestock production. It is also the fundamental condition of primary industry and farmer's incomes (See 2.1.1). For crops, water usage is related to crop yield. The main water supply is provided by irrigation. We use the crop coefficient method to estimate crop water demand based on the Food and Agricultural Organization report No. 56 (FAO-56) (Allen et al., 1998). For each crop, its growth process can be separated into several stages that have different potential crop water demands (Allen et al., 1998; Smilovic et al., 2016):

$$W_p = \int_{t_0}^{t_n} K_c(t) \cdot ET_0 dt \tag{4a}$$

$$W_a = W_p - P_e \tag{4b}$$

where W_P is potential crop water demand, and can also be called reference crop demand of crop i, $K_c(t)$ is the crop coefficient of stage t for a specific crop, t_0 and t_n is the first and last stage of the growth process of a specific crop. W_a is the irrigation water demand. The maximum crop yield is based on the hypothesis that the crop water supply (including precipitation) can meet W_p (Allen et al., 1998). According to FAO-56, crop growth is usually divided into four phenological stages: initial, development, middle, and end, and corresponds to three different crop coefficients: $K_{c,ini}$, $K_{c,mid}$ and $K_{c,end}$. For details, see Allen et al. (1998). For each crop, the crop yield is presented as follow (Smilovic et al., 2016):

$$\frac{Y_s}{Y_p} = \prod_{t=t_0}^{t_n} \frac{Y_{s,t}}{Y_{p,t}} = \prod_{t=t_0}^{t_n} \left[1 - K_{y,t} \left(1 - \frac{W_{s,t} + P_{e,t}}{W_{p,t}} \right) \right]$$
(5)

where $W_{s,t}$ is the actual irrigation water supply for crop i at time t, Y_s and Y_p is the crop yield under actual and ideal condition (both irrigation water supply W_s and precipitation P_e can meet the crop water demand W_p), $K_{y,t}$ is yield response factor of the crop i at time t. Due to the limitation of local water resources conditions, crop water supply is usually equal to or less than crop water demand. That is, $(W_s+P_e) \leq W_p$, and crop water supply is greatly related to crop yield. The value of Y_s/Y_p is also equal to or less than one, and it takes the "=" sign when the crop yield attains the maximum. In this case, the water supply also attains the maximum.

For meat production, it is reflected by the production of livestock (pork and beef) and poultry

(chicken, duck, and goose). The calculation of water usage of livestock is the same as Eq.(1a), and here N and q are the total livestock population and its corresponding water use. The production of livestock and poultry can be solved by linear regressive calculation based on local statistical yearbooks and water resources bulletin over the historical years (Li et al., 2019):

$$Y_L = a_L W_L + b_L \tag{6}$$

where Y_L is the production of a certain livestock (10⁴t) and W_L is the actual water use of a certain livestock (10⁴m³), a_L and b_L are primary coefficient and constant term of the stock-water production function.

S3. Constraints of the model

(1) Constraints of continuity equation between subareas and reservoir

For each water supply subsystem, a reservoir supplies water to each subarea (the lower level in Fig.3). Therefore, reservoir is interconnected with each subarea. Among subareas, they also have the continuity relationship of the upper and lower reach of the river. It can be expressed as follows:

$$I_{kt} = \sum_{j=1}^{J} WS_{jkt}^{rsv} + \sum_{k \in \Omega} WR_{k-1,t} + WIF_{kt}$$
(7)

where I_{kt} is the total water income of subarea k in time t, WS^{rsv} is water supply only from reservoir, WR is water recession to the downstream subarea(s). Subscript j represents different water users. WIF is the intermediate flow between (k-1)th and kth subarea. Ω is the summary of the direct upper reaches of kth subarea.

(2) Constraints of the water balance of reservoir

$$V_{t} + QN_{t} - \sum_{j=1}^{J} \sum_{k=2}^{K} WS_{jkt}^{rsv} - W_{t}^{loss} - Q_{t} = V_{t+1}$$
(8)

where V_t is water volume in the reservoir at time t, W^{loss} is the water loss of evaporation and leakage of the reservoir.

(3) Constraints of the water balance of subarea

$$W_{kt} + I_{kt} - \sum_{j=1}^{J} WS_{jkt} - WR_{kt} = W_{k,t+1}$$
(9)

where W_{kt} is the total quantity of water resources in subarea k in time t.

(4) Water supply constraint

Water allocated to each subarea should not exceed the capacity of each water project.

$$WS_{i,t} \le WS_{i,\max}$$
 (10)

(5) Water demand constraint

For decreasing the waste of water resources, water allocated to each subarea should not exceed the water demand. If there is abundant water, the extra water that exceeds the water demand should be stored in the water project.

$$0 \le WS_{ikt} \le WD_{ikt} \tag{11}$$

(6) Reservoir volume constraint

The lower and upper limit of the reservoir should be considered to keep the reservoir safety.

$$V_{\min} \le V_t \le V_{\max} \tag{12}$$

(7) Non-negative constraint

All the variables in this model should be non-negativity.

S4. Whole procedure of decomposition-coordination and dynamic programming

The total procedure of DC is classified into four steps. First, the whole system is decomposed into a three-level hieratical structure (upper level, middle level, and lower level) and subsystems (see Fig.2 and Fig.3). The upper level represents the whole system, middle level a reservoir subsystem, and lower level represents an individual reservoir & subarea. The DC process is classified into two layers: the internal subsystem of water supply and the relation between water supply subsystems. For each internal reservoir subsystem, the Lagrange function is presented to describe the model objective:

$$L = \alpha \left(F_{ecnmy} + F_{veg} + F_{food} \right) + \theta F_{riv} + \sum_{t=1}^{T} \sum_{k=1}^{K_{1}} \lambda_{kt} \left(\sum_{j=1}^{J} WS_{jkt}^{rsv} + \sum_{k \in \Omega} WR_{k-1,t} + WIF_{kt} - I_{kt} \right)$$

$$+ \sum_{t=1}^{T} \mu_{1,kt} \left(V_{t} + QN_{t} - \sum_{j=1}^{J} \sum_{k=1}^{K_{1}} WS_{ikt}^{rsv} - W_{t}^{loss} - Q_{t} - V_{t+1} \right)$$

$$+ \sum_{t=1}^{T} \sum_{k=1}^{K_{1}} \mu_{2,kt} \left(W_{kt} + I_{kt} - \sum_{j=1}^{J} WS_{jkt} - WR_{kt} - W_{k,t+1} \right)$$

$$(7)$$

where λ , μ_1 and μ_2 are slack variables, K₁ is the number of subareas in a reservoir water supply subsystem. The last two items of Eq.(S1) are 0 when the water balance equation is satisfied (Li et al.,2015). Thus, the Lagrange function can be rewritten as the additive separable form (Jia et al., 2015):

$$L = \sum_{t=1}^{T} \left\{ \left[\theta F_{riv} + \sum_{i=1}^{I} \sum_{k=1}^{K_1} \lambda_{kt} W S_{ikt}^{rsv} \right] + \sum_{k=1}^{K_1} \left[\alpha \left(F_{ecnmy} + F_{veg} + F_{food} \right) + \lambda_{kt} \left(\sum_{k \in \Omega} W R_{k-1,t} + W I F_{kt} - I_{kt} \right) \right] \right\}$$
(8)

Eq.(S2) is the Lagrange function that summarizes the objective function of each subarea and reservoir. For the layer that describes the relationship between water supply subsystems, the optimal solution for the whole system is the summary of Eq.(S2) of each water supply subsystem.

Following the objective function between subareas is the coordination between those subareas and reservoirs in each reservoir supply subsystem. Coordinate variables are treated as independent variables. According to the dual theory, the necessary condition of the optimal solution of Lagrange function is that the derivative to the model variables should be zero (Jia et al., 2015), and the gradient method was used to solve the optimal coordinate variables:

$$\lambda_{kt}^{m+1} = \lambda_{kt}^{m} + \sigma_m \cdot \frac{\partial L}{\partial \lambda_{kt}^{m}} \tag{9}$$

The third step is the optimization of the subareas and reservoir. Considering water management can be divided into several time steps, dynamic programming (DP) is used in the optimization process. DP mainly includes four elements that listed below:

(1) Stage variable: each time step is selected as the stage variable.

(2) State variable: the initial water amount in each subsystem is selected as a stage variable. In this case, it is reflected by the initial storage of the reservoir and the total amount of water in each administrative region.

(3) Decision variable: total water supply for each subarea and actual streamflow of the reservoir is selected as a decision variable.

(4) Recurrence formulation:

$$f\left(S_{t}\right) = \min\left\{\nu\left(S_{t}, D_{t}\right) + f\left(S_{t+1}\right)\right\}$$
(10)

where S_t and D_t is the state and decision variable at the stage, $f(S_t)$ is the optimal benefit of the whole system at the state S_t ; $v(S_t, D_t)$ is the benefit with the decision D_t at the state S_t .

The last step is to combine the first three steps because the process of decomposition, coordination, and subsystem optimization is interrelated. The procedure of the whole DC method is as follows:

(1) Generate an initial solution of each subarea and reservoir with a given initial value. The solution includes the actual reservoir streamflow and the total water supply of each subarea.

(2) Calculate the coordinative variables based on the initial solution based on Eq.(9), and optimizing the solution of each subsystem by using DP based on the calculated coordination variables.

(3) Compare the optimized solution in (2) with the initial solution. If the error is within the given precision (ϵ =0.0001), it is the final solution. Otherwise, recalculate the new coordinative variables and repeat the procedure until the error is within the specified range.

(4) Optimize the next reservoir supply subsystem, and the summary of each subsystem is the global optimal solution.



S5. Detailed flowchart of system dynamics and equations of EEF nexus

Fig.S2 Dynamic analysis framework of EEF nexus based on SD model

To distinguish, the variable that can reveal the coevolution of EEF nexus is shown in different colors. Red for economic, orange for food and green for ecology. The main equations of SD model are shown in Table S1.

Variables	Unit	Equations		
Birth rate	%	See Table 4		
Industrial growth rate	%	See Table 4		
GDP	10 ⁴ yuan	Primary industrial production + Secondary industrial		
		production + Tertiary industrial production		
Industrial water	$10^{4}m^{3}$	$GDP \times Water consumption per 10000RMB of GDP$		
demand				
Urbanization rate	%	=WITHLOOKUP {Time, [(2016,0.3317)-		
		(2040,0.4958)], (2016,0.3499), (2017, 0.3550),		
		(2018,0.3601), (2019,0.3652), (2020,0.3704),		
		(2021,0.3780), (2022,0.3856), (2023, 0.3933),		
		(2024,0.4010), (2025,0.4088), (2026,0.4166),		
		(2027,0.4245), (2028,0.4323), (2029,0.4403),		
		(2030,0.4482), (2031,0.4530), (2032,0.4578),		
		(2033,0.4625), (2034,0.4673), (2035,0.4720),		
		(2036,0.4768), (2037,0.4815), (2038,0.4863),		
		(2039,0.4910), (2040,0.4958)}		
Water quota for urban	L/person/d	200		
Water quota for rural	L/person/d	120		
Urban population	People	Population × Urbanization rate		
Rural population	People	Population × (1-Urbanization rate)		
Water demand for	10 ⁴ m ³	See Eq.(1a)		
urban household				
Water demand for	$10^{4}m^{3}$	See Eq.(1a)		
urban household				
Household water	10 ⁴ m ³	Water demand for urban household + Water demand for		
demand		urban household		
Water demand for	$10^{4}m^{3}$	Household water demand + Industrial water demand		
socio-economic				
development				
Urban household water	$10^{4}m^{3}$	Solved by optimal model		
supply				
Rural household water	$10^{4}m^{3}$	Solved by optimal model		
supply				
Water supply for socio-	$10^{4}m^{3}$	Urban household water supply + Rural household water		
economy development		supply + Reuse water resources		
Urban population	people	Urban household water supply \times 1000 / (Water quota for		
carrying capacity		urban \times day of the year)		
Rural population	people	Rural household water supply \times 1000 / (Water quota for		
carrying capacity		rural ×day of the year)		

Table S1. Main equations of SD model

Population carrying	people	Urban population carrying capacity + Rural population		
capacity		carrying capacity		
Overload index of	-	Population/Population carrying capacity		
population				
Industrial water supply	$10^{4}m^{3}$	Solved by optimal model		
GDP capacity	10 ⁴ yuan	Industrial water supply/Water consumption per		
		10000RMB of GDP		
Overload index of	-	GDP/GDP capacity		
GDP				
Household sewage	-	0.75		
discharge coefficient				
Household sewage	$10^{4}m^{3}$	Household water demand ×Household sewage discharge		
discharge		coefficient		
Household sewage	-	0.75		
treatment rate				
Household sewage	$10^{4}m^{3}$	Household sewage discharge × Household sewage		
treatment		treatment rate		
Industrial sewage	-	0.7		
discharge coefficient				
Industrial sewage	$10^{4}m^{3}$	Industrial water demand ×Industrial sewage discharge		
discharge		coefficient		
Industrial sewage	-	0.7		
treatment rate				
Industrial sewage	$10^{4}m^{3}$	Industrial sewage discharge × Industrial sewage		
treatment		treatment rate		
Total sewage treatment	$10^{4}m^{3}$	Household sewage treatment + Industrial sewage		
		treatment		
Reuse water utilization	-	0.2		
rate				
Reuse water resources	$10^{4}m^{3}$	Total sewage treatment ×Reuse water utilization rate		
Number of livestock	10 ⁴ number	=WITHLOOKUP {Time, [(2016,256)-(2040,306)],		
		(2016,256), (2017,258), (2018,260), (2019,262),		
		(2020,263), (2021,265), (2022,267), (2023, 269),		
		(2024,271), (2025,274), (2026,276), (2027,278),		
		(2028,280), (2029,282), (2030,284), (2031,286),		
		(2032,288), (2033,290), (2034,293), (2035,295),		
		(2036,297), (2037,299), (2038,301), (2039,304),		
		(2040,306)}		
Water quota for big	L/number/d	100		
livestock				
Big livestock water	$10^{4}m^{3}$	See Eq.(1a)		
demand				
Number of poultries	10 ⁴ number	=WITHLOOKUP {Time, [(2016,6870)-(2040,8220)],		
		(2016,6870), (2017,6922), (2018,6974), (2019,7026),		

		(2020,7078), (2021,7132), (2022,7186), (2023,7239),
		(2024,7294), (2025,7348), (2026,7404), (2027,7459),
		(2028,7515), (2029,7571), (2030,7628), (2031,7685),
		(2032,7743), (2033,7801), (2034,7859), (2035,7918),
		(2036,7977), (2037,8037), (2038,8098), (2039,8159),
		(2040,8220)}
Water quota for	L/number/d	1.5
poultries		
Poultries water	$10^{4}m^{3}$	See Eq.(1a)
demand		
Livestock water	$10^{4}m^{3}$	Big livestock water demand + Poultries water demand
demand		
Reference crop	$10^{4}m^{3}$	Potential evapotranspiration for crops × Crop coefficient
demand		(See Eq.(5))
Irrigation water	$10^{4}m^{3}$	Reference crop demand- effective precipitation for crop
demand		
Water demand for food	$10^{4}m^{3}$	Livestock water demand + Irrigation water demand
production		
Crop yield	10 ⁴ t	f(Water supply for crops, water demand for food
		production), see Eq.(6)

S6. Three-level hieratical structure model in ULRB

As mentioned in section 2.2.1, the optimal model can be conceptualized as a three-level hieratical structure model. In ULRB, there are seven reservoirs, and their corresponding water recipient regions are listed in Table S1. Therefore, there are seven reservoir supply systems, i.e., seven subsystems. For each subsystem, it includes a reservoir and subareas and is listed in each row in Table S2.

			1	0	1	8
Abbreviation	Full name	Initial year	Total	Dead	Yearly	Subareas/Water
(Shown in		constructed	storage	storage	average	recipient region
Fig.4)			(10 ⁴	(10^4 m^3)	inflow	(City or county)
			m ³)		(m ³ /s)	
FZK	Fuzikou	2011	18000	920	8.53	Xing'an
CJ	Chuanjiang	2009	9787	346	15.44	Xing'an
XRJ	Xiaorongjiang	2010	16200	670	13.34	Xing'an
QST	Qingshitan	1964	41500	4600	28.09	Guilin urban
						area,
						Lingchuan,
						Lingui
SAJ	Si'anjiang	2006	8323	213	26.94	Lingchuan,
						Yangshuo
JS	Junshan	1990	12000	590	27.61	Pingle,
						Gongcheng
DJ	Dajiang	1960	8140	530	12.52	Lipu

Table S2. Parameters of reservoirs and corresponding water recipient regions

In this table, we can see that some counties receive water from more than 1 reservoir. For example, Xing'an county receives water from FZK, CJ, and XRJ, while Lingchuan county receives water from XRJ, QST, and SAJ. To overcome this problem, these counties can be further split into towns. As there are three towns named Huajiang, Rongjiang, and Yanguan that belong to Xing'an County, FZK, CJ, and XRJ was set to supply water for Huajiang, Rongjiang, and Yanguan towns, respectively. For the same reason, as Lingchuan county is big and receives water from 2 reservoirs (QST and SAJ), it can also be split into towns, and the reservoirs supply water for the nearest towns. The detailed for Lingchuan county is shown in Table S3.

Table S3. Water recipient regions for Lingchuan County

Reservoirs	Water recipient region (town)
Qingshitan	Sanjie, Lantian, Qinshitan, Tanxia, Lingchuan, Dingjiang, Gantang
Si'anjiang	Dajing, Lingtian, Haiyang, Dawei, Chaotian

Also, according to the three-level hierarchical structure presented in Fig.3 of Section 2.2.1 and the physical condition of ULRB, the three-level hierarchical structure of ULRB is shown in Fig.S2.



Notes: 1. Huajiang, Rongjiang and Yanguan town belong to Xing`an county; 2. Lingchuan county I and II are the water recipient region of QST and SAJ reservoir, the corresponding towns are shown in Table S3.

Fig.S3 Three-level hierarchical structure of ULRB

S7. Data sources and parameter initialization of ULRB

S7.1 Data sources

Data	Sources	Usage
Population, GDP as well	Ching City Statistical Yearbook	Predict future population
as natural growth rate,	(2000-2014)	including livestock
livestock numbers	Socio-economic statistical yearbook	
	of Guilin city (2000-2014);	
	Socio-economic statistical yearbook	
	of Guangxi (2000-2014);	
	Urban comprehensive planning of	
	Guilin City	
	Kandasamy et al., (2014)	
Meteorological data	Weather stations (shown in Fig.5)	Main input (ET ₀) of crop
(Precipitation,	(<u>http://data.cma.cn</u>) (1958-2013)	yield equation and vegetation
temperature, relative		water demand
humidity, sunshine		
duration)		
Water use quota	Water industry standard of People's	Predict water demands of
	Republic of China	water users
Crop & vegetation area	Resource and Environment Data	Crop and vegetation water
	Cloud Platform, China Academy of	demand
	Sciences (REDCP-CAS)	
	(<u>http://www.resdc.cn</u>) (2015)	
Reservoir inflow	Hydrological yearbooks (1958-	Input of optimal model
	2013)	
Historical water usage of	Water Resources Bulletin of Guilin	Building regression equation
livestock	(2000-2014)	of livestock number and its
		water usage
Sewage treatment rate &	Water Resources Bulletin of Guilin	Calculating reuse water
reuse water recycling rate		

Table S4. Data sources and its usages

S7.2 Initialized parameters

Table S5. Initial parameter setting of EEF nexus model

	10010 0.	. minu	1 purumen	a setting of EET nexus model	
Parameter	Notation	Unit	Eq.	Value	Data sources
Population growth	-	%	(1c)	Stage1: 1.23	http://data.cnki.net;
rate				Stage2: 3.41	MGGC;
				Stage3: 1.24	Kandasamy et al.;
Tertiary industrial	-	%	(1c)	Stage1: 1.99	(2014)
product growth rate				Stage2: 4.11	
				Stage3: 2.36	
Industrial product	-	%	(1c)	Stage1: 3.04	
growth rate				Stage2: 5.33	

				Stage3: 1.24	
Correction	Ks	-	(3a)(3b)	0.9	Shi et al., (2016);
coefficient of soil				Saxton et al., (1986	
moisture					
Correction	Kc	-	(3a)(3b)	Forest: 1.00	
coefficient of canopy				Open forest: 0.73	
				Shrubbery: 0.65	
Vegetation area	-	km ²	-	Forest: 2373	http://www.resdc.cn
				Open forest: 356	
				Shrubbery: 764.2	
Crop coefficient in	K _{c,ini} ,	-	(5)	Rice: 1.05, 1.2, 0.75	Allen et al., (1998)
different stages	Kc,mid,			Corn: 0.3, 1.2, 0.6	FAO, 2012
	K _{c,end} ,			Vegetables: 0.65, 1.1, 0.95	
Crop area	-	km ²	-	Rice: 1239	http://www.resdc.cn
				Corn: 208.83	
				Vegetables: 670.43	
Initial streamflow of	Q _{mj}	m^3/s	(4)	Ecological basic flow, i.e.,	Hong et al., 2016;
reservoir(s) for				30% of average annual flow	Tennant et al., 1976;
monthly average				from April to September, 10% Hydrological yearb	
				from October to March, based	of Xijiang River Basin
				on Tennant method.	(1956~2013)
Coefficient of big	a_L	-	(7)	0.002	Regressive calculation
livestock production					based on Water
equation					resources bulletin of
Coefficient of big	b_{L}	-	(7)	0.0405 Guilin (2005~20	
livestock production				and Socioeconom	
equation				Bureau of Statistics of	
Coefficient of poultry	a_L	-	(7)	0.0028 Guilin Ci	
production equation					(2005~2014).
Coefficient of poultry	b_{L}	-	(7)	0.00002	
production equation					

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