Modeling the integrated framework of complex water resources system considering socioeconomic 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.

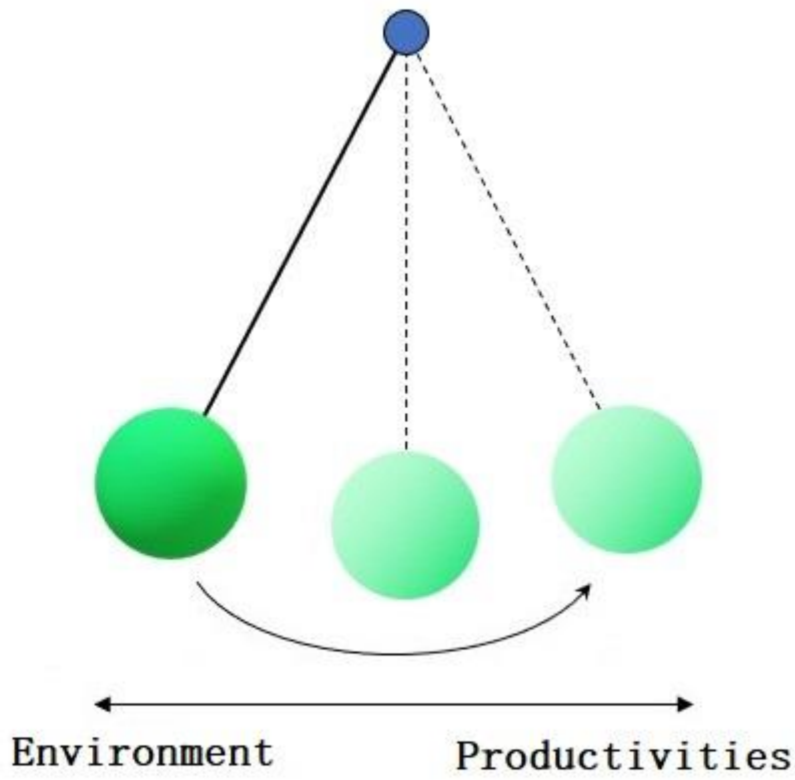


Fig S1. Illustration of pendulum dynamics

S2. System dynamic equations

S2.1 Socioeconomic agent

1. GDP = Primary Industrial Production + Secondary Industrial Production +Tertiary Industrial Production

2. Urban population = Population * Urbanization rate

3. Rural population = Population – Urban population

4. Urbanization rate = WITHLOOKUP {Time, [(2021, 0.3317)-(2045, 0.4958)], (2021, 0.3499), (2022, 0.3550), (2023, 0.3601), (2024, 0.3652), (2025, 0.3704), (2026, 0.3780), (2027, 0.3856), (2028, 0.3933), (2029, 0.4010), (2030, 0.4088), (2031, 0.4166), (2032, 0.4245), (2033, 0.4323), (2034, 0.4403), (2035, 0.4482), (2036, 0.4530), (2037, 0.4578), (2038, 0.4625), (2039, 0.4673), (2040, 0.4720), (2041, 0.4768), (2042, 0.4815), (2043, 0.4863), (2044, 0.4910), (2045, 0.4958)}

5. Water demand for socioeconomy = Domestic water demand + Industrial water demand

6. Domestic water demand = Water demand for urban domestic + Water demand for rural

domestic

7. Water quota for urban = WITHLOOKUP {Time, [(2021, 170)-(2045, 160)], (2021, 170), (2022, 170), (2023, 170), (2024, 170), (2025, 170), (2026, 170), (2027, 170), (2028, 170), (2029, 170), (2030, 170), (2031, 170), (2032, 170), (2033, 170), (2034, 170), (2035, 170), (2036, 169), (2037, 168), (2038, 167), (2039, 166), (2040, 165), (2041, 164), (2042, 163), (2043, 162), (2044, 161), (2045, 160)}

8. Water quota for rural = WITHLOOKUP {Time, [(2021, 120)-(2045, 110)], (2021, 120), (2022, 120), (2023, 120), (2024, 120), (2025, 120), (2026, 120), (2027, 120), (2028, 120), (2029, 120), (2030, 120), (2031, 120), (2032, 120), (2033, 120), (2034, 120), (2035, 120), (2036, 119), (2037, 118), (2038, 117), (2039, 116), (2040, 115), (2041, 114), (2042, 113), (2043, 112), (2044, 111), (2045, 110)}

9. Water consumption per 1000 RMB of GDP = WITHLOOKUP {Time, [(2021, 55)-(2045, 45)], (2021, 55), (2022, 55), (2023, 55), (2024, 55), (2025, 55), (2026, 55), (2027, 55), (2028, 55), (2029, 55), (2030, 55), (2031, 55), (2032, 55), (2033, 55), (2034, 55), (2035, 55), (2036, 54), (2037, 53), (2038, 52), (2039, 51), (2040, 50), (2041, 49), (2042, 48), (2043, 47), (2044, 46), (2045, 45)}

S2.2 Update process of SD model and water supply simulation

1. Total water demand = Domestic water demand + Industrial water demand + Irrigation water demand + water demand for vegetation

2. Domestic water supply = Domestic water demand * (1 – Domestic water shortage ratio)

3. Industrial water supply = Industrial water demand * (1 – Industrial water shortage ratio)

4. Crop water supply = Irrigation water demand * (1 – Agriculture water shortage ratio) + Effective precipitation

5. Vegetation water supply = Vegetation water demand * (1 – Vegetation water shortage ratio) + Effective precipitation

6. Domestic water shortage ratio = 0.05

7. Industrial water shortage ratio = 0.05

8. Agricultural water shortage ratio = 0.15

9. Vegetation water shortage ratio = 0.15

10. Flow percentage = 0.4 (Apr~Oct); 0.2 (Nov~Mar)

11. Domestic sewage discharge = Domestic water demand * Domestic sewage discharge coefficient

12. Domestic sewage treatment = Domestic sewage discharge * Domestic sewage treatment rate

13. Industrial sewage discharge = Industrial water demand * Industrial sewage discharge coefficient

14. Industrial sewage treatment = Industrial sewage discharge * Industrial sewage treatment rate

15. Total sewage treatment = Domestic sewage treatment + Industrial sewage treatment

16. Reuse water resources = Total sewage treatment * Reuse water utilization rate

17. Domestic sewage discharge coefficient = 0.6

18. Industrial sewage discharge coefficient = 0.6

19. Domestic sewage treatment rate = 0.75

20. Industrial sewage treatment rate = 0.75

21. Reuse water utilization rate = 0.2

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:

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

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

$$V_t + QN_t - \sum_{j=1}^{J}\sum_{k=2}^{K} WS_{jkt}^{rsv} - W_t^{loss} - Q_t = V_{t+1} \tag{2}$$

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

$$W_{kt} + I_{kt} - \sum_{j=1}^{J} WS_{jkt} - WR_{kt} = W_{k,t+1} \tag{3}$$

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.

$$WS_{i,t} \le WS_{i,\max} \tag{4}$$

(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.

$$0 \le WS_{jkt} \le WD_{jkt} \tag{5}$$

(6) Reservoir volume constraint

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

$$V_{\min} \le V_t \le V_{\max} \tag{6}$$

(7) Non-negative constraint

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

S4. Description of decomposition-coordination (DC) and discrete differential dynamic programming (DDDP)

S4.1 DC process

S4.1.1 System decomposition

The whole system is decomposed into a three-level hieratical structure (upper level, middle level, and lower level) and subsystems (see Fig.5 and Fig.6 in the main text). The upper level represents the whole system, middle level a reservoir subsystem, and lower level represents an individual reservoir & subarea. It is clear that each subsystem has their spacial relationships (e.g., upstream and downstream) that is reflected by continuity of each subarea (see Eq.(1)), which contributes to the complexity of the structure of water resources system. The water recession mainly includes the reused water from the current subarea and flow to the downstream subarea and act as the part of water supply. The system decomposition considering interconnection of each subsystem is based on the theory of Lagrange multiplier by introducing coordinate variables (Jia et al., 2015; Li et al., 2015). For each internal reservoir subsystem, the Lagrange function is presented to describe the model objective:

$$
\begin{aligned}
L = {} & \alpha\left(F_{socemy} + F_{veg} + F_{food}\right) + \theta F_{riv} + \sum_{t=1}^{T}\sum_{k=1}^{K_1}\lambda_{kt}\left(\sum_{j=1}^{J} WS_{jkt}^{rsv} + \sum_{k\in\Omega} WR_{k-1,t} + WIF_{kt} - I_{kt}\right) \\
& + \sum_{t=1}^{T}\mu_{1,kt}\left(V_t + QN_t - \sum_{j=1}^{J}\sum_{k=1}^{K_1} WS_{ikt}^{rsv} - W_t^{loss} - Q_t - V_{t+1}\right) \\
& + \sum_{t=1}^{T}\sum_{k=1}^{K_1}\mu_{2,kt}\left(W_{kt} + I_{kt} - \sum_{j=1}^{J} WS_{jkt} - WR_{kt} - W_{k,t+1}\right)
\end{aligned}
\tag{7}
$$

where λ, μ_1 and μ_2 are slack variables, K_1 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):

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

Eq.(8) 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.(8) of each water supply subsystem. Then, the optimal problem of each subarea can be outlined by follows:

Objective (reservoir):

$$
L = \sum_{t=1}^{T}\left(\theta F_{riv} + \sum_{i=1}^{I}\sum_{k=1}^{K_1}\lambda_{kt} WS_{ikt}^{rsv}\right)
\tag{9}
$$

Objective (subarea):

$$
L = \sum_{t=1}^{T}\left[\alpha\left(F_{socemy} + F_{veg} + F_{food}\right) + \lambda_{kt}\left(\sum_{k\in\Omega} WR_{k-1,t} + WIF_{kt} - I_{kt}\right)\right]
\tag{10}
$$

Constraints: see section S2.

S4.1.2 System coordination

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:

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

S4.2 DDDP algorithm

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 (t) is selected as the stage variable. The t is the time step of multiyear reservoir streamflow.

(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:

$$f\left(S_t\right) = \min\left\{v\left(S_t, D_t\right) + f\left(S_{t+1}\right)\right\} \tag{10}$$

where S_t and D_t is the state and decision variable at tth 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.

However, when the dimensionality of the system is too high, it may cause the amount of calculation to increase exponentially, which will extend the calculation time, and the computer's memory cannot accommodate such a high-dimensional amount of data, so that the optimal solution cannot be effectively obtained (Cheng et al., 2014), which is generally called "curse of dimensionality". In order to solve this problem, Larson et al., (1968) proposed an improved dynamic programming algorithm called "Discrete Differential Dynamic Programming" (DDDP). Compared with traditional dynamic programming, the core step of this dynamic programming method is assuming that there is an upper boundary condition and a lower boundary condition in each optimization calculation period. For the optimal trajectory, the upper and lower boundaries of each period are connected to form an optimal corridor.

Within the optimal trajectory, the traditional dynamic programming algorithm is used to find the optimal value. Therefore, setting the width of the corridor is an important part of DDDP optimization. Generally speaking, during the first cycle, the optimization corridor can be appropriately widened to find the initial optimal solution, and at the same time, the optimization corridor is reconstructed. The solution obtained in this iteration is taken as the second iteration. Initial solution, until the error of the optimization results from two adjacent iterations is less than the specified range. Then, reduce the width of the optimization corridor (this time is the second cycle), repeat the above process and repeat the iterations until the global optimal solution.

S5. 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.

Table S2. Parameters of reservoirs and corresponding water recipient regions

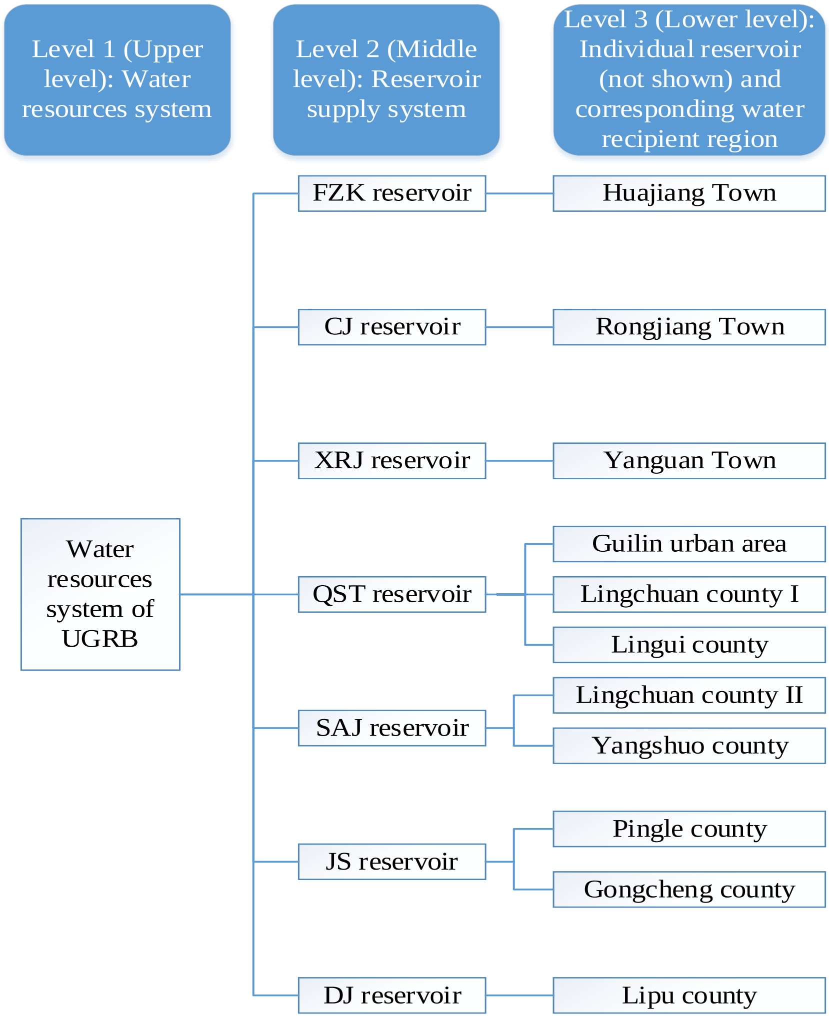
Abbreviation (Shown in Fig.4)	Full name	Initial year constructed	Total storage (10^4 m^3)	Dead storage (10^4 m^3)	Yearly average inflow (m^3/s)	Subareas/Water recipient region (City or county)
FZK	Fuzikou	2011	18000	920	8.53	Xing'an
CJ	Chuanjiang	2009	9787	346	15.44	Xing'an
XRJ	Xiaorongjiang	2010	16200	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

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

S6. Data sources and parameter initialization of ULRB

S6.1 Data sources

Table S4. Data sources and its usages

Data	Sources	Usage
Population, GDP as well as natural growth rate, livestock numbers	Ching City Statistical Yearbook (2000-2014) 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)	Predict future population

Meteorological data (Precipitation, temperature, relative humidity, sunshine duration)	Weather stations (shown in Fig.5) (http://data.cma.cn) (1958-2013)	Main input (ET_0) of crop yield equation and vegetation water demand
Water use quota	Water industry standard of People's Republic of China	Predict water demands of water users
Crop & vegetation area	Resource and Environment Data Cloud Platform, China Academy of Sciences (REDCP-CAS) (http://www.resdc.cn) (2015)	Crop and vegetation water demand
Reservoir inflow	Hydrological yearbooks (1958-2013)	Input of optimal model
Sewage treatment rate & reuse water recycling rate	Water Resources Bulletin of Guilin	Calculating reuse water

S6.2 Initialized parameters

Table S5. Initial parameter setting of EEF nexus model

Parameter	Notation	Unit	Eq.	Value	Data sources
Population growth rate	-	%	(1c)	Stage1: 1.23 Stage2: 3.41 Stage3: 1.24	http://data.cnki.net; MGGC; Kandasamy et al.; (2014)
Tertiary industrial product growth rate	-	%	(1c)	Stage1: 1.99 Stage2: 4.11 Stage3: 2.36	
Industrial product growth rate	-	%	(1c)	Stage1: 3.04 Stage2: 5.33 Stage3: 1.24	
Correction coefficient of soil moisture	K_s	-	(3a)(3b)	0.9	Shi et al., (2016); Saxton et al., (1986)
Correction coefficient of canopy	K_c	-	(3a)(3b)	Forest: 1.00 Open forest: 0.73 Shrubbery: 0.65	
Vegetation area	-	km^2	-	Forest: 2373 Open forest: 356 Shrubbery: 764.2	http://www.resdc.cn
Crop coefficient in different stages	$K_{c,ini}$, $K_{c,mid}$, $K_{c,end}$,	-	(5)	Rice: 1.05, 1.2, 0.75 Corn: 0.3, 1.2, 0.6 Vegetables: 0.65, 1.1, 0.95	Allen et al., (1998) FAO, 2012
Crop area	-	km^2	-	Rice: 1239 Corn: 208.83 Vegetables: 670.43	http://www.resdc.cn
Initial streamflow of	Q_{mj}	m^3/s	(4)	Ecological basic flow, i.e.,	Hong et al., 2016;

reservoir(s) for monthly average		30% of average annual flow from April to September, 10% from October to March, based on Tennant method.	Tennant et al., 1976; Hydrological yearbook of Xijiang River Basin (1956~2013)

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