An integrated modeling framework for coevolution and feedback loops of nexus across economy, ecology and food systems based on the sustainable development of water resources

By Yaogeng Tan*, Zengchuan Dong, Sandra M. Guzman, Xinkui Wang, Wei Yan

Appendix B: Supplementary materials (Data availability)

S1 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 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.

S2. 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 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 and individual reservoir & subarea. The DC process is classified into 2 layers: 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:

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

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 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):

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

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

Following the objective function between subareas is the coordination between those subareas and reservoir in each reservoir supply subsystem. Coordinate variables are treated as the independent variables. According to the dual theory, the necessary condition of optimal solution of Lagrange function is that the derivative to the model variables should be zero (Jia et al., 2015), and 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 subareas and reservoir. Considering water management can be divided into several time steps, dynamic programming (DP) is used in 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 stage variable. In this case, it is reflected by the initial storage of reservoir and total amount of water in each administrative region.

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

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 initial solution of each subarea and reservoir with a given initial value. The solution includes the actual reservoir streamflow and 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 specific range.

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

S3. Detailed flowchart of system dynamics and equations of EEF nexus

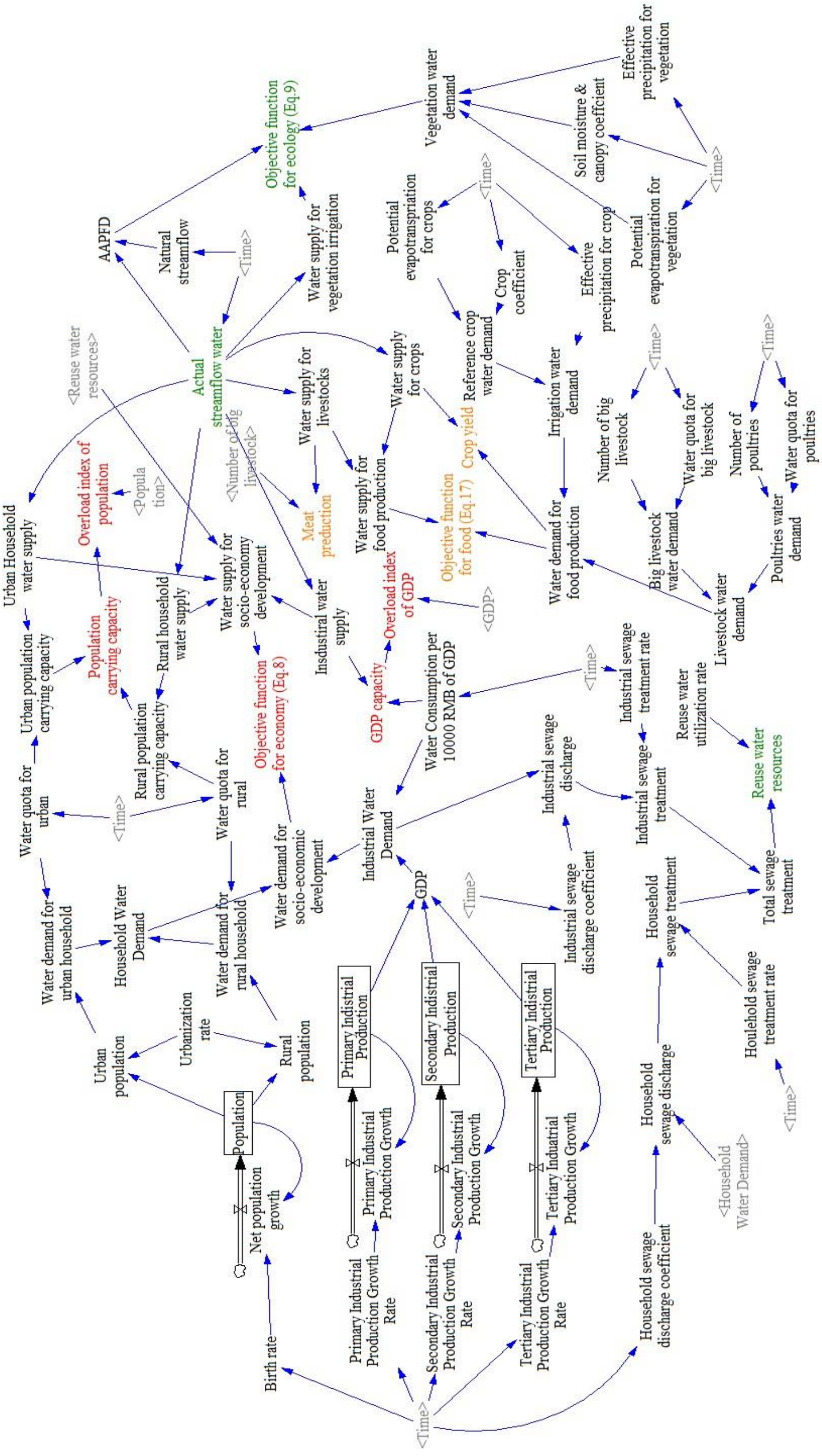


Fig.S1 Dynamic analysis framework of EEF nexus based on SD model

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.

Table S1. Main equations of SD model

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 demand	10^4m^3	GDP × Water consumption per 10000RMB of GDP
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 urban household	10^4m^3	See Eq.(1a)
Water demand for urban household	10^4m^3	See Eq.(1a)
Household water demand	10^4m^3	Water demand for urban household + Water demand for urban household
Water demand for socio-economic development	10^4m^3	Household water demand + Industrial water demand
Urban household water supply	10^4m^3	Solved by optimal model
Rural household water supply	10^4m^3	Solved by optimal model
Water supply for socio-economy development	10^4m^3	Urban household water supply + Rural household water supply + Reuse water resources
Urban population carrying capacity	people	Urban household water supply × 1000 / (Water quota for urban × 365)
Rural population carrying capacity	people	Rural household water supply × 1000 / (Water quota for rural × 365)
Population carrying capacity	people	Urban population carrying capacity + Rural population carrying capacity

Overload index of population	-	Population/Population carrying capacity
Industrial water supply	10^4m^3	Solved by optimal model
GDP capacity	10^4yuan	Industrial water supply/Water consumption per 10000RMB of GDP
Overload index of GDP	-	GDP/GDP capacity
Household sewage discharge coefficient	-	0.75
Household sewage discharge	10^4m^3	Household water demand ×Household sewage discharge coefficient
Household sewage treatment rate	-	0.75
Household sewage treatment	10^4m^3	Household sewage discharge × Household sewage treatment rate
Industrial sewage discharge coefficient	-	0.7
Industrial sewage discharge	10^4m^3	Industrial water demand ×Industrial sewage discharge coefficient
Industrial sewage treatment rate	-	0.7
Industrial sewage treatment	10^4m^3	Industrial sewage discharge × Industrial sewage treatment rate
Total sewage treatment	10^4m^3	Household sewage treatment + Industrial sewage treatment
Reuse water utilization rate	-	0.2
Reuse water resources	10^4m^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 livestock	L/number/d	100
Big livestock water demand	10^4m^3	See Eq.(1a)
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 poultries	L/number/d	1.5
Poultries water demand	10^4m^3	See Eq.(1a)
Livestock water demand	10^4m^3	Big livestock water demand + Poultries water demand
Reference crop demand	10^4m^3	Potential evapotranspiration for crops × Crop coefficient (See Eq.(5))
Irrigation water demand	10^4m^3	Reference crop demand- effective precipitation for crop
Water demand for food production	10^4m^3	Livestock water demand + Irrigation water demand
Crop yield	10^4t	f(Water supply for crops, water demand for food production), see Eq.(6)

S4. Three-level hieratical structure model in ULRB

As mentioned in section 2.2.1, the optimal model can be conceptualized as three-level hieratical structure model. In ULRB, there are seven reservoirs and their corresponding water recipient regions is 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 listed in each row in Table S3.

Table S3. 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 receive water from XRJ, QST and SAJ. To overcome this problem, these counties can be further spilt into towns. As there are 3 towns, named Huajiang, Rongjiang and Yanguan that belongs 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 receive water from 2 reservoirs (QST and SAJ), it can be also split into towns and the reservoirs supply water for the nearest towns. The detailed for Lingchuan county is shown in Table S4.

Table S4. Water recipient regions for Lingchuan County

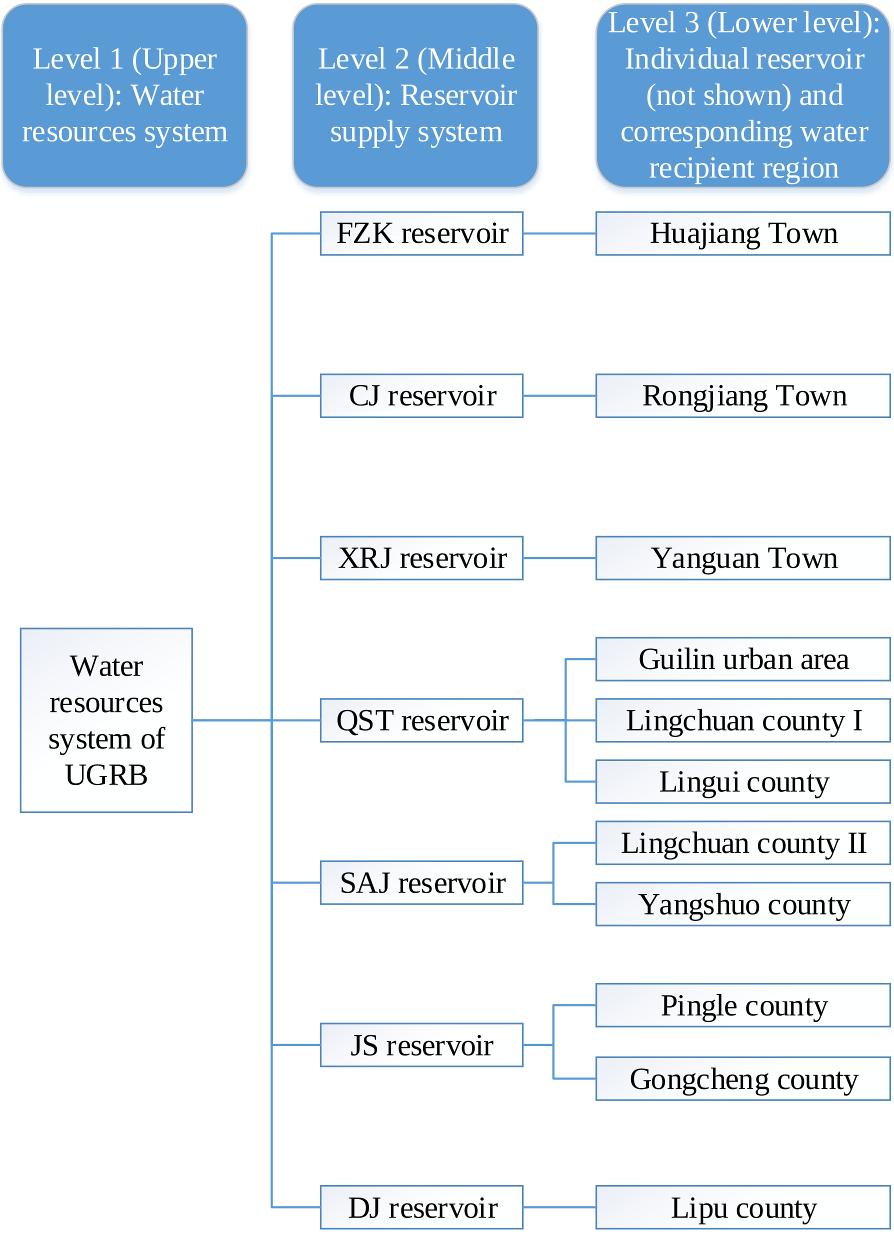
Reservoirs	Water recipient region (town)
Qingshitan	Sanjie, Lantian, Qinshitan, Tanxia, Lingchuan, Dingjiang, Gantang
Si'anjiang	Dajing, Lingtian, Haiyang, Dawei, Chaotian

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.

S5. Data sources of ULRB

Table S2. 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 including livestock
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
Historical water usage of livestock	Water Resources Bulletin of Guilin (2000-2014)	Building regression equation of livestock number and its water usage
Sewage treatment rate & reuse water recycling rate	Water Resources Bulletin of Guilin	Calculating reuse water



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 S4.

Fig.S2 Three-level hierarchical structure of ULRB

References

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