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

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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:

\[ I_{kt} = \sum_{j=1}^{J} WS_{jk}^{rsv} + \sum_{k \in \Omega} WR_{k-1,j} + WIF_{kt} \]

(1)

where \( I_{kt} \) is the total water income of subarea \( k \) in time \( t \), \( WS_{jk}^{rsv} \) 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 \(k\)th subarea. \( \Omega \) is the summary of the direct upper reaches of \( k\)th subarea.

(2) Constraints of the water balance of reservoir

\[ V_t + QN_t - \sum_{j=1}^{J} \sum_{k=2}^{K} WS_{jk}^{rsv} - W_{t}^{loss} - Q_t = V_{t+1} \]

(2)

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

(3) Constraints of the water balance of subarea

\[ W_{kt} + I_{kt} - \sum_{j=1}^{J} WS_{jk} - WR_{kt} = W_{k,t+1} \]

(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.

\[ WS_{i,j} \leq WS_{i,\text{max}} \]

(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.

\[ 0 \leq WS_{jk} \leq WD_{jk} \]

(5)
Reservoir volume constraint
The lower and upper limit of the reservoir should be considered to keep the reservoir safety.

\[ V_{\text{min}} \leq V_t \leq V_{\text{max}} \]  

(6)

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 hierarchy 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:

\[
L = \alpha \left( F_{\text{energy}} + F_{\text{vegetation}} + F_{\text{food}} \right) + \theta F_{\text{irr}} + \sum_{i=1}^{T} \sum_{k=1}^{K_{i}} \lambda_{ik} \left( \sum_{j=1}^{J} W_{jkt}^{\text{irr}} + \sum_{k=1}^{K_{i}} W_{k,1,t} + W_{\text{IRF}} - I_{kt} \right) 
+ \sum_{i=1}^{T} \mu_{1,kt} \left( V_{i} + QN_{i} - \sum_{j=1}^{J} W_{jkt}^{\text{irr}} - W_{\text{loss}} - Q_{i} - V_{i+1} \right) 
+ \sum_{i=1}^{T} \sum_{k=1}^{K_{i}} \mu_{2,kt} \left( W_{ir} + I_{ir} - \sum_{j=1}^{J} W_{jkt}^{\text{irr}} - WR_{k} - W_{k,1} \right)
\]  

(7)

where \( \lambda, \mu_1 \) and \( \mu_2 \) are slack variables, \( K_{i} \) 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):

\[
L = \sum_{i=1}^{T} \left[ \theta F_{\text{irr}} + \sum_{k=1}^{K_{i}} \lambda_{ik} W_{jkt}^{\text{irr}} \right] + \sum_{k=1}^{K_{i}} \left[ \alpha \left( F_{\text{energy}} + F_{\text{vegetation}} + F_{\text{food}} \right) + \lambda_{k} \left( \sum_{i=1}^{T} W_{k,1,i} + W_{\text{IRF}} - I_{k} \right) \right]  
\]  

(8)

Eq.(S2) is the Lagrange function that summarizes the objective function of each subarea and reservoir. For the layer that describes the 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:

\[
\lambda_{k+1}^{m} = \lambda_{k}^{m} + \sigma_{m} \frac{\partial L}{\partial \lambda_{k}^{m}}
\]  

(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:

\[
 f(S_t) = \min \left\{ v(S_t, D_t) + f(S_{t+1}) \right\}
\]

where \( S_t \) and \( D_t \) is the state and decision variable at \( t \)th 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 (\( \varepsilon=0.0001 \)), 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    | 10^4 m³    | 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 | 10^4 m³  | See Eq.(1a)                                                               |
| Water demand for urban household | 10^4 m³  | See Eq.(1a)                                                               |
| Household water demand     | 10^4 m³    | Water demand for urban household + Water demand for urban household       |
| Water demand for socio-economic development | 10^4 m³ | Household water demand + Industrial water demand                          |
| Urban household water supply | 10^4 m³  | Solved by optimal model                                                   |
| Rural household water supply | 10^4 m³  | Solved by optimal model                                                   |
| Water supply for socio-economy development | 10^4 m³ | 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     | $10^3 \text{m}^3$ | Solved by optimal model |
| GDP capacity                | $10^8 \text{yuan}$ | 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  | $10^3 \text{m}^3$ | Household water demand $\times$ Household sewage discharge coefficient |
| Household sewage treatment rate | - | 0.75 |
| Household sewage treatment  | $10^3 \text{m}^3$ | Household sewage discharge $\times$ Household sewage treatment rate |
| Industrial sewage discharge coefficient | - | 0.7 |
| Industrial sewage discharge  | $10^3 \text{m}^3$ | Industrial water demand $\times$ Industrial sewage discharge coefficient |
| Industrial sewage treatment rate | - | 0.7 |
| Industrial sewage treatment  | $10^3 \text{m}^3$ | Industrial sewage discharge $\times$ Industrial sewage treatment rate |
| Total sewage treatment      | $10^4 \text{m}^3$ | Household sewage treatment $+$ Industrial sewage treatment |
| Reuse water utilization rate | - | 0.2 |
| Reuse water resources       | $10^3 \text{m}^3$ | Total sewage treatment $\times$ Reuse water utilization rate |
| Number of livestock         | $10^4 \text{number}$ | =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  | $10^4 \text{m}^3$ | See Eq.(1a) |
| Number of poultries         | $10^4 \text{number}$ | =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), (2028,7509), (2029,7561), (2030,7613), (2031,7665), (2032,7717), (2033,7769), (2034,7821), (2035,7873), (2036,7925), (2037,7977), (2038,8029), (2039,8081), (2040,8133)} |
Water quota for poultries L/number/d 1.5

Poultries water demand $10^3$m$^3$ See Eq.(1a)

Livestock water demand $10^4$m$^3$ Big livestock water demand + Poultries water demand

Reference crop demand $10^4$m$^3$ Potential evapotranspiration for crops \times Crop coefficient (See Eq.(5))

Irrigation water demand $10^4$m$^3$ Reference crop demand-effective precipitation for crop

Water demand for food production $10^4$m$^3$ Livestock water demand + Irrigation water demand

Crop yield $10^4$t 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.

| 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, Qingshitan, 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

| Data                                     | Sources                                                                 | Usage                                                                 |
|------------------------------------------|------------------------------------------------------------------------|----------------------------------------------------------------------|
| Population, GDP as well as natural growth rate, livestock numbers | Ching City Statistical Yearbook (2000-2014) | Predict future population including livestock                          |
|                                          | 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 (Precipitation, temperature, relative humidity, sunshine duration) | Weather stations (shown in Fig.5) (http://data.cma.cn) (1958-2013) | Main input ($E_{T0}$) 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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