Identifying the dynamic evolution and feedback process of water resources nexus system considering socioeconomic development, ecological protection, and food security: A practical tool for sustainable water use

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Abstract: The accelerated consumption of water resources caused by the rapid increase of population and urbanization is intensifying the complex interactions across water resources, socioeconomic development, ecological protection, and food security (WSEF), which causes not only the imbalance between water supply & demand but also the vulnerability of both food and ecological systems. Therefore, identifying the dynamic coevolution and feedback process is one of the most crucial ways to achieve the goal of sustainable water use. In this study, we developed an integrated modeling framework to better identify the dynamic interaction and coevolution process of the nexus across WSEF systems in the context of sustainable water uses by coupling system dynamic model (SD) and multi-objective optimization model. The SD model is used to simulate both the dynamic interaction of each agent and the coevolution process of the whole nexus system by positive/negative feedback loops. The multi-objective optimization model is used to quantify the negative feedback loops of the SD model by generating the optimal scheme of different water users. Finally, the model uncertainty considering different weighting factors is analyzed. The framework is applied to the Upper Reaches of Guijiang River Basin, China. Results show that: (i) the rapid economic growth rises the conflict between the water uses for the socioeconomic development and ecological protection, intensifying the ecological awareness and resulting in more water shortages of socio-economy and food agents, which is unable to support such rapid development. (ii) Once the economic growth rate decreases, water resources are able to support economic development with decreased overload index and stable crop yield, which further contributes to water sustainability. (iii) The river ecological agent is the critical factor that affects the robustness of the model. (iv) The equal consideration of each water usage is the most beneficial to sustainable development. These results highlight the importance of water resources management considering the tradeoffs across multiple stakeholders and give a strong reference to policymakers for comprehensive urban planning.

Key words: Sustainable water uses; WSEF nexus system; SD model; optimization model; feedback linkages

1. Introduction

In recent years, the rapid increase of economic development and urbanization is accelerating the consumption of water resources, further contributing to the imbalances and conflicts between water supply and demand (Carpenter et al., 2011; Yaeger et al., 2014; Perrone and Hornberger, 2014). The accelerated consumption of water resources not only influences the natural hydrological cycle and the process of agricultural water demand, affecting the agricultural water uses and eventually giving the vulnerability of food security but also reduces the ecological streamflow, deteriorating the river ecological health and affecting the aquatic biodiversity (Bei et al., 2009; Yang et al., 2019; Tan et al., 2019). The resulting huge pressure on food security, river ecosystem, and socioeconomic development presents the characteristics of universality and complexity, seriously restricting the achievement of regional sustainable development goals (Walter et al., 2012; Liu et al., 2014; Yang et al., 2019). Therefore, detecting the sustainable balance across the different water needs has become one of the hotspots of water resources planning and management communities (Baron et al., 2002; Falkenmark, 2003; Rockstrom et al., 2009; Perrone and Hornberger., 2016; Zhang et al., 2018; Luo and Zuo, 2019). At present, the water resources system is composed of numerous water sectors and is susceptible to the influence of external conditions, intensifying their complex dynamic interactions under external changes (Phillips, 2001; Thomas, 2001; Liu et al., 2007a; Parker et al., 2008; Wagener et al., 2010; Secchi et al., 2011; Yaeger et al., 2014). However, the dynamic interactions are usually characterized by high dimensionality and non-linearity, which challenges the goal of sustainable water uses (Gastélum et al., 2010; Yaeger et al., 2014). Thus, identifying the coevolution process and dynamic interactions across multiple water uses is one of the crucial and effective approaches on how the water resources system performs more sustainably (Sivapalan et al., 2012; Collins et al., 2011; Yaeger et al., 2014; Thompson et al., 2013; Wagener et al., 2010).

The water resources system is composed of spatial subsystems that include multiple water users, which contributes to its hierarchy and multiplicity. Thus, the systematic analysis approach (SAA) is one of the most effective methods to solve water resources management problems. Although SSA is characterized by its complexity, it has been carried out by many scholars (Faridah et al., 2014; Liu et al., 2008; Li et al., 2015; Jia et al., 2015). There are many approaches that are based on SAA, such as optimal algorithms (Abdulbaki et al., 2017), decision support system (Chandramouli and Deka, 2005), Multi-criteria Decision Analysis (MCDA) (Afify, 2010), etc. Among all the SAAs, the system optimization approach is one of the most practical options to manage complex water resources systems in a nonlinear, integrated, and comprehensive way (Moraes et al., 2010; Singh, 2014; Chen et al., 2017; Li et al., 2019a). It gives insights on how to allocate the water resources on a regional or watershed scale in a balanced way (Li et al., 2015; Liu et al., 2019). The optimization approach is essentially an adaptive system adjustment, or a “complex adaptive system” (CAS) (Holland, 1995), that is susceptible to external conditions. As for the water resources system, external conditions are able to stimulate both the entire system and its agents (i.e., water users) to adjust and strengthen themselves to better adapt to the external changes. However, the system optimization approach usually puts emphasis on how to attain the optimal value of each water user and neglects the dynamic interactions and relations among these users.

The core content of sustainable water resources is to emphasize the value of water resources and the protection of the ecological environment while ensuring socioeconomic development and food security (Gohari et al., 2013). It also stresses the relevance and dynamic interactions of those water uses instead of their individual properties. In this respect, the term "nexus" is emerged to reveal the multiple components and their interlinkages within a system. This term is first conceived by World Economic Forum (2011) to promote and discuss the indivisible relationships between the multiple uses of resources. It provides the universal rights of water, energy, and food, and developed the water-energy-food (WEF) nexus framework (Hoff, 2011; Biggs et al., 2015). The definition of nexus thinking can be classified into two categories (Zhang et al., 2018): First, the nexus is interpreted as the interactions among different subsystems (or sectors) within the nexus system. Second, it is presented as an analytical approach to quantify the links between the nexus nodes. The feedback mechanism not only includes the inner features of the coupled system by capturing the interactions between different sectors but also the external forces or actors that drive nexus system dynamics. However, nexus thinking includes but is not limited to WEF (Duan et al., 2019), such as water-energy-food-environment nexus (Hellegers et al., 2008), energy-water-environment (EWE) nexus (Shahzad et al., 2017), water-power-environment (WPE) nexus (Feng et al., 2016, 2019), etc. In addition, the components of the water resources system also include the interaction between the natural hydrological cycle and human society, which can be regarded as a human-natural nexus system and is usually assessed on a watershed scale (Liu et al., 2007b). Although those nexus systems are made of different components, their common feature is that the coevolution and feedback process of such components are considered in a dynamic and integrated way.

Recently, many new technical methods based on nexus systems have emerged to deal with the problem of performances and interactions of a complex system in a more advanced and comprehensive way. Nair et al., (2014) stressed the energy uses in an urban water system are from both water supply and wastewater, and suggested that life cycle analysis (LCA) is one of the most widely used approaches in the water-energy nexus. LCA is addressed based on the different stages of the evolution of the whole system and its components. Apart from LCA, Ecological network analysis (ENA) is another systematic method that can provide a consolidated analysis for both direct and indirect flows reflected in complicated chains of production and consumption, indicating the potential to investigate the trade-off between multiple elements (Chen and Chen, 2016). System dynamic (SD), that based on the computer simulation method, is one of the most visualized approaches for analyzing information feedback systems (Forrester et al., 1971). It can link different elements for analyzing the dynamic simulation under different external conditions. Its ability to dynamically simulate the system characterized by non-linearity, multiple feedbacks, and complexity makes it popular among many scholars (Venkatesan et al., 2011; Li et al., 2018; Yang et al., 2019). Although those advanced systematic methods made decent contributions on simulating and characterizing a real system, there are still some shortcomings and limitations in applying to comprehensive water resources management including (1) those methods are used to simulate the dynamic status and feedbacks in an objective way but no optimal function inherently, which limits the goal of sustainable water uses to some extent; (2) optimization algorithms are commonly addressed on water resources planning and allocation facing multiple water users, but rarely evaluated in a dynamic way taking in account other interactions. Therefore, coupling systematic methods of both SD and optimization approaches can integrate their advantages and further achieve the goal of accurate coordination among different water users of the nexus system.

To achieve the abovementioned goal, the objectives of this study are, (1) to develop a nexus system that couples the water uses across the socioeconomic development, ecological protection, and food security (WSEF) and explore its dynamic interaction and feedback loops under external changes by using system dynamic model, (2) to identify their dynamic evolution and feedback process in a perspective of sustainable water use by coupling the system dynamic (SD) model and optimization model and (3) identify the model uncertainty to assess the various tradeoffs to stakeholders and recognize the main factor(s) that most influences the model robustness to improve the reliability of the integrated framework.

2. Methodology

2.1 Outlines of the integrated modeling framework

Nexus thinking is one of the crucial methods to deal with complex systems and their dynamic interactions. Sustainable uses of water resources (i.e., **Water**) are composed of that for socioeconomic development (i.e., **Socioeconomic**), ecological protection (i.e., **Ecology**), and food security (i.e., **Food)** and their interactions (Hunt et al., 2018; Uen et al., 2018; Perrone and Hornberger., 2016; Feng et al., 2019), which is investigated as WSEF nexus system. The external changes that affect the performances and interactions of WSEF nexus systems can be addressed by the “pendulum model” outlined by Kandasamy et al. (2014). He stressed that the term "pendulum swing" refers to the shift in the balance of water utilization between economic development and environmental protection. It has periodic changes that can be classified into several stages in a relatively long-term period. In short, it can be classified into the "initial" stage that productivity is about to emerge, "developing" stage that production activities are negatively affecting the environment, and "environmental protection" stage to which environmental issue is paid great attention. The detailed description of the "pendulum model" can be found in **Supplementary material S1**.

The external changes, which are quantified by the abovementioned “pendulum model”, are one of the main sources that affect the status of the entire WSEF nexus system. It not only influences the system’s dynamic status but also starts the self-adjust process of both the whole system and its components to attain the adaptive status. The system dynamic (SD) model is a powerful tool to simulate the dynamic interaction of the water resources system and its components. The self-adjust process in this model can be outlined by the theory of complex adaptive system (CAS) that is first addressed by Holland (1995). He stressed that CAS is developed based on the system theory, indicating that each agent has its learning ability and stress mechanism to the external changes, and then becomes a stronger agent through such self-adjust process, to adapt to the change of external environment. The self-adjust process of each agent is substantially the optimal process, and the system optimization approach is thereby the effective tool that can quantify such self-adjust process of each agent

The overall research framework that couples SD and optimization model of the WSEF nexus system is shown in **Fig.1** and the detailed model description is provided in the following sections. First, the external drivers of the whole nexus system are the changes in the development level of the socio-economy that can be separated into several time steps (here we use "τ" to nominate). Both the initial ecological streamflow and the initial water supply scheme, along with their interactions can be simulated by the SD model under each τ. Next, the initial scheme is acted as the input of the optimization model (Li et al., 2018). SD model includes positive and negative feedback loops and the optimization model is used to quantify the negative feedback loop of SD. The optimization result is generated by iteration of the optimal algorithm with the initial value. The iteration process will not be terminated until the adjacent iteration result is within the specific error. Then, the optimization result will transfer back to update the system status of the current τ, and start a new simulation with the next τ. If τ=T, end the whole process, otherwise, repeat this process. Here T is the total length of simulation time. Finally, the dynamic process of the WSEF nexus system can be embodied by the trajectories of system variables connecting each τ, including water supply/demand, carrying capacity, ecological flow, crop yield, etc.

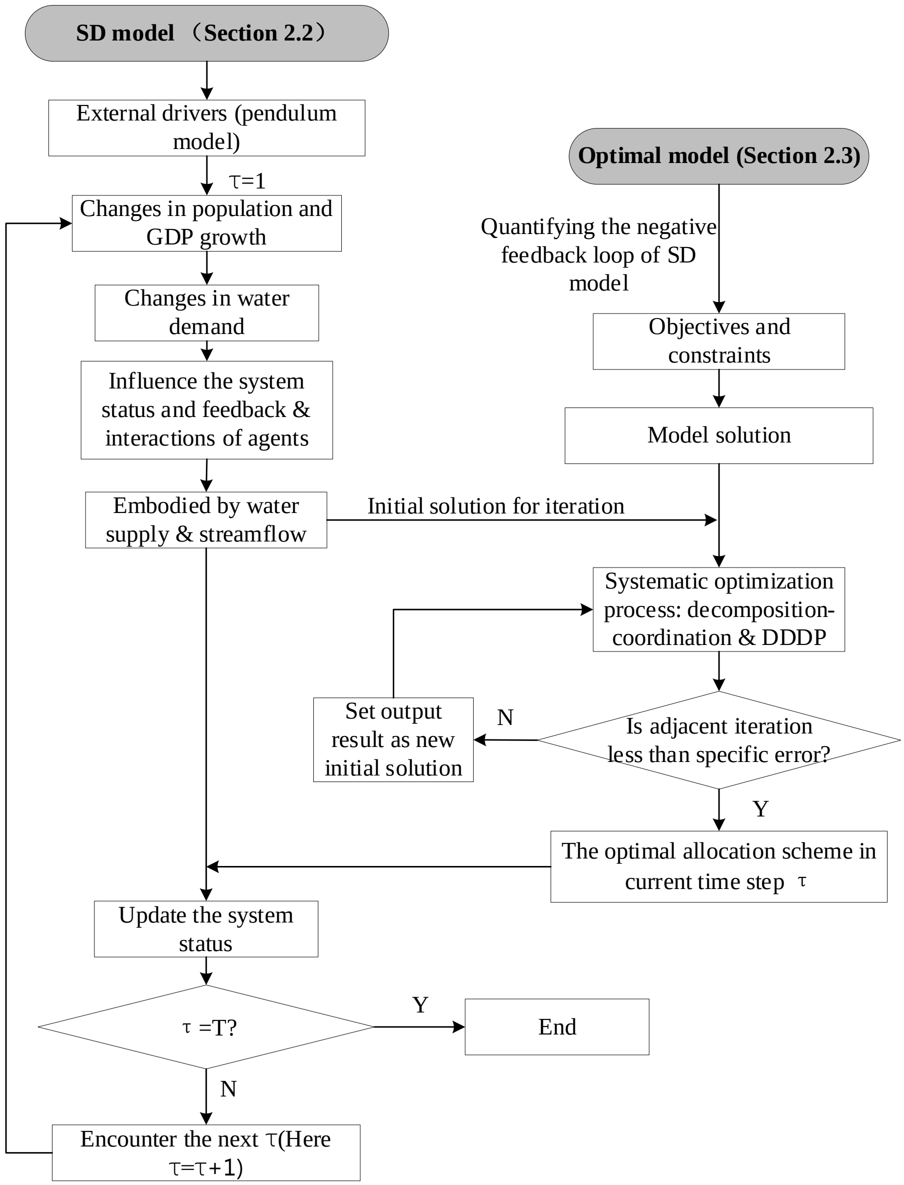


Fig.1 Overall research framework of the integrated modeling approach

2.2 WSEF nexus system developed by SD model

WSEF nexus system includes water resources, socioeconomic development, ecological protection, and food security agents, with water resources supplying water for the other three agents. In addition, these three agents are greatly affected by water usage. Therefore, the dynamic interactions of such three agents are discussed.

2.2.1 Socioeconomic agent

The socioeconomic agent describes the regional population rate, urbanization rate, and GDP products. Their dynamic changing process in water recipient regions can be described within the logistic model, which can be expressed by the following differential equations (Jørgensen and Bendoricchio, 2001; Feng et al., 2019):

$$\frac{dN}{dt} = rN, \frac{dI}{dt} = rI \tag{1}$$

where N and I are population size and the total amount of GDP, r is the natural growth rate of GDP or population. The natural growth rate can be assessed by collecting and analyzing the statistical data of the urban population, rural population, and the total amount of GDP (including primary, secondary, and tertiary industry). The water demand of socioeconomic agents can be outlined by the following equation:

$$WD_{dom} = \frac{q_{dom} \times N \times d}{1000} \tag{2}$$

$$WD_{indus} = I_{GDP} \times q_{indus} \tag{3}$$

where WD_{dom} and WD_{indus} are the annual domestic (including urban and rural) and industrial (including secondary and tertiary) water demand (m^3), q_{dom} 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 10^4 Yuan ($m^3/10^4$ Yuan), respectively. It should be also noted that the economy also includes the agricultural economy. For the agricultural economy, the economic basis of farmer's response is reflected by average incomes that can be expressed by the following:

$$I = \frac{1000\sum_{i=1}^{n} Y_i p_i}{N_r} \tag{4}$$

where I is the farmer's average income, Y_i is the ith crop yield, N_r is the rural population. Crop yield is a significant component of both primary industry values and can measure farmers' income because farmers sell these foods to customers and get profits. The calculation of crop yield is shown in Section 2.2.3. The system dynamic model of the Socioeconomic agent is presented in Fig.2. The external changes outlined by the pendulum model are exactly embodied by the changing rate of population and GDP expressed by Eq.(1). In the scope of SD, the dynamic process of population growth can be expressed as follow:

$$population(\tau) = population(\tau - d\tau) + (net\ population\ growth) \times d\tau \tag{5}$$

The dynamic growth of the three industries is similar to Eq.(5). From Fig.2 we can see that the changing population and GDP (i.e., the external drivers), will result in the changing water demand, which further affects the water supply and eventually the status of the entire nexus system (See 2.2.4).

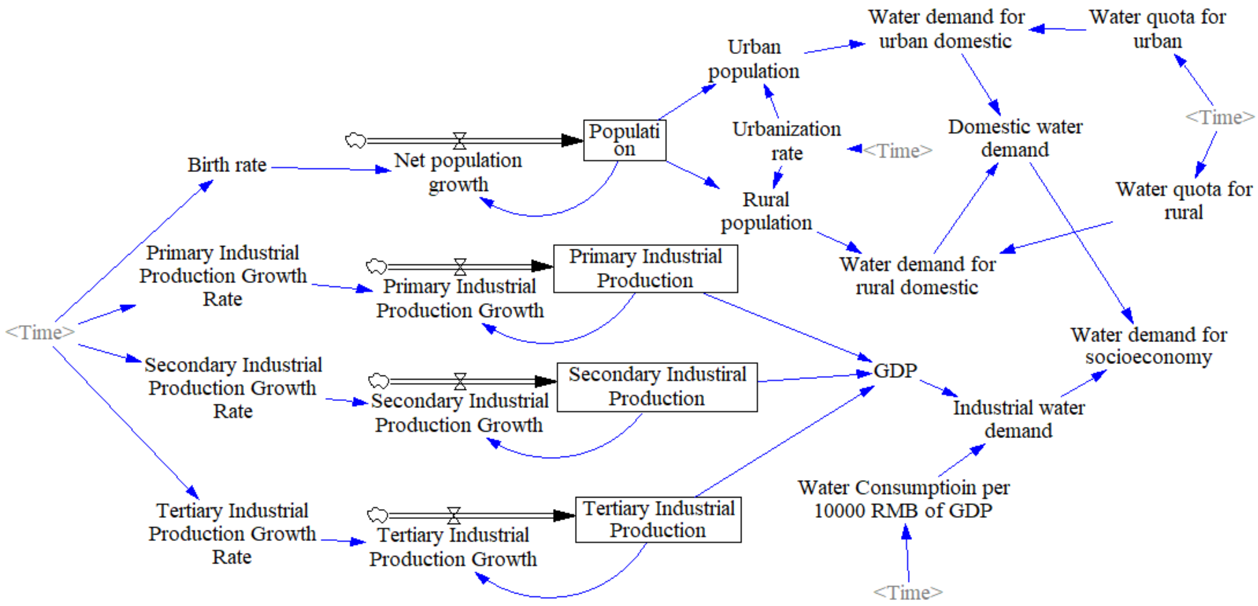


Fig.2 The inner stimulus and feedbacks of socioeconomic agent

2.2.2 Ecological agent

Ecological water demand includes vegetation and river streamflow. The ecological water demand of vegetation is used to maintain the physiological function of canopies. 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):

$$WD_{veg} = K_s \cdot K_c \cdot ET_0 - P_e \tag{6a}$$

$$ET_0 = \frac{0.408\Delta\left(H_{net} - G\right) + \gamma \frac{900}{T+273} u_2 \left(e_0 - e_z\right)}{\Delta + \gamma\left(1 + 0.34u_2\right)} \tag{6b}$$

$$K_s = \frac{\ln\left[100 \times \frac{S - S_w}{S_c - S_w} + 1\right]}{\ln 101} \tag{6c}$$

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.

For river streamflow, the Tennant method is adopted in this study:

$$W_{eco} = 86400 \times \sum_{m=1}^{12} d_m Q_m P_m \tag{7}$$

where W_{eco} is the ecological streamflow in the annual average level (m^3), d_m is the day number of month m, Q_m is the observed streamflow (m^3/s). P_m is the percentage of observed streamflow of the month m. It should be noted that the river streamflow calculated by Eq.(7) is just the initial value with given P_m's, and it will be input to the optimization model for an optimized solution.

2.2.3 Food agent

The food agent is mostly related to agricultural water usage, including crop water requirements based on phenological stages. It is also the fundamental condition of primary industry and farmer's income (See 2.1.1). For crop production, water usage is directly related to crop yield becoming a crucial part of food security. The main water supply is provided by precipitation and 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):

$$W_p = \int_{t_0}^{t_n} K_c(t) \cdot ET_0 dt \tag{8a}$$

$$W_a = W_p - P_e \tag{8b}$$

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):

$$\frac{Y_s}{Y_p} = \prod_{t=t_0}^{t_n} \frac{Y_{s,t}}{Y_{p,t}} = \prod_{t=t_0}^{t_n} \left[1 - K_{y,t} \left(1 - \frac{W_{s,t} + P_{e,t}}{W_{p,t}} \right) \right] \tag{9}$$

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 resource conditions, crop water supply is usually equal to or less than crop water demand. That is, $(W_s+P_e) \leqslant W_p$, 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.

It should be noted that the agricultural and vegetation water demand in the future will be hard to predict because these demands are related to meteorological and land-use variables, that will require long-time global scenario analysis. Fortunately, the statistical characteristics of regional weather data are usually assumed to be consistent on a multiyear scale (Feng et al., 2019). That is, the characteristics of the future precipitation can be captured by multiannual historical data. Therefore, the average level of water demand of historical multi-year is proposed in this study because historical data can represent the hydrological conditions of a certain area.

2.2.4 Overall simulation of SD and system status update

The overall simulation of the SD model is to reveal the dynamic interactions influenced by dynamic external drivers and the update process. The dynamic interactions are embodied by the positive/negative feedback linkages/loops among different agents (includes their water supply and demand). The update process of the SD model is reflected by some relevant variables that are greatly affected by the water supply of different agents. The relevant variables include water shortage (aiming at all agents), carrying capacity & overload index & farmer's income (socioeconomic agent), the deviation between ecological and observed streamflow (ecological agent), and crop yield (food agent). These variables are shown in the boxes in Fig.3.

2.2.4.1 Dynamic interactions revealed by positive/negative feedback loop

Fig.3 outlines the overall simulation process of the SD model, including the interaction between each agent of the SD model and how the initial water supply and other variables are simulated. The symbol "+" and "-" besides the arrows represents the positive/negative feedback linkage, respectively. The words in grey represent the shadow variables. The feedback linkages among socioeconomic and ecological agent under external drivers are revealed as follows (the arrows in the bracket indicates "increase" and "decrease"):

- Population (↑) → Domestic water demand (↑) → Domestic water supply (↑) → Ecological streamflow (↓)
- GDP (↑) → Industrial water demand (↑) → Industrial water supply (↑) → Ecological streamflow (↓)
- Domestic/Industrial water supply (↑) → Carrying Capacity (↑) → Population/GDP (↑)

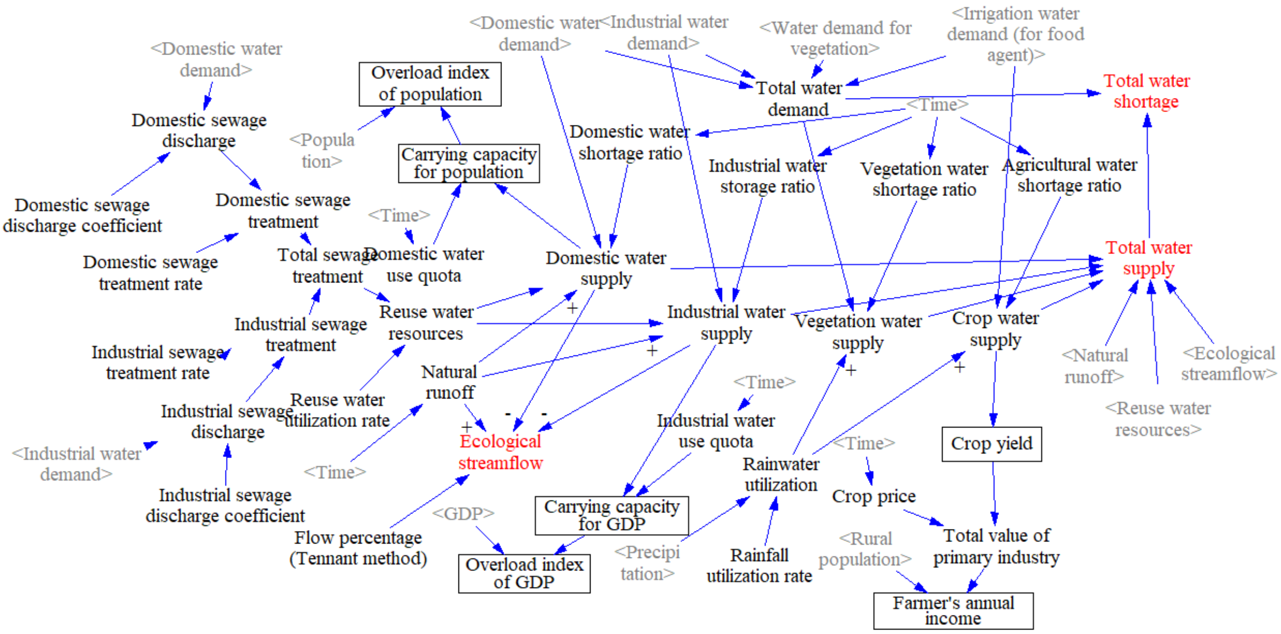


Fig.3 Total simulation and update process of SD model

Here "carrying capacity" quantifies the population/GDP that can be supported by a certain amount of water resources. The overload index is given by dividing predicted population/GDP by carried population/GDP. The higher value of the overload index, the more serious degree of overload. The feedback linkages also occur in other agents. For example, socioeconomic agent affects food agent and finally transfers back to socioeconomic itself:

- Precipitation (↑) → Crop/vegetation water supply (↑ → Crop yield (↑)
- Population (↑) → Food demand (↑) → Crop water supply (↑) → Crop yield (↑)
- Crop yield (↑) → Crop carrying capacity (↑) → Population (↑)
- Crop yield (↑) → Primary industrial production (↑) → Farmer's income (↑) → GDP (↑)

Here "crop carrying capacity" quantifies the population size that can be supported by a certain amount of crop yield. Those feedback linkages can be expressed by the causal loop diagram (Fig.4). The symbol "+" and "-" beside the arrow is the positive/negative feedback linkage, respectively. The clockwise arrow with a "+" inside is a positive feedback loop, while the counterclockwise arrow with a "-" inside is a negative feedback loop.

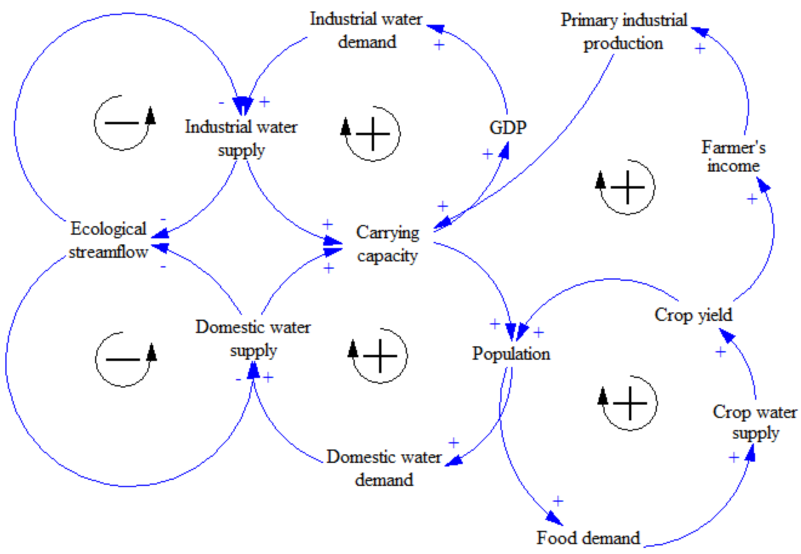


Fig.4 Causal loop diagram

Adequate water supply is one of the most important conditions to ensure socioeconomic development and is also a prerequisite for crop yield. Therefore, in socioeconomic agent, policymakers expect to decrease the water shortage by increasing water supply to ensure socioeconomic development, since increased population/GDP is accompanied by increased water demand (Li et al., 2019b). Then, the increasing water supply leads to the increased carrying capacity, and the population/GDP will increase again. Such linkage can be regarded as a positive feedback loop. Similarly, in food agent, increased population intensifies crop demand, and more water supply is needed to increase the crop yield, which can eventually support more population size. This linkage can also be regarded as a positive feedback loop. Adequate water supply can be embodied by the following equation by minimizing the water shortage ratio:

$$WS_j = WD_j \times \left(1 - WSR_j\right) \tag{10}$$

where WS_j, WD_j, and WSR_j are water supply, water demand, and water shortage ratio for jth sector, respectively. Here j is each component of the WSEF nexus system. Crop and vegetation water supply also include effective precipitation (P_e).

It should be noted that the water supply expressed by Eq.(10) is just the expected value for policymakers. However, water for socioeconomic development and river ecological health always conflict with each other as both of them consume natural runoff. In the scope of SD, it is embodied by the negative feedback loop. That is, the increased (domestic and industrial) water supply will contribute to decreased river streamflow that deteriorates ecological health (Yin et al., 2010; 2011; Yu et al., 2017), and vice versa. To consider this issue, a certain percentage of streamflow (usually for ensuring basic flow) are the rigid constraint for the ecological agent, and the water supply considering ecological basic flow is expressed as follow:

$$WS = \min(\sum_{j=1}^{J} WS_j, R + W_{reuse} - W_{eco}) \quad (11)$$

where R and W_{reuse} are the natural runoff and reused water (includes rainfall utilization and recycled). The water supply presented in Eq.(11) is the initial water supply simulated by SD.

2.2.4.2 Update process of the SD model

Considering the certain percentage of streamflow is still not enough for considering each aspect of water use, because if the adequate water supply is ready for ensuring socioeconomic development and crop yield, the ecological streamflow will be decreased. Even the ecological basic flow is ensured, the ecological function of a river will be limited. Therefore, the optimization model is presented in this study to reveal the negative feedback loop and then achieve the sustainable water uses of each agent (see next section) by inputting the initial simulated result of SD and iteration (Li et al., 2018). The simulated result is calculated by Eq.(11). Finally, the optimal scheme of water supply and ecological streamflow is transferred back to the SD model to update the status of the current time step (as shown in **Fig.1**). The update process of the SD model refers to the variables listed in Table 1. Then all the dynamic changes of each variable can be assessed. Other variables and equations can be seen in **Supplementary materials S2**.

Table 1 Main equations for model update

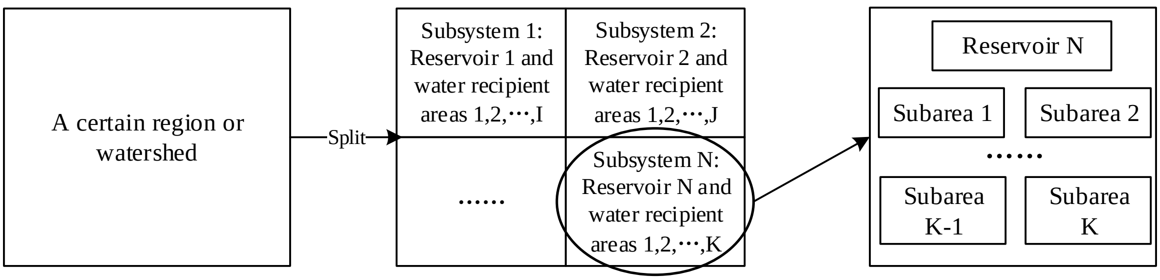
Variables	Units	Mathematics	Remarks
Water supply for each sector	$10^8 m^3$	Corresponding water demand × (1 – corresponding water shortage ratio)	This is valid for each sector. For example, if calculating domestic water supply, just multiply domestic water demand with the domestic water supply coefficient. Others are the same.
Total water supply	$10^8 m^3$	min (Water storage + reuse water resources – ecological streamflow, sum (Domestic water supply, Industrial water supply, Agricultural water supply, Vegetation water supply))	See Eq. (11)
Ecological streamflow	$10^8 m^3$	Water storage × Flow percentage	Tennant method, see Eq.(7). The initial percentage is set as 0.2 (Oct~Mar) and 0.4 (Apr~Sep) to consider the basic streamflow
Carrying capacity: population	people	Domestic water supply × 1000/(water quota for domestic × day of a certain year)	The unit of water quota for domestic is L/people/d. Both urban and rural are calculated like this.
Carrying capacity: GDP	10^8 yuan	(Industrial water supply + tertiary water supply) / Water consumption per 10000RMB of non-agricultural industry + Total value of primary industry	

Crop yield	10^4t	Crop yield is the nonlinear function of crop water supply and demand, see Eq.(9)	
Overload index		Predicted economic index/ Carrying capacity	Valid for both population and GDP
Total value of primary industry	10^8yuan	Crop yield × crop price per unit	
Farmer's annual income	10^4 yuan	Total value of primary industry/rural population	Eq.(4)

2.3 Optimization approach of the WSEF nexus system

2.3.1 Model conceptualization

In a water system inside a watershed or a region, there are multiple water supply projects to different water users. This system in a watershed is called a "large water resources system" (**Fig.5**a). It is subdivided into multiple sub-watershed or subregions that are called "subsystems" (**Fig.5**b). In this case, reservoirs can provide not only socio-economic developments but also environmental impacts. They are constructed across the rivers for both water supply of the whole region or watershed and adjust the downstream river streamflow, which should be considered individually to target the river ecology concerns.



(a) A large water resources system (b) Large system separated into subsystem based on reservoirs (c) Components of each subsystem

Fig.5 Water resources system and its decomposition

The whole system is separated into subsystems that contain one individual reservoir and several corresponding water recipient areas (**Fig.5**b) as there is usually more than one reservoir in a certain region. We call these subsystems "reservoir supply subsystems". Such a subsystem can be further separated into the smallest unit: a reservoir and each water recipient region (or called "subarea") (**Fig.5**c). In this view, the total system of the water resources in a certain region (watershed) can be divided into several subsystems or subareas that consist of a three-level hierarchical structure.

It should be noted that the term "large water resources system" is not the same thing as the framework of the WSEF nexus system presented in this study. To combine these two terms, each agent of the WSEF nexus system can be distributed to each subarea (with the objective of food, socio-economy, and vegetation) and reservoir (river ecology) (see **Fig.6**). Therefore, we can coordinate these objectives to achieve sustainable development by setting up a multi-objective optimization model.

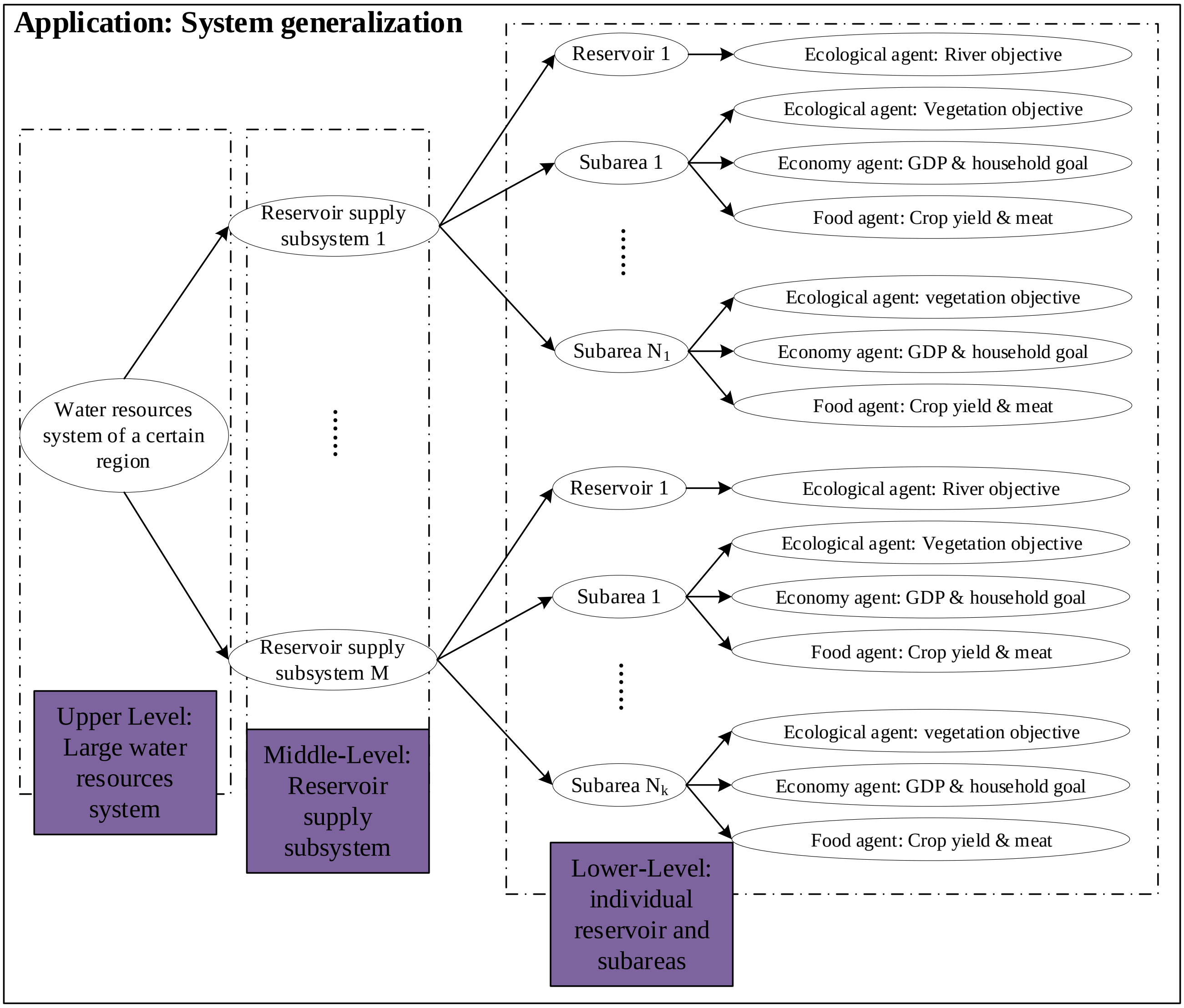


Fig.6 Large water resources system considering the WSEF nexus

2.3.2 Objective function

(1) Socioeconomic development agent

The objective of the socioeconomic agent is expressed by the minimum water shortage rate:

$$F_{socemy} = \frac{1}{T}\min\sum_{k=1}^{K}\sum_{t=1}^{T}\left(\frac{WD_{socemy,kt} - WS_{socemy,kt}}{WD_{socemy,kt}}\right)^2 \tag{12}$$

where F_{socemy} is the objective function of the socioeconomic agent. WD and WS are the total water demand and supply (including reservoir and other water projects) of this agent. T is the time length of the reservoir operation horizon. Subscript k and t are the number of subarea and time steps, respectively. It should be noted that the farmer's income affiliated with the socioeconomic agent is greatly related to crop yield. Thus, this goal will be discussed in food agent.

(2) Ecological protection agent

Ecological protection comprises two aspects: river ecology and vegetation ecology. For river ecology, the artificial intervention in the natural flow regime is a crucial factor in the severe deterioration of river ecosystems (Shiau et al., 2013; Tan et al., 2019). It has been proved that the term "amended annual proportional flow deviation" (AAPFD) is used to embody the river's health degree and used in many studies in terms of river ecology and assumed that the minimum deviation between observed (natural) and actual streamflow contributes to the healthy status of river ecological health (Gehrke et al., 1995; Ladson and White, 1999; Liu et al., 2019; Feng et al., 2019). The objective function can be expressed as follow:

$$F_{riv} = \min \frac{AAPFD}{5} = \min \frac{1}{5n} \sum_{j=1}^{n} \sqrt{\sum_{m}^{12} \left(\frac{W_{eco,mj} - QN_{mj}}{\overline{QN_j}} \right)^2} \tag{13a}$$

where the subscript "riv" represents river ecology, QN is the observed streamflow. The variable AAPFD ranges from zero to five and the minimum value represents the best status of the river's ecological health (Gehrke et al., 1995; Ladson and White, 1999; Yin et al., 2010). Thus, we divided it by five to normalize the objective function and make it range from zero to one. The subscript n, m, and j are the total year number, mth month, and jth year.

Vegetation, similar to the river environment, is also an indispensable part of ecology because it produces oxygen to improve air pollutions and purifies water bodies. The abundant water supply contributes to these goals. Therefore, the objection of vegetation is expressed as follow:

$$F_{veg} = \frac{1}{T} \min \sum_{k=1}^{K} \sum_{t=1}^{T} \left(\frac{WD_{veg,kt} - WS_{veg,kt}}{WD_{veg,kt}} \right)^2 \tag{13b}$$

where the subscript “veg” represents vegetation ecology.

The objective of the ecological agent is reflected by maintaining both aspects, reflected by the following normalized form (from zero to one):

$$F_{eclgy} = \frac{F_{veg} + F_{riv}}{2} \tag{13c}$$

where F_{eclgy} is the total objective function of the ecological agent.

(3) Food agent

The goal of the food agent is to maximize crop yield and is the indispensable condition of increase primary industry products and farmer's income. Also, food is the most fundamental prerequisite for people's survival and farmer’s income. The mathematical expression is presented as follow:

$$F_{food} = \max \sum_{n=1}^{N} \left(\frac{Y_a}{Y_p} \right)_n \tag{14a}$$

where N and L are the total number of crops and livestock, respectively. Y_a and Y_p are the crop yield under the actual and ideal conditions, respectively.

The calculation of crop yield is based on the Food and Agricultural Organization report No. 56 (FAO-56) (Allen et al., 1998). According to the crop yield equation based on FAO-56 (see Eq.(9)), crop yield that determines the farmer's profit is directly related to irrigation water (FAO, 2012; Liu et al., 2002; Lyu et al., 2020). Therefore, the maximum supply of crops (includes both precipitation and artificial water supply for crops) is the most critical condition for maximum crop yield. Thus, the normalized objective of the food agent can be rewritten as:

$$F_{food} = \frac{1}{T}\min\sum_{k=1}^{K}\sum_{t=1}^{T}\left(\frac{WD_{food,kt} - WS_{food,kt}}{WD_{food,kt}}\right)^2 \tag{14c}$$

2.3.3 Tradeoffs between objectives

As can be seen in objective functions, three benefits are set minimum (Eqs. (12)(13c)(14c)), which may contribute to the conflict between objectives. The tradeoffs across WSEF nexus can be reflected by Pareto frontier that can describe a set of non-dominated optimal solutions that any one of these three objectives are unable to be improved unless sacrificing other objectives (Reddy and Kumar, 2007; Feng et al., 2019; Beh et al., 2015; Burke and Kendall., 2014). We can reclassify all the water users from each of the three agents into two categories: Instream and off-stream water users (Hong et al., 2016). River ecological water demand can be regarded as an instream water user, and all others can be considered as off-stream water users. Therefore, according to the objective function expressed by Eqs. (12), (13c), and (14c)), the weighted objective function can be rewritten by:

$$\begin{aligned}\min F &= F_{socemy} + F_{eclgy} + F_{food} = \alpha\left(F_{socemy} + F_{veg} + F_{food}\right) + \theta F_{riv} \\ &= \sum_{j=1}^{J}\sum_{k=1}^{K}\sum_{t=1}^{T}\alpha_j\left(\frac{WD_{jkt} - WS_{jkt}}{WD_{jkt}}\right)^2 + \theta\frac{1}{5n}\sum_{j=1}^{n}\sqrt{\sum_{m}^{12}\left(\frac{Q_{mj} - QN_{mj}}{\overline{QN}_j}\right)^2}\end{aligned} \tag{15}$$

where (F_{socemy}+F_{veg}+F_{food}) is off-stream water users, and F_{riv} is the instream water user. The subscript j is the index of the off-stream water users, respectively. j=1,2,3 represents socio-economic, food, and vegetation water usage, which corresponds to the subscript "socemy", "eclgy" and "food". α and θ are weight factors and $\sum_{j=1}^{J}\alpha_j + \theta = 1$. Previous literature demonstrated the optimal solution shaped like Eq.(15) is Pareto-optimal because of the positive weights and concave objectives, and the non-dominated sorting process is used to find the optimal solution of Eq.(15) because the characteristic of either concave or convex is difficult to be proven (Marler and Arora., 2009; Feng et al., 2019; Goicoechea et al., 1982; Zadeh, 1963). For each given combination set of α and θ, the optimal solution can be attained by decomposition-coordination (DC) principle and discrete differential dynamic programming (DDDP) (see section 2.3.5).

The tradeoff across objectives is reflected in the values of multiple sets of weighting factors $\boldsymbol{r} = \left(\alpha_1, \alpha_2, \alpha_3, \theta\right)^T$, revealing different decision-makers' preferences. Considering that the contradictions also occur in off-stream water users, the balanced priority should be addressed to consider each off-stream water user (Casadei et al., 2016), that is, $\alpha_1=\alpha_2=\alpha_3$. Therefore, the tradeoff and decision preference between instream and off-stream is reflected by the different values of θ (0≤θ≤1). The larger value of θ represents more concerns about river ecology. In this study, the parameter θ is initially set as 0.5 to give an equal consideration of both instream and off-stream water usage. It should be noted that this weight combination is one possible set that considers the equal use of instream and off-stream water uses, and different weight of weighting factor reveals the preferences of stakeholders. Different vectors of ***r*** can affect the performance of the WSEF nexus and are used to assess the uncertainty and robustness of the model to improve its reliability (see Section 5.2 & 5.3).

2.3.4 Constraints

The model constraints include the connection of subsystems, the water balance equation, and the upper and lower limits. The details are found in **Supplementary material S3**.

2.3.5 Overall model solution

The WSEF nexus system of water resources sustainability is a compound system that is classified into multiple hierarchical structures (**Fig.6**). Therefore, the model solution of this structure should be solved by systematical analysis techniques. In this study, we use the decomposition-coordination (DC) method to solve this model. The core procedure of this method comprises two parts: first, the large system is decomposed by several subsystems (i.e., reservoir and recipients) using Lagrange function considering the interrelations between subsystems, and its coordination process is performed by coordination variables; second, the optimization process using DDDP method of each subsystem. The monthly historical streamflow observations with the length of decades are the important model input for DDDP method (i.e., subscript t in the variables of the entire optimization model), assuming that the characteristics of future streamflow are captured by the historical data (Feng et al., 2019). The detailed descriptions are found in **Supplementary material S4**. The entire procedure for the overall framework of the model is outlined below:

Step1: Initialize the parameters, including initial reservoir storage, water recession coefficient, the total amount of water resources of the recipient area, etc.

Step2: For each reservoir supply system, calculate the initial water supply of each subarea and reservoir streamflow at $\tau=1$ (set as S_0). These variables can be simulated by the SD model (see 2.2.4 and Table 1).

Step3: Using the DDDP algorithm to optimize each subsystem decomposed by the Lagrange function with coordinate variables. The expression of coordinate variables is the function of the initial scheme, which is shown in **Supplementary material S4**. To use DDDP, the width of the corridor is given (set as ΔI), and the traditional DP is optimized within ΔI. Mark the result generated by DP (include both water supply and river streamflow) as S1. If $|S_1-S_0|<\varepsilon$, go to the next step, otherwise repeat this step.

Step4: Narrow the width of the corridor and continue the DP process, and set Si as the optimal result, where i is the iteration number. If $|S_i-S_{i-1}|<\varepsilon$, go to the next step, otherwise repeat this step.

Step5: Update the coordinate variables and compare them with the initial coordinate variables. If the error is within ε, the optimal solution (i.e., water supply and streamflow) will be generated, otherwise, repeat step3~5.

Step6: Optimize the next reservoir supply subsystem by repeating step2~5, and the summary of each subsystem is the global optimal solution.

Step7: The optimal result in Step6 is under $\tau=1$, and prepare to encounter the next time step ($\tau=2$) of external drivers by repeating overall procedures until $\tau=T$.

2.4 Sustainable development degree (SDD) assessment

The evaluation index system is used in this study as the WSEF nexus system includes different agents, and each agent includes several variables. The water resources agent is used to supply water for other agents and other agents are the key factor to influence the sustainable development degree. Therefore, we selected the indicators listed in **Table 2** based on the three agents and are used to evaluate the impact of sustainable development.

Table 2 Sustainable development evaluation index system of three agents

Agent	Indicators	Property
	Overload index of population	-
Socioeconomy	Overload index of GDP	-
	Per capita GDP (RMB/people)	+

	Water consumption per 10000RMB of GDP ($m^3/10^4$RMB)	-
	Farmer's income (RMB/people)	+
Food (Agriculture)	Crop yield (t)	+
	Effective irrigation area for crops (km^2)	+
Ecology	Effective irrigation area for vegetation (km^2)	+
	AAPFD	-

The property (+, -) of indicators denotes positive and negative indicators, respectively. The positive/negative indicators mean they have positive (negative) impacts on the corresponding agent and were termed as a development/constraint index (Yang et al., 2019). Considering the ranges of indicators listed in **Table 2** are different, they should be normalized before evaluation. The positive and negative indicators normalization is shown by Eq.(16a) and (16b).

$$y_{ij} = \frac{x_{ij} - \min_{i=1}^{m} x_{ij}}{\max_{i=1}^{m} x_{ij} - \min_{i=1}^{m} x_{ij}} \tag{16a}$$

$$y_{ij} = \frac{\max_{i=1}^{m} x_{ij} - x_{ij}}{\max_{i=1}^{m} x_{ij} - \min_{i=1}^{m} x_{ij}} \tag{16b}$$

where x_{ij} and y_{ij} are the original and normalized indicator j in sample i, and m is the total number of samples. The entropy weight method is then adopted to calculate SDD, which calculates the information entropy of indicators that reflect their relative change degree on the whole WSEF nexus system (Wang et al., 2019). The information entropy of indicator j in sample i is expressed by:

$$E_j = -\frac{1}{\ln m}\sum_{i=1}^{m} d_{ij} \ln d_{ij} \tag{17a}$$

$$d_{ij} = \frac{y_{ij}}{\sum_{i=1}^{m} y_{ij}} \tag{17b}$$

Finally, the entropy weight of each indicator is expressed by:

$$\omega_j = \frac{1 - E_j}{\sum_{j=1}^{n}\left(1 - E_j\right)} \tag{18}$$

where n is the total number of indicators in a certain agent.

The SDD is calculated based on the coupling coordination degree (Sun and Cui, 2018), reflecting the degree of coordination of various factors or subsystems. In this study, SDD is calculated based on the coordination of three agents and expressed by:

$$SDD = \sqrt{C_1 C_2} \tag{19a}$$

$$C_1 = \left[\frac{SOCEMY(t) \cdot ECLGY(t) \cdot FOOD(t)}{\left(SOCEMY(t) + ECLGY(t) + FOOD(t)\right)^3} \right]^{\frac{1}{3}}$$

$$= \left[\frac{\sum_{p=1}^{P} \omega_{pj} y_{pj} \cdot \sum_{q=1}^{Q} \omega_{qj} y_{qj} \cdot \sum_{r=1}^{R} \omega_{rj} y_{rj}}{\left(\sum_{p=1}^{P} \omega_{pj} y_{pj} + \sum_{q=1}^{Q} \omega_{qj} y_{qj} + \sum_{r=1}^{R} \omega_{rj} y_{rj} \right)^3} \right]^{\frac{1}{3}} \quad (19b)$$

$$C_2 = \frac{1}{3}\left(SOCEMY(t) + ECLGY(t) + FOOD(t)\right)$$

$$= \frac{1}{3}\left(\sum_{p=1}^{P} \omega_{pj} y_{pj} + \sum_{q=1}^{Q} \omega_{qj} y_{qj} + \sum_{r=1}^{R} \omega_{rj} y_{rj} \right) \quad (19c)$$

where SOCEMY(t), ECLGY(t), and FOOD(t) are the coordination degree of socioeconomy, ecology, and food agent, respectively. P, Q, R is the total indicator number in socioeconomy, ecology, and food agent.

3. Study area and data sources

3.1 A brief description of the study area

Guijiang River Basin (GRB) is one of the most important branch basins of the Pearl River Basin (PRB) in South China. PRB belongs to the typical karst area and is the second-largest river basin in China in terms of total runoff and also the third largest river basin in terms of total area. The upper reach of Guijiang River Basin (UGRB) (24°6' ~25°55'N, 110°~111°20'E) is selected as a case study as it represents the highly conflicts between socio-economic growth and ecological protection in karst areas. Furthermore, reservoirs are widely constructed in UGRB to supply water for socio-economy but are likely to deteriorate the river ecological health by alternating natural flow (Yin et al., 2010; 2011). UGRB is also a karst area with a total area of 13,131 km^2, with about three million people. Also, UGRB has a total crop planting area of about 2,400 km^2, a total vegetation area of about 3,700 km^2, and yearly average precipitation of about 1600mm. UGRB is located in Guilin City and refers to eight administrative regions (or counties). Seven reservoirs are constructed in UGRB to provide water resources support for maintaining socioeconomical development. The detailed parameters of seven reservoirs and their three-level hieratical structure, including subareas, are found in **Supplementary material S5**. Guilin city is both a heavy industrial city and a national major tourist city, and the population and economic development is expected to continue rapidly increasing in the near term. It will exacerbate the conflicts between social development, food security, and environmental protection, especially for water use of the river ecological environment, resulting in severe ecological deterioration of the lower Guijiang River basin and even lower XRB. Therefore, how to achieve coordination and sustainable development in UGRB between these aspects is becoming a challenging problem in the upcoming years and is necessary to be solved.

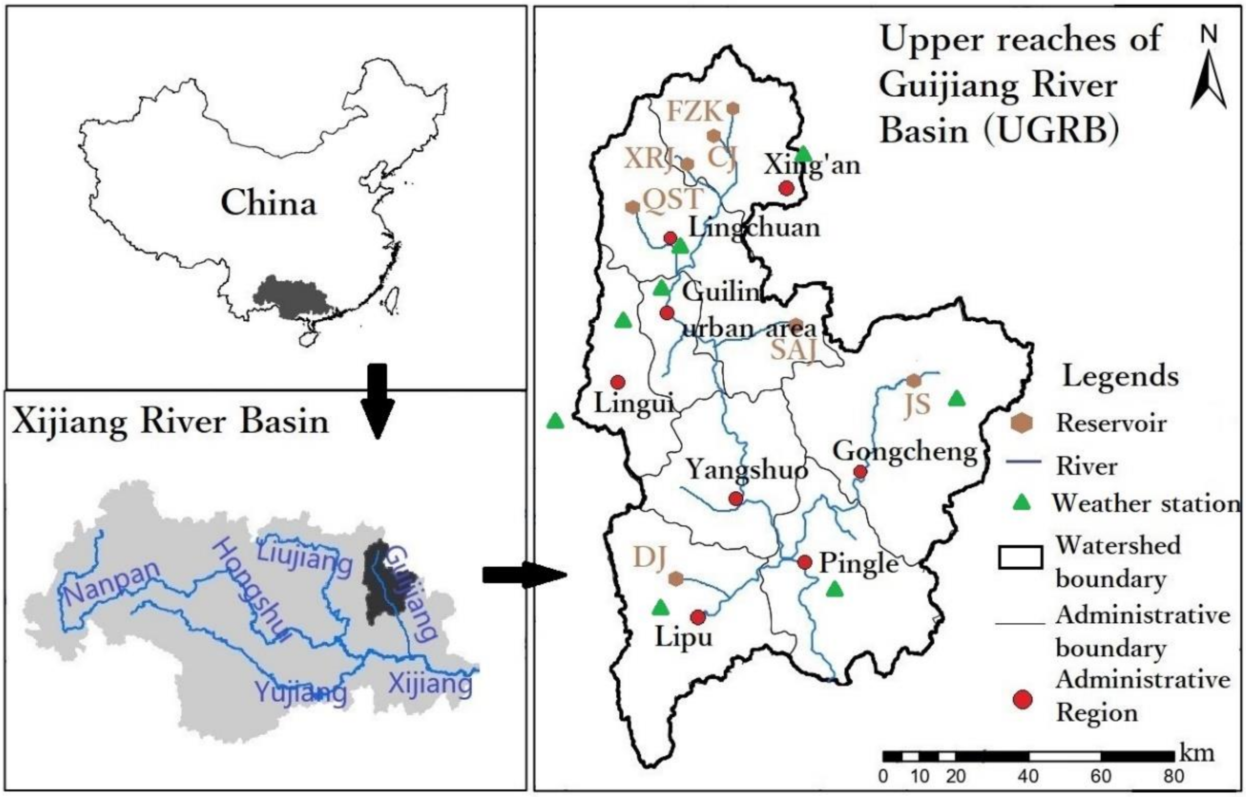


Fig.7 A brief location of UGRB

3.2 Datasets and parameter initialization

Datasets of the case study include socio-economic, water use, land use, meteorological and hydrological data. The major source of socio-economic data, including population and GDP, are the statistical yearbooks of both Guilin City and Guangxi autonomous region from 2005-2019. The Municipal Government of Guilin City (MGGC) predicted population and GDP till 2045, along with per capita water use from the water industry standard of the People's Republic of China, to predict the water demand of socioeconomic agent (Venkatesan et al., 2011). These predicted socioeconomic indexes are exactly the external drivers of the whole integrated modeling framework (see Section 2), and the corresponding growth rate in different stages is shown in **Table 3**. Water use data include historical water usage and total water amount found in the Guilin water resources bulletin (2005~2019). Land use data contain the spatial distribution of crops and vegetations with a resolution of 1km×1km that can be found in the Resource and Environment Data Cloud Platform, China Academy of Sciences (REDCP-CAS). The crops in the study areas are mainly corns, rice, and vegetables, and their crop coefficients are found in FAO-56 (the detailed values are found in **supplementary material S6**). Meteorological data from 1956 to 2013, including daily average wind speed, sunshine duration, maximum and minimum temperature, relative humidity, and precipitation, are found in meteorological stations. The hydrological data from 1958 to 2013, including the monthly inflow of each reservoir, can be found in hydrological stations for the input of the optimal algorithm. All the initialized parameters and the total index of the data sources can be found in **Supplementary material S6**

Table 3 External drivers (i.e. socio-economic changes) of the entire research framework based on pendulum model

Yearly growth rate (%)	Stage 1 (2021~2025)	Stage 2 (2026~2035)	Stage 3 (2036~2045)
Population	1.23	3.41	1.24
Secondary industry	1.99	4.11	2.36
Tertiary industry	3.04	5.33	1.24

4. Results

4.1 Model calibration and validation

Before the model can be simulated, the main parameters in this model should be calibrated and validated. The historical data of socioeconomic and water usage from 2012 to 2016 is used to calibrate the model, while the data from 2017 to 2019 is used to validate the model. Domestic, industrial, and agricultural water use from 2017 to 2019 are calculated by calibrated results and are used to validate the model by comparing them with their observed value. The calibration and validation result are shown in **Supplementary material S7**, and from the validation result, we can see that the relative error of domestic and industrial water uses is around 1%, while that of agricultural water uses is less than 2%, which can reveal the general situation of the current area.

4.2 Coevolution process of WSEF nexus

The coevolution trajectories of population, GDP, water supply & demand, streamflow, and objective function (F_{SOCEMY}, F_{eclgy}, F_{food}, based on Eq.(10)(11)(12)) referring to each component of the WSEF nexus is shown in **Fig.8**. As can be seen in **Fig.8**, the coevolution process of all the items depicts the characteristics of different stages. Then, the (quasi-)stable state is converged, i.e., the variations of each variable are small or close to zero. It happens because the rate of external changes in the last stage (i.e., economic indexes) is much lower than in the previous stage, which decreases the internal changes (i.e., Streamflow water and three objective functions). In the first stage, the growth rate is relatively low and is based on the historical data, and the growth rate of F_{socemy}, $F_{eclgy,}$ and F_{food} is also slow. When entering the second stage, the economic growth will lead to increased water demand. However, according to the achievement of sustainable development based on the optimization model, ecological concerns should not be neglected. Therefore, the increase of river streamflow will also happen driven by the optimization model to maintain the river ecological health, consequently reducing the total water supply and increasing the water shortage of water users (**Fig.8**c). As F_{food} and F_{SOCEMY} can reflect the water shortage of the corresponding water users, their value will also increase sharply (**Fig.8e** and **8g**) due to the rapid increase of socio-economic indexes. When entering the last stage, the development of the socio-economy will tend to be stable, and the increasing speed of F_{food} and F_{SOCEMY} will decrease compared with that in the second stage. This is because the relatively stable development of the socio-economy does not need too much increased streamflow water (i.e., the increasing rate of streamflow water is closed to a relatively stable state), and both changing rates of water supply and demand tend to be stable consequently (**Fig.8**c).

We can also see that the off-stream water supply system competes for the instream ecological system. As shown in **Fig.8**, especially in stage 2, increased streamflow is accompanied by increased F_{SOCEMY} and F_{food} (**Fig.8e** and **8g**), reflecting the decreased satisfaction degree of the water supply of socio-economy and agriculture, thereby revealing the competition use between instream and off-stream water uses. The tradeoff between instream and off-stream water users can be obtained by the optimization model to solve for the best coordination status between them by adjusting economic development modes and balance the priority of each water user. It should be noted that the ecological objective (F_{eclgy}) is in a relatively stable status in all stages compared with other objectives (**Fig.8**f). This is because the ecological agent contains not only river streamflow but also the vegetation. The booming economy drives the optimization model to focus more on river ecological health (F_{riv}), and there are limited water resources for off-stream water users including vegetation. The dual effect of increasing streamflow water and decreasing water for vegetation makes the F_{eclgy} relatively stable. However, the optimization model takes the effect that the optimal allocation scheme is obtained by shifting streamflow water because instream and off-stream water use is intrinsically conflicted with each other, and should be coordinated by adjusting different weights of each component (see section 5.2 and 5.3).

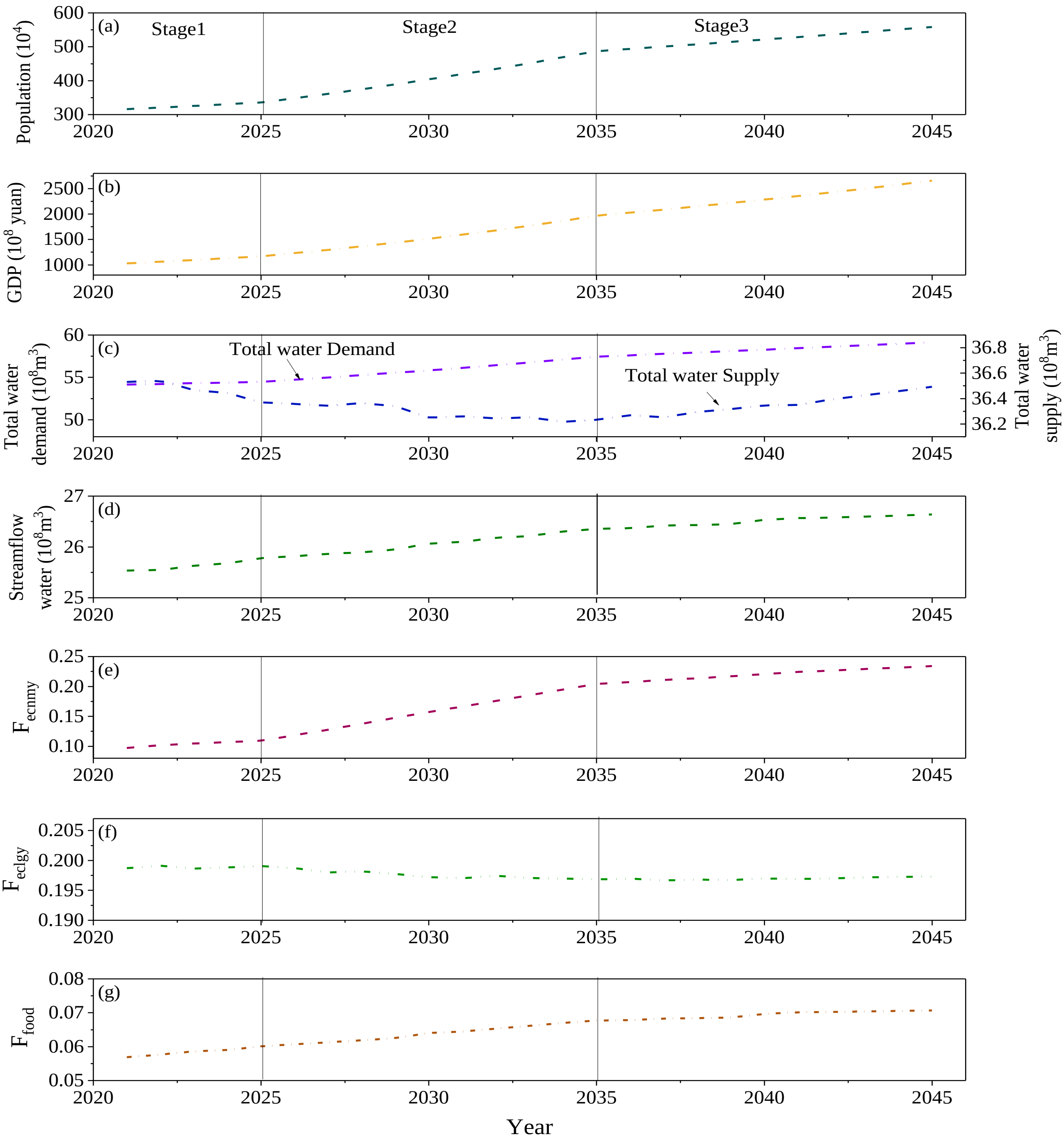


Fig.8 Coevolution process of WSEF nexus model

4.3 Dynamic interactions of WSEF nexus system

4.3.1 Socioeconomic-ecology response linkages

Fig.9 illustrates the loop of socioeconomic-ecology feedback. As demonstrated in **Fig.9**, the response linkage of carrying capacity and overload index involves the changes of economic indexes, water supply & demand, and streamflow water (Feng et al., 2019). In the beginning, the economy is still increasing slowly, and the increasing rate of water demand is also slow. The population and GDP are near the carrying capacity in this stage (i.e., the value of OI is near 1). In the following stage, both increasing population and GDP intensify the water demand (**Fig.9a** and **b**). To satisfy socio-economic development demands, the water supply of economic agent has also increased. However, there will be a more significant concern of the river ecological system (**Fig.8**c, **Fig.9**c) because ecological streamflow is an important part of sustainable water use, simulated by the optimization model. In this view, the growing rate of the water supply of domestic and industry (**Fig.9**d) will be less than the growth rate of water demand (**Fig.9**b) and therefore contributes to the increase of water shortage, which is in accordance with the performance shown in **Fig.8**e. The increasing water shortage will generate the gap between carrying capacity (**Fig.9**e) and predicted economic indexes (**Fig.9**a). Then, the overload index will further increase, consequently affecting socio-economic development. It further contributes to the overload of the WSEF nexus system, which even restricts the socio-economy instead. In the last stage, as the growth rate of population and GDP alleviates (**Fig.9a**), there will be a relatively slower increase rate of streamflow water, and there will be more water space for socio-economic development. Although the water shortage is increasing, its rate is lower than that in the second stage. The carrying capacity will be able to catch the predicted economic index if the stable or slower growth rate continues. The overload index is also decreased (**Fig.9f**, and the whole system tends to be stable. This response linkage indicates that the excessive population and GDP growth will eventually lead to increased overload status by increased ecological streamflow, and moderate socioeconomic growth will promote the best status of both each agent and the entire WSEF nexus system, and eventually promote sustainable water use.

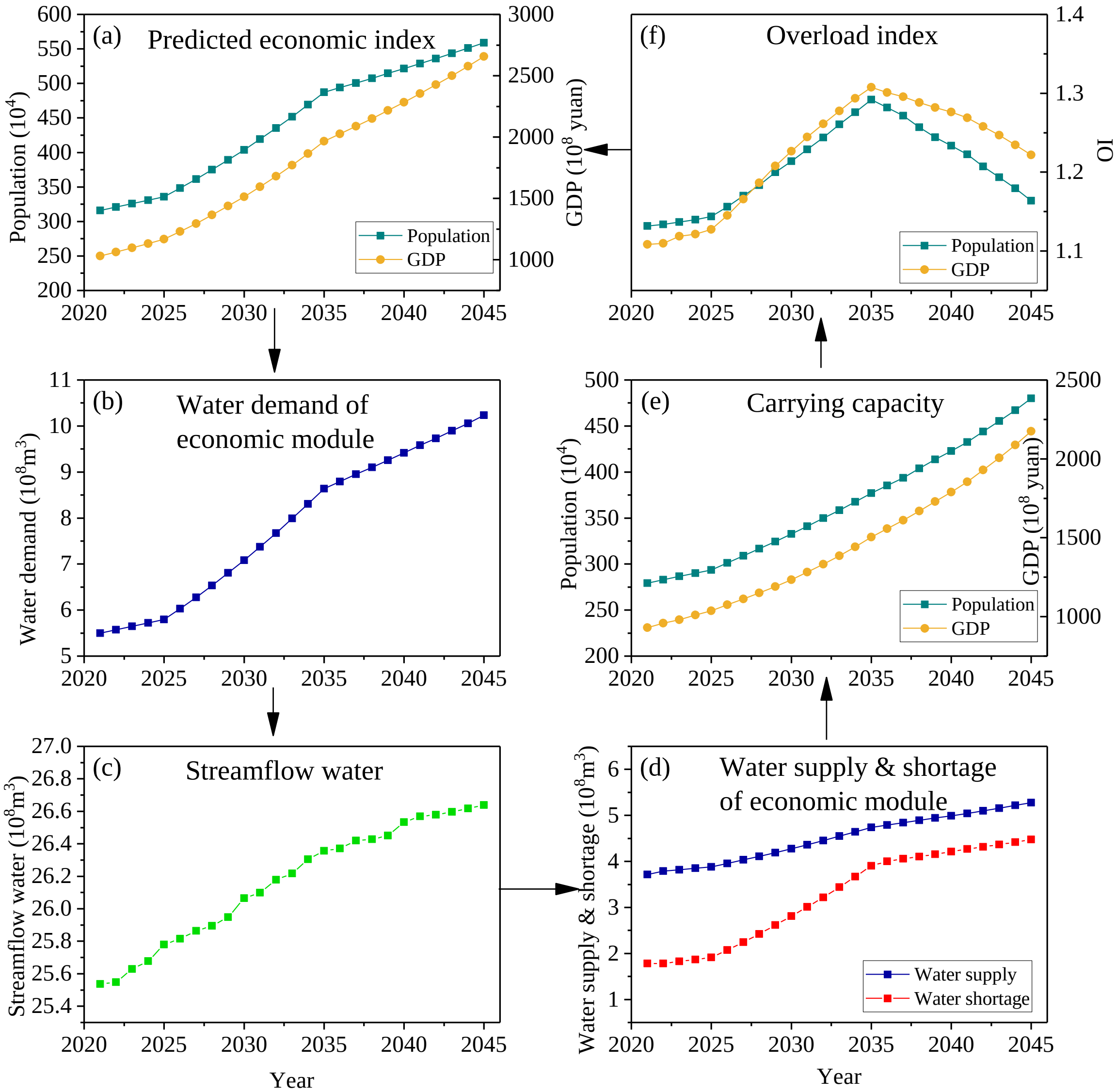


Fig.9 Response linkage of socioeconomy-ecology feedback loop

4.3.2 Ecology-food response linkages

Another performance is the ecology-food response linkage and as shown in **Fig.10**. It not only illustrated the linkage between crop and ecological water usage but also demonstrated the coevolution of ecology components of both instream (river ecology) and off-stream (vegetation) aspects. **Fig.10** shows that the increased streamflow water is the driving force of the ecology-food response. However, the increasing streamflow of water was driven by the rapidly increasing socio-economic scale. The optimization model is used to achieve the goal of sustainable development to balance the need of different users, especially that of instream and off-stream. The increased streamflow has two effects on the ecology-food response linkage. First, the variable F_{riv} describes the ecological health of a certain river. According to the definition of AAPFD, the higher value of streamflow water indicates the lower value of F_{riv}, which indicates that the river ecology is getting better. Second, the increasing streamflow water restricts the water supply of all off-stream water users, including agricultural and vegetation water (**Fig.10**b).

Irrigation and vegetation water use is the largest off-stream water consumer, and their increased water shortage was also driven by increased streamflow water (**Fig.10**d).

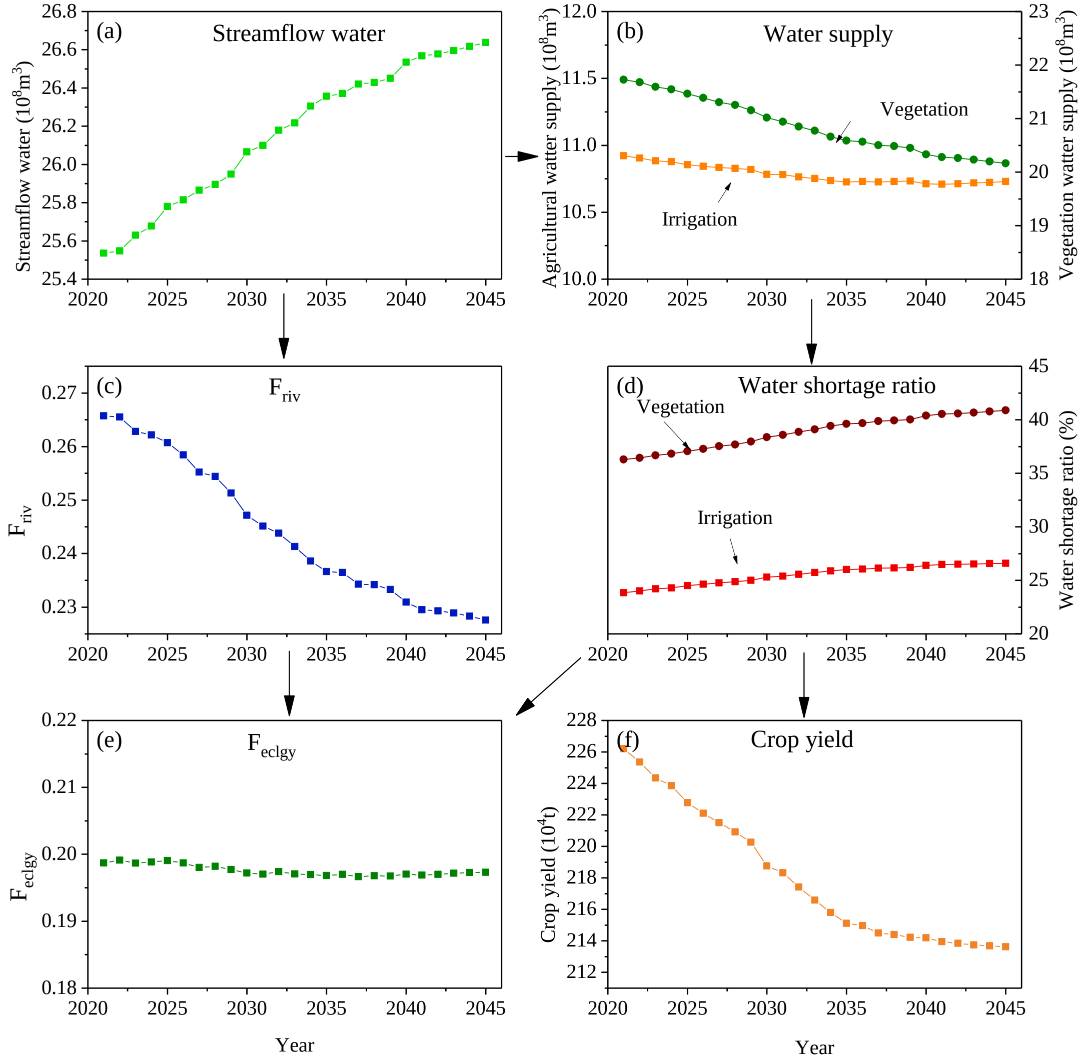


Fig.10 Ecology-food response linkage

For ecological agent, the dual effect of increased streamflow water and decreased vegetation water makes the stable change of F_{eclgy} (**Fig.10**e), indicating that the ecological aspect of UGRB is maintaining a good status. For food agent, crop yield is strongly affected by the satisfaction degree of irrigation water, and the increased water shortage of crop water will, therefore, indicate the decrease of crop yields (**Fig.10**f). But it tends to be stable in stage 3 because of the slower growth rate of the socioeconomic index, which contributes to the stable changing trend of streamflow water and further contributes to the stable changes of crop yield.

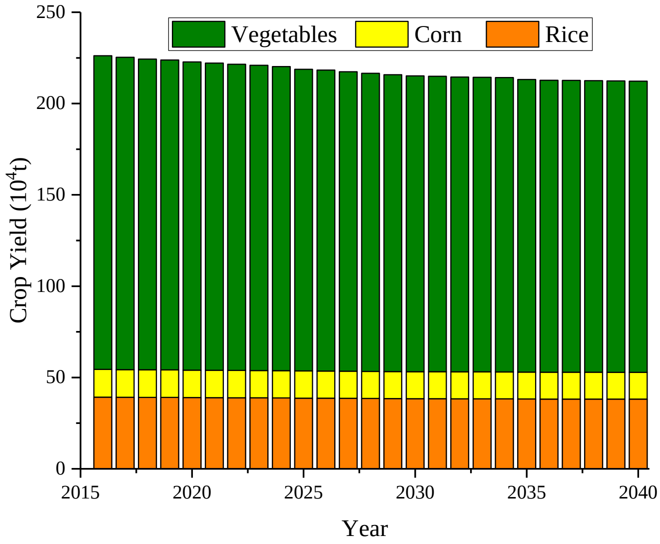


Fig.11 Detailed crop yield

4.3.3 Socioeconomic-food response linkage

Because food security ensures people's survival, The decreased crop yield is driven by the increased streamflow water that also caused an increasing overload index (**Fig.9**f) in the second stage, which is reflected by socioeconomic-food response linkage (**Fig.12**). The detailed crop yield is shown in **Fig.11**. Due to the sharply increased population and GDP, the increased water shortage of agricultural water contributes to the decreased crop yield (**Fig.12**b), which also results in the stagnant farmer's income (**Fig.12**c). The increased water shortage happens because of the socioeconomic-ecology linkage, the increased ecological streamflow reduces crop water supply. The stagnant farmer's income is the result of the dual effect of both decreased crop yield and increased population. The total value of the primary industry is considerably related to crop yield. The reduced crop yield increases the crop price, but its rate is still less than the rate of population growth. As crop yield and income are greatly related to people's survival, the stagnant income and decreased crop yield will finally decrease carrying capacity and further intensify the overload index (**Fig.12**d). If the growth rate of the predicted population decreases (stage 3), there will be less pressure for water supply and can well balance the agricultural and streamflow water, further contributing to stable crop yield, increased farmer's income, and decreased overload index. Hence, how crop yield affects socioeconomic in this linkage can be embodied by the following three aspects: First, the decreased crop yield may lead to food crisis to come extent, which contributes to decreased population because of the limited access to food; Second, the main source of farmer's income is the total value of the primary industry, which is directly embodied by yield, and less income caused by decreased crop yield make it hard for farmer's survival; third, the declined population also decreases the labor force, which also hinders the socioeconomic development.

So far, the linkage of socioeconomic-food, socioeconomic-ecology, and ecology-food were all presented, which indicated that the three components interact and respond with each other.

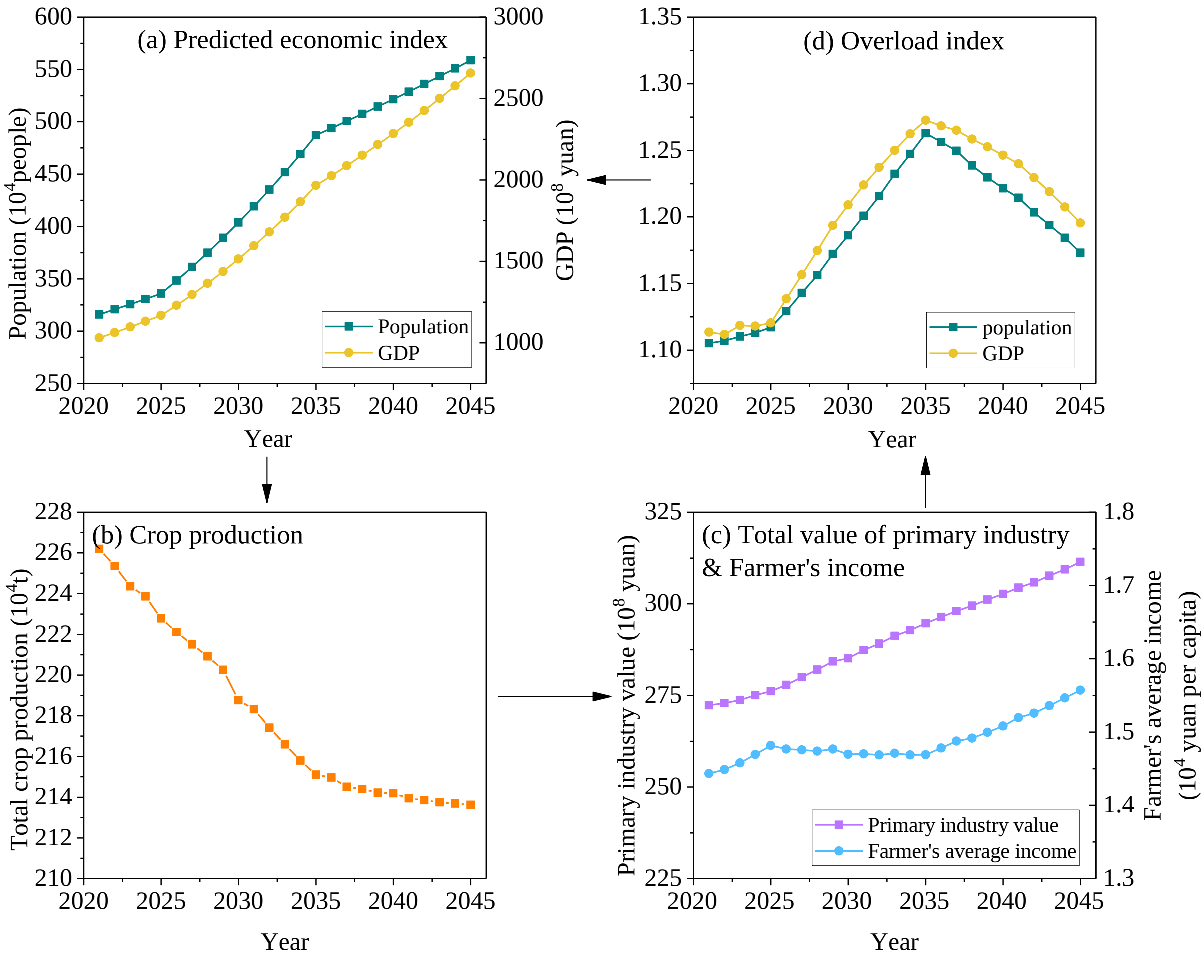


Fig.12 Socioeconomic-food response linkage

4.4 Assessment of coordinative degree of each subsystem and SDD

The calculation result of SDD of WSEF nexus and coordination degree of the socioeconomy (SOCEMY), ecology (ECLGY), and food (FOOD) is demonstrated in **Fig.13**. We can see that the variation of the four variables is also showing the state characteristics. The SOCEMY in the first stage is increasing, but it had an either decreasing (UGRB, Guilin urban area, Lingui, etc.) or stable (Xing'an, Yangshuo) trend in the second stage, indicating the coordinative status of socio-economy is not good caused by the excessive growth rate of the economy. The decreased coordinative status of the socioeconomic subsystem also influences other subsystems and the SDD of total WSEF nexus, reflected by the decrease of ECLGY, FOOD, and further SDD. Fortunately, the decreasing rate of ECLGY is smoother compared with that of FOOD, indicating the performance of the ecology of UGRB is relative well compared with socioeconomics and agriculture. This performance could be due to the dual effect of increasing streamflow water and decreasing vegetation irrigation. The same was true for other administrative regions of UGRB. Moreover, for the whole basin, the value of SOCEMY in the later period of the second stage (about 2033~2035) is even lower than FOOD and ECLGY. From the perspective of administrative regions, it is more obvious in Guilin urban area, Pingle, and Lipu counties. It happens because the economic-stressed stage has lasted almost ten years in 2035, which is similar to the "pendulum model" that takes the effect that the pendulum "swings" towards the economic-stressed system (See 2.1). As socio-economic index increases sharply and continuously, the ecological protection mechanism will also be continuously triggered to increase the overload index, resulting in both SOCEMY and SDD reaching the minimum.

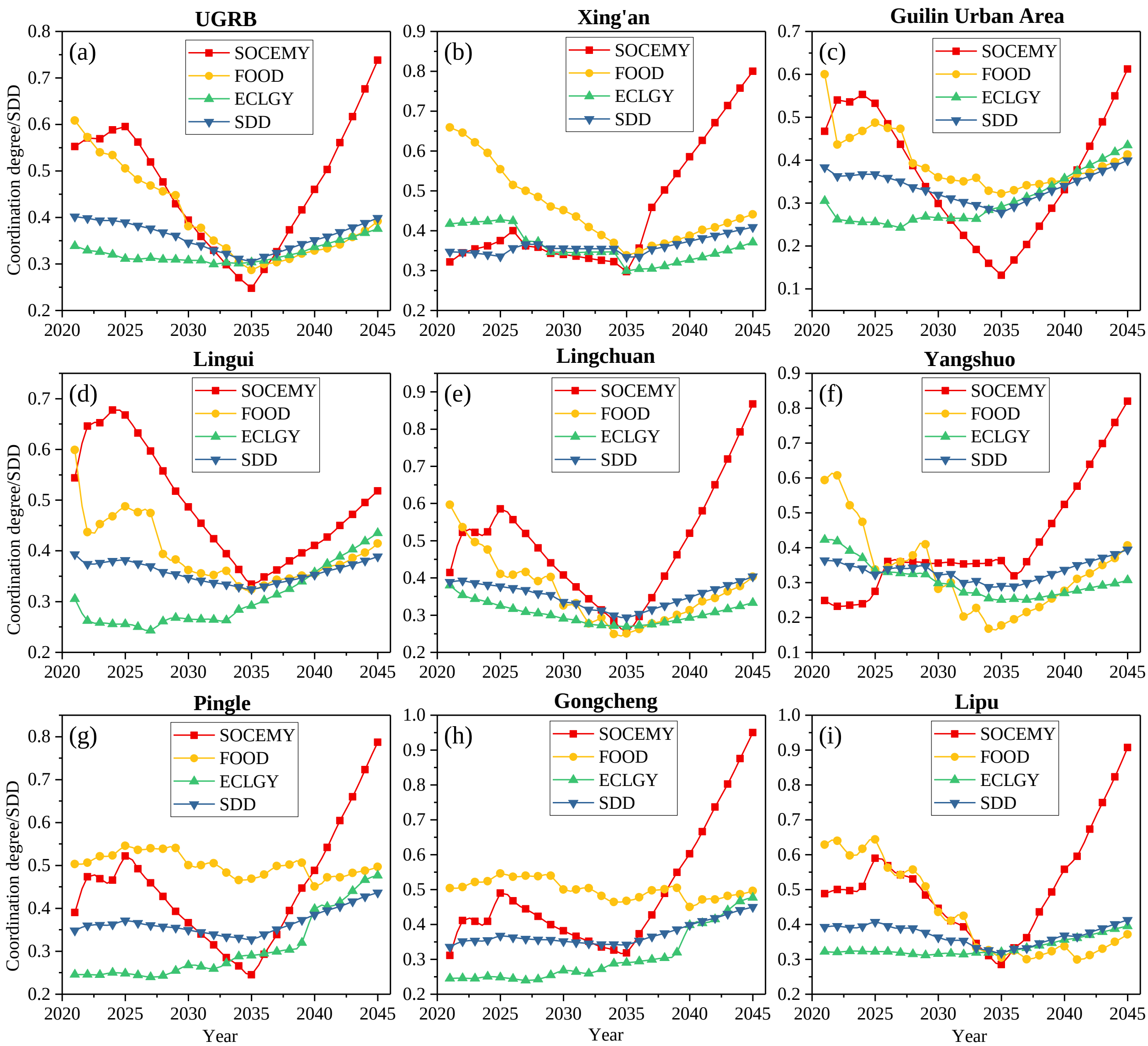


Fig.13 Time variation of sustainable development degree (SDD) of WSEF nexus and coordination degree of each agent

When it comes to the third stage, the value of SOCEMY increases, indicating the coordination of the socioeconomic subsystem is improving. It revealed the decreasing of overload index and the increased carrying capacity due to the relatively slower increasing rate of water demand of economic agent. The increasing value of SOCEMY promotes the coordinative degree of ecology and food, and the value of SDD is consequently increased, revealing that stable economic growth will promote the sustainable development of the WSEF nexus. The good phenomenon of the last stage happens because the relatively slow growth rate of water demand for the economic agent will generate more water for food and ecological agent, and the increasing sewage and recycled water treatment rate will provide relatively more water for users. The coevolution process assumes the "pendulum model" presented by Van et al. (2014) and Kandasamy et al. (2014), where environmental awareness has been raised, and a stable population rate occurred in the last era. The result presented in this study is similar to the findings in Van et al. (2014) and Kandasamy et al. (2014). Furthermore, we can speculate that in the 2045s, the pendulum of ULRB will also "swung" back to the stage of protective resources & environment and stable development of socio-economy.

5. Discussions

5.1 The reasons for coevolution trends and model performances

The overall coevolution changes and performances are affected by the external drivers embodied by the growth rate of population and GDP (see **Table 3**). The sharply increased rate in the second stage exactly corresponds to the era that "heavy government policy support and investment" and "population grow rapidly", which stressed in the "pendulum model" by Kandasamy et al. (2014) (see Section 2 and **Supplementary material S1**). The growth rate from 2036 to 2045 is lower compared with that from 2026 to 2035, which corresponds to the era of "remediation and emergence of the environmental customer". That's why the coevolution process of all the items depicts the characteristics of different stages. Although the optimization model is used in this study, the objective function of both socioeconomic and food agents still increases in stage 2, accompanied by the decreased crop yield (**Fig.12**b), increased overload index (**Fig.9**f), and even lower SDD (**Fig.13**). This is because the optimization model is just the crucial tool for achieving sustainable water use in which the ecological agent is an indispensable part. Ecological streamflow must be guaranteed to maintain river health and, hence we can see the river streamflow increase rapidly in this stage simulated by the optimization model, and further intensifies the water shortage.

The positive feedback loop in the SD model (see Fig.4) will take effect if the optimization model is not coupled with the entire framework. However, this positive linkage will lead to divergence in the socioeconomic agent subsystem. That is, both water supply and population will increase circularly, and likely to result in unlimited growth of socioeconomic, which directly reduces the river streamflow and cause severe ecological problems. That's also the reason why the value of SDD is decreasing (see Fig.14). The socioeconomic/food agent and ecological agent constitute the negative feedback loop, and the optimization model will then be coupled with SD to help find the balance from this loop. With sharply increased population/GDP, the optimization model intensified the ecological streamflow to ensure river health. The optimization model does help to try its utmost to achieve the sustainable goal but there is no guarantee that the ideal status (higher SDD) will be achieved. The accelerated growth of water demand, caused by a rapid growth rate of population, is the main factor for the negative performance of the WSEF nexus (e.g., high overload index). Fig.14 demonstrated the comparison of model performances between two cases (SD model only and SD & optimization model) of the entire UGRB. Fig.14 shows that the value of SDD of coupled SD and optimization model is higher than that of only SD model, indicating that the coupled model performs better and is able to increase the accuracy and reliability of the SDD model. In addition, the situation in stage 3 has been improved, with decreased overload index, stable streamflow and crop yield. The moderate growth rate contributes to more water supply for supporting reasonable economic development. We can conclude that the technologies (such as optimization approaches) are just a tool that helps water sustainability, but management regimes and policy adjustment on external drivers is the fundamental approach to achieve this goal.

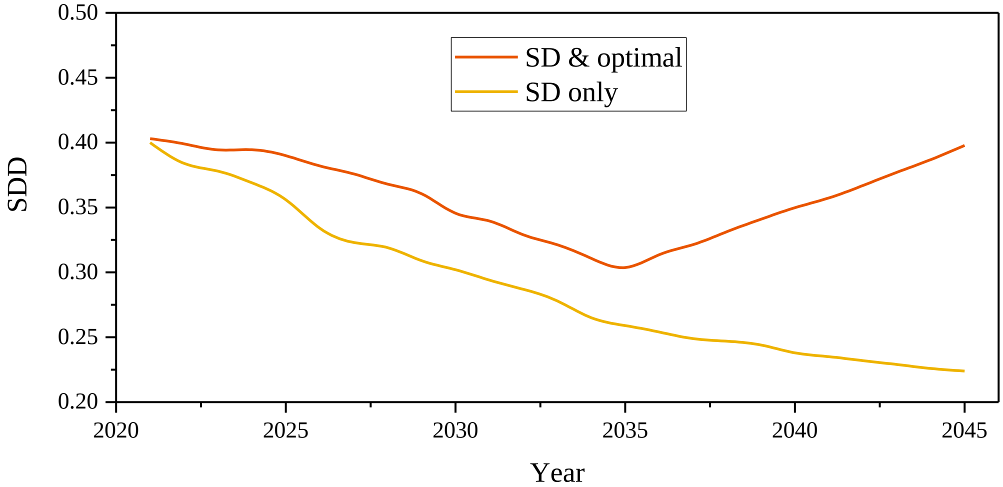


Fig.14 Performance of model results under different scenarios of entire UGRB

5.2 Decision making performance considering model uncertainty

The chain of the model is complex and usually contains lots of uncertainties, and decision-makers usually aim to achieve multiple performance objectives and have to make tradeoffs among those conflicting objectives, which arises from uncertainties (Herman et al., 2014, 2015). For uncertainties of the multi-objective model, it is reflected mathematically by the portfolios of all the non-dominant optimal solutions (also called Pareto frontier) (**Fig.15**). Each dot in **Fig.15**, correspond to a certain weight vector $\boldsymbol{r}=(\alpha_1,\alpha_2,\alpha_3,\theta)$, that represents one possible alternative. Therefore, the way we choose those optimal solutions from the Pareto alternative is the main source of the model uncertainty by which the weight of each objective is reflected (Tingstad et al., 2014; Liu et al., 2019), that is, the tradeoff analysis. This study provides several alternatives based on different weighting factors to assess model performances. Twelve alternatives are presented in Table 4 and represent the preferences of decision-makers, and the different performances are shown in Fig.16.

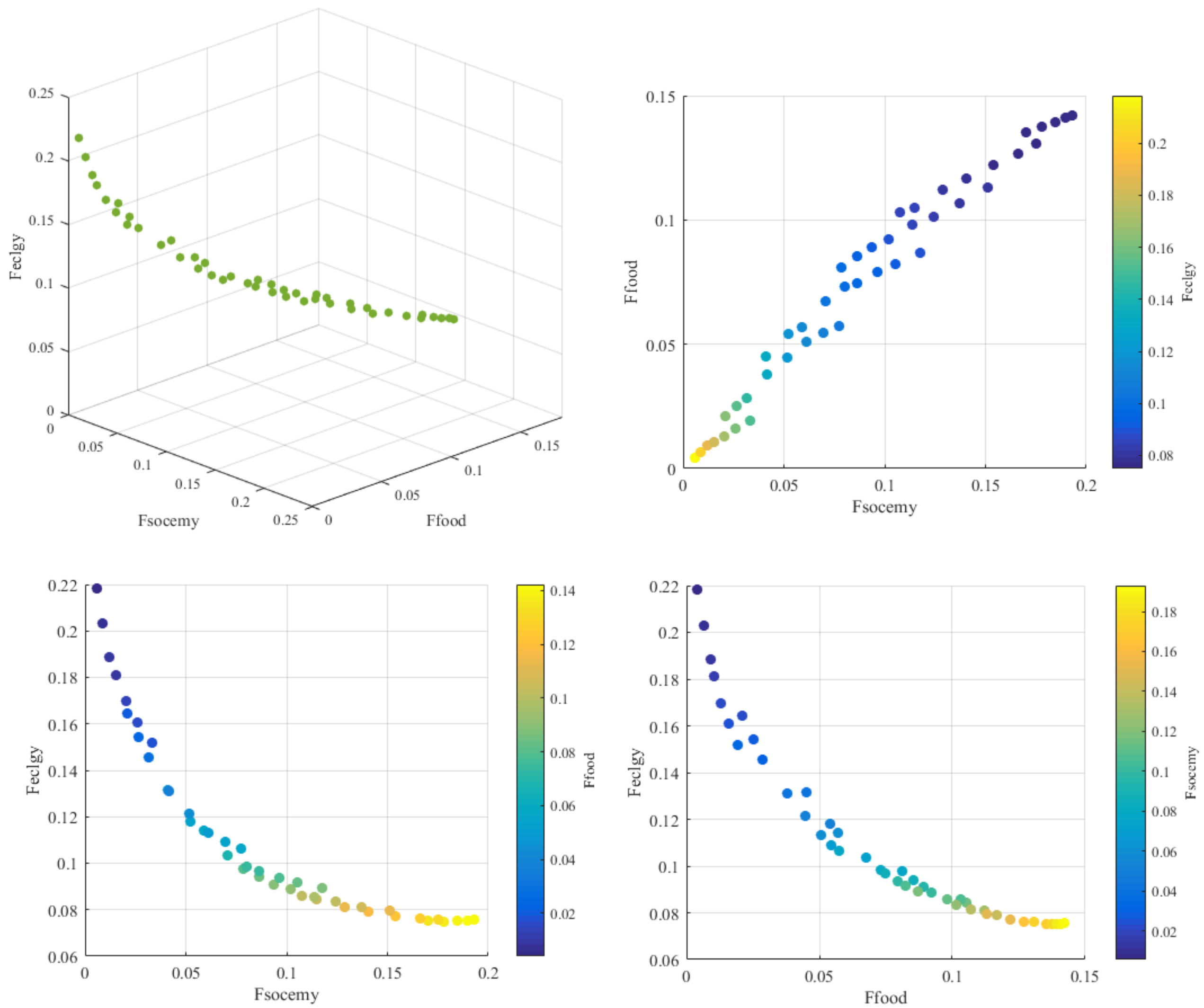


Fig.15 Portfolios of all the non-dominant optimal solutions of 2020.

Table 4 Twelve alternatives based on weighting factors for uncertainty assessment

Alternatives	Weighting factors				Alternatives	Weighting factors			
	α_1	α_2	α_3	θ		α_1	α_2	α_3	θ
A1	0.2	0.1	0.2	0.5	A7	0.2	0.2	0.4	0.2
A2	0.2	0.1	0.3	0.4	A8	0.5	0.2	0.1	0.2
A3	0.2	0.2	0.2	0.4	A9	0.4	0.2	0.2	0.2
A4	0.1	0.2	0.4	0.3	A10	0.5	0.1	0.2	0.2
A5	0.2	0.1	0.4	0.3	A11	0.4	0.1	0.2	0.3
A6	0.3	0.1	0.4	0.2	A12	0.25	0.25	0.25	0.25

Approximately, A1 to A3 focus more on ecological streamflow with higher θ, while that of A4~A7 and A8~A10 is lower. A4~A7 focus more on food agent while A8~A11 focus more on the economic agent. A11 focuses on both economic and streamflow issues. A12 is the average level that each weight is set as equal. The value of both objective functions of each agent and SDD under each alternative is shown in Fig.16. From Fig.16, we can see that the values of SDD under A1~A5 and A11 are smaller than those under other alternatives. Meanwhile, the objective function of both economy and food agents under A1~A5 and A11 is higher than that under other alternatives, suggesting more water shortage. On the contrary, the objective function of the ecology agent shows the opposite trend. We can contribute this result to the relatively higher weighting factor of θ and the lower weighting factor of α in those alternatives, resulting in the relatively less water serving for economic and food agents. Moreover, of all the alternatives, A12 performs the best with an equal value of weighting factor (0.25), suggesting that equal consideration to each agent is more likely to attain sustainable development. The value in other alternatives is either more or less than 0.25, suggesting that excessive or lower weighting factors prevent the sustainable development of water resources to some extent. Therefore, this uncertainty analysis can serve as a reference for the decision-making process in water resources management. based on the primary needs of each stakeholder, multiple weighting scenarios can be identified and explored.

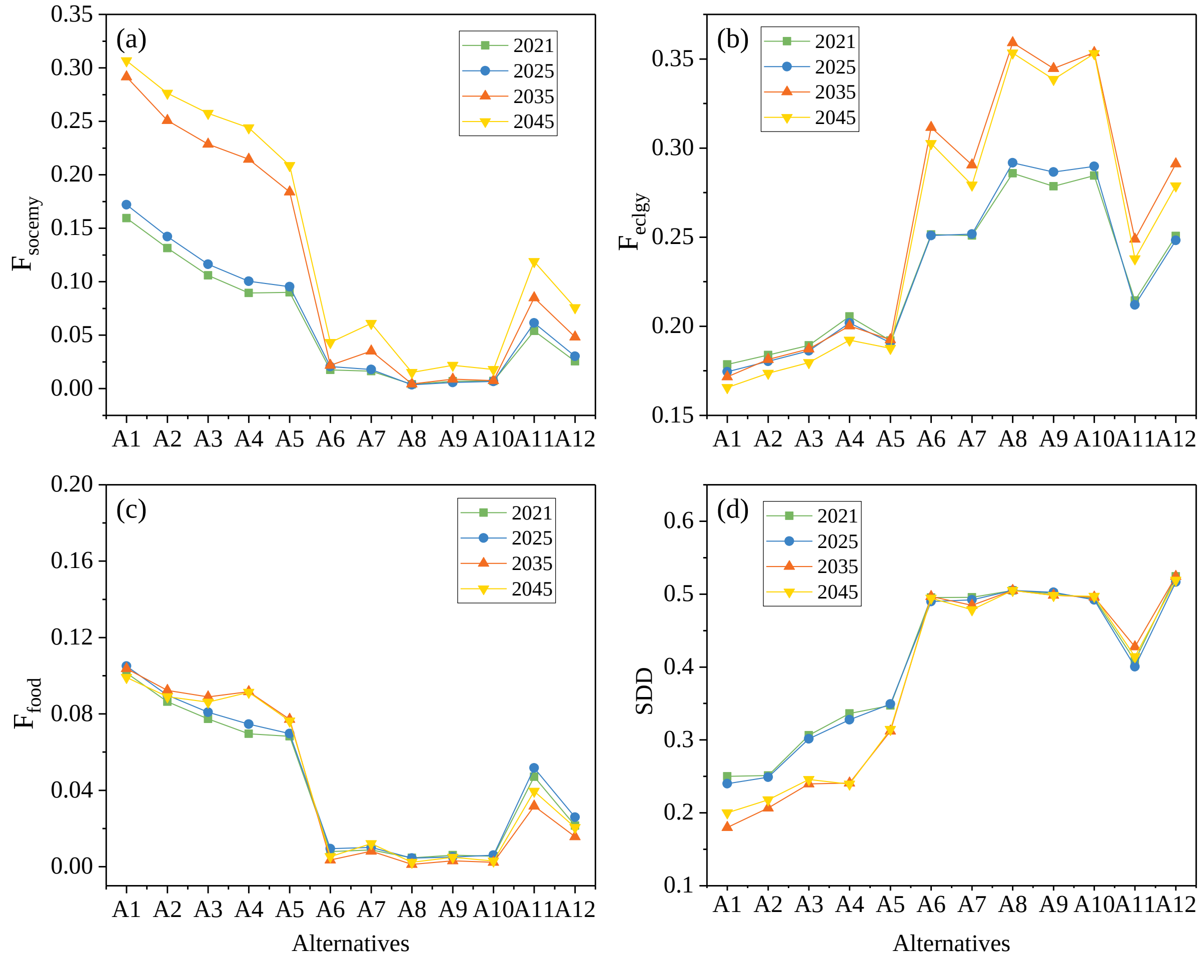


Fig.16 Sustainable development degree of different alternatives

5.3 Robustness analysis for WSEF nexus

The key factor(s) that affect the robustness of the WSEF nexus system is/are assessed to improve its reliability. The alternatives of A5, A7, A9, A11 are set particularly by controlling relative variables to assess the robustness of the WSEF nexus. In the case of both A5 vs. A7 and A9 vs. A11, we change θ while α_1 and α_3 remain unchanged to assess the influences of river ecology water changes on the performance of the WSEF nexus. While in the case of both A5 vs. A11 and A7 vs. A9, we change α_1 and α_3 while θ and α_2 remain unchanged to assess the influences of water changes of both economic and food agents on the performance of WSEF nexus. According to Fig.16, the differences between both cases are shown in Table 5. To illustrate, the SDD value of 0.06 in row "A5 vs. A11" and column "2016" means that the difference of SDD value between A5 and A11 in 2016 is 0.06. From Table 5, we can see that the values in the lower two rows are smaller than those in the upper two rows. It indicates that when the weighting factors of both socioeconomic and food agents are certain, changing the weighting factor of streamflow will have a relatively significant impact on the performance of the WSEF nexus in both objective function and sustainable development degree. Additionally, changing the weighting factor of both socioeconomic and crop water uses will have less influence on model performance. In other words, the streamflow agent has a relatively great influence on the robustness of the WSEF nexus model.

Table 5 Comparison of the performance of WSEF nexus between different alternatives

Case comparisons	Uses	F_{socemy}				F_{food}				SDD			
		2021	2025	2035	2045	2021	2025	2035	2045	2021	2025	2035	2045
A5 vs. A7	Influence of changing river ecology on WSEF performance	0.07	0.08	0.15	0.15	0.06	0.06	0.07	0.06	0.15	0.14	0.17	0.16
A9 vs. A11		0.05	0.06	0.11	0.12	0.04	0.05	0.05	0.05	0.09	0.10	0.12	0.12
A5 vs. A11	Influence of changing socioeconomy and food on WSEF performance	0.04	0.03	0.08	0.06	0.02	0.02	0.02	0.02	0.06	0.05	0.07	0.07
A7 vs. A9		0.01	0.01	0.03	0.04	0.00	0.01	0.00	0.01	0.01	0.01	0.01	0.02

The robustness of river ecology can also be reflected in the model performance of different years. From Fig.16, we can also see that both objective functions and SDD under A1~A5 have a greater difference between 2021&2025 and 2035&2045 compared with other alternatives. There will be a rapid economic increase from 2025 to 2035 and the ecological awareness in these alternatives outweighs other alternatives (with higher θ), which is more likely to trigger the adaptive adjustment of the WSEF nexus system and further accelerates river streamflow. Then, there will be not enough economic water services, and the overload index will increase, further decreasing SDD in 2035 compared with 2025.

5.4 Simplifications of model dynamics and limitations

The proposed model simulates the dynamic evolution and feedback loops based on the three agents: socioeconomic, food, and ecology. The findings proposed in this study are similar to those in Kandasamy et al. (2014). This study stressed that environmental awareness arises when an accelerated population is about to consume freshwater. This is translated into population decrease to protect the environment. The study also showed the stable status of sustainability of both social productivity and environmental issues because the population growth rate is moderate and steady in the third stage, this to pay more attention to environmental awareness.

These individual three nexus agents have also prominent theories or disciplines that contain numerous individual principles. Therefore, several assumptions and simplifications are often conducted to develop the nexus models that are, to some extent, one of the most necessary and significant ways for natural resources management practices for sustainable development. For example, the linkage between crop yield and carrying population may not be as easy as a linear relationship (Lyu et al., 2020). The main goal of this study is to assess the viability of WSEF nexus models as a framework for decision-making. For individual dynamics between two agents, a simplified version of our proposed model, incorporating more detailed and localized assumptions that incorporate non-linear relationships, could be used. Our study focuses on linear-based relationships as a practical way to develop a more comprehensive analysis. Also, the proposed model was used in humid areas but may not be suitable in dry areas, which can be conducted in further studies.

Moreover, it should be noted that the analysis in Section 5.3 is one of the most used methods of robust analysis, which is based on changes in the weighting factors (Herman et al., 2015; Liu et al., 2019). Also, Feng (2019) established the integrated framework of the water resources system and applied it in Danjiangkou Reservoir by introducing many parameters. The robust analysis is conducted based on the changes of these parameters, and the model performance (revealed by certain variables) under the different values of these parameters are analyzed. Other methods use weight analysis to assess model changes and scenario analysis. For example, the robust analysis presented in Tan et al., (2019) is conducted by changing the reservoir's streamflow and comparing the value of the objective function of both in-stream and off-stream water users. The increasing streamflow results in decreasing water supply of off-stream, which leads to the higher increasing rate of the off-stream objective function. In terms of robust analysis, both Tan et al., (2019) and this study attempt to make the initial analysis and develop practical frameworks that could be implemented by water resources managers and other stakeholders. Further research should evaluate the effect of more advanced analysis methods on the efficiency and practicality of WSEF nexus models.

6. Conclusions

This paper presented a new integrated framework that is used to analyze the dynamic interactions within coupled human and natural systems in the context of socio-economic development, food security, and environmental protection by establishing system dynamic and optimization modeling. The system dynamics gives how the dynamic status of water supply is performed, while optimization modeling gives insights on how sustainable water uses can be achieved. The dynamic optimal results are generated by using as input the initial result of the SD model of each time step and iteration process. The changing external conditions, i.e., the socio-economic development changes, result in nonlinear and multiscale feedback responses. The uncertainty analysis is also helpful for multiple tradeoffs and robustness analysis in the decision-making process. The result can give a firm reference and provide a practical tool for sustainable water use from the following two aspects:

This coupled modeling tool enables dynamic evolution and feedback process by generating the whole scale of future trajectories that reveals the interactions across socioeconomic development, food security, and ecological protection dynamically and optimally. All the trajectories differed in different stages. That is, depending on the external drivers in terms of different stages, the dynamic changes manifest differently in water supply, streamflow water, farmer's profit, and population size. There are no obvious changes in the performances of the model in the first stage. In stage 2 (2026~2035), the severe increase of the economy intensifies the water for increased population and the need for economic productivities, which contributes to the positive feedback loop. However, it deteriorates the river health in ecological agents, and the negative feedback loop is used to find their balance. Therefore, the interaction of the entire WSEF nexus system is intensified by triggering more streamflow water of reservoirs for the ecological agent. It results in less water for agriculture and social economy and cannot afford the rapidly increasing population and economy (increased overload index), and decreased crop yield. In stage 3 (2035~2045), concerning moderate socioeconomic development, the interaction of the WSEF nexus system will be alleviated, that is, the changes of streamflow water will tend to be stable, and there will be more water to support the proper population size and economy, as well as crop yield. In terms of sustainable development degree, the increasing trend occurred in stage 3 compared with the declining trend in stage 2. These results suggest that only considering the economic benefits (stage 2) will rather accelerate the overload process of the overall WSEF nexus system, which inversely affects the socio-economic development and cannot achieve sustainable water use. If ecological awareness arises and the economic growth rate tends to be stable, it will be beneficial for the sustainability of water. Thus, the coevolution process and dynamic interactions between human society and natural systems can provide valuable information and guidelines for policymakers on how to decide the development degree and manage water resources on a regional scale considering economic development, food security, and ecological protection.

The uncertainty analysis result of the coupled model also revealed the different performances considering the need of various stakeholders, giving references to multiple tradeoffs influencing the WSEF nexus system and stakeholders, notably the tradeoffs between water for social development, food security, and ecological protection. The Pareto portfolio of the multi-optimization model based on different weighting factors reveals the competitive mechanism of the three agents of the coupled model. The alternatives based on different weighting factors show the varied sustainable development degrees and objective functions of each agent. Of all the alternatives, the equal consideration of each stakeholder (weighting factor) is more likely to achieve sustainable development (with the greater SDD). Therefore, policymakers can explore the future water allocation scheme among different needs of stakeholders based on those different alternatives. Of all the agents within the WSEF nexus system, the river ecological part is more likely to influence its robustness. This result suggests that the ecological agent of the WSEF nexus system should be paid more attention to the process of both water allocation and the policymaking process compared with other aspects. This paper not only reveals the dynamic evolution and feedback responses across multiple agents more precisely by coupling SD with the optimization model, improving the model's reliability compared with the traditional SD model but also provides valuable predictive insights into the decision-making process of nexus systems.

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Supplement: Supplementary materials (Data availability)

(Supplementary materials, uploaded to the supplementary links of journal's website)

Author contribution

Yaogeng Tan prepared the manuscript and developed the model. Zengchuan Dong and Sandra Guzman revised the manuscript. Xinkui Wang and Wei Yan helped collect the data.

Competing interests

The authors declare that they have no conflict of interest.

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