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Original Research

Optimizing sustainable development in arid river basins: A multi-objective approach to balancing water, energy, economy, carbon and ecology nexus

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ABSTRACT

The ongoing water crisis poses significant threats to the socioeconomic sustainability and ecological security of arid and semi-arid river basins. Achieving Sustainable Development Goals (SDGs) within a complex socio-ecological nexus requires effective and balanced resource management. However, due to the intricate interactions between human societies and environmental systems, the tradeoffs and synergies of different SDGs remain unclear, posing a substantial challenge for collaborative management of natural resources. Here we introduce a gray fractional multi-objective optimization (GFMOP) model to balance multi-dimensional SDGs through a novel water–energy–economy–carbon–ecology nexus perspective. The model was applied to a typical arid river basin in Northwest China, where thirty-two scenarios were explored, considering factors such as shared socioeconomic pathways, carbon removal rates, water conveyance efficiencies, and ecological requirements. The results reveal a strong tradeoff between marginal benefit and carbon emission intensity, indicating that improving the economic efficiency of water use can simultaneously reduce emissions and protect the environment. Given the immense power generation potential, wind power development should be prioritized in the future, with its share in the energy structure projected to increase to 23.3% by 2060. Furthermore, promoting carbon capture technologies and expanding grassland coverage are recommended to achieve regional carbon neutrality, contributing 39.5% and 49.1% to carbon absorption during 2021–2060, respectively. Compared with traditional single-objective models, GFMOP demonstrates a superiority in uncovering interrelationships among multiple SDGs and identifying compromised alternatives within the compound socio-ecological nexus. The model also provides detailed strategies for resource allocation and pollutant control, offering valuable guidance to policymakers and stakeholders in pursuing sustainable and harmonious watershed management.

1. Introduction

1.1. Background

Concerns about water scarcity, energy crisis, ecological degradation, and intensive carbon emissions have prompted the formulation of the 2030 global agenda on the Sustainable Development Goals (SDGs) set by the United Nations. The 17 SDGs are dedicated to promoting sustainability in resource management and ensuring water, food, energy, and ecological security for human society. As an essential resource, water is pivotal in supporting the SDGs aimed at poverty reduction, economic growth, and environmental sustainability [1]. However, relentless economic development, continuing urbanization, and booming population have accelerated the rate of resource depletion worldwide over the past decades [2]. The global population is projected to reach around nine billion by 2050, leading to an 80% increase in energy consumption and a 60% rise in food demand. To meet the demands for food and energy production, water withdrawals are anticipated to surge by

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50% in developing nations from 2017 to 2025 [3,4]. As the fundamental physical and socioeconomic−political unit for water management, river basins are under enormous environmental pressure and even face ecosystem collapse due to increasing water consumption and the associated pollutant emissions. Globally, over 60% of rivers have experienced significant declines in their ecological flows. By 2100, the expansion of arid watersheds is projected to affect 5.17 billion people, 64% of whom will reside in developing countries [5]. Against that background, ensuring a stable supply of essential resources has become one of the most significant challenges for achieving regional SDGs in the future. To overcome that challenge, it is necessary to explore the interactions among water, energy, and ecology, as well as strengthen social and environmental security in river basins facing water scarcity.

Northwest China is one of the world's most severely arid and ecologically fragile regions. Water resources in Northwest China account for only 8% of the national total, while the land and coal resources of the region account for 35% and 70% of the national total, respectively [6,7]. This spatial mismatch in energy and land resources exacerbates the water scarcity in the region. The Tarim River Basin in Northwest China is one of the world's largest inland and represents the most important water resource for regional development. Since 2000, a major tributary of the Tarim River Basin, the Kaidu−Kongqi River Basin (KKRB), has suffered severe river channel cutoffs and ecological degradation downstream due to intensive agricultural irrigation and energy generation. The KKRB is a primary cotton and grain production base for Xinjiang Uygur Zizhiqu, with 69.8% of its water used for agricultural irrigation. Moreover, under the west−east natural gas transmission project, the energy consumption of industrial enterprises in the KKRB increased from 1.89 million tons of coal equivalent (tce) in 2000 to 8.72 million tce in 2022, with an average annual growth rate of 15.5%, accompanied by massive water consumption [8]. The growing water demand and industrial expansion in the area are incompatible with the low quality of human habitat and aggravate desertification. To guarantee the ecological security and socioeconomic sustainability of the KKRB, there is an urgent need for integrated management of water resources, energy, and ecology; such efforts will work toward achieving sustainable development goals. In practice, the SDGs are highly interrelated; achieving one may affect the achievement of others, some positively and others negatively. In detail, water allocation and energy supply should be ensured for food production, industrial activities, and domestic demands (corresponding to SDGs 6 and 10). Energy production consumes large amounts of water and is deemed the major emitter of CO_2, especially from fossil fuels (SDGs 7 and 12). All the active economic and energy sectors squeeze the water available for ecosystem services, which impacts the carbon sink capacity and environmental quality (SDG 15). In this context, formulating a comprehensive framework for managing the synergies and trade-offs among different SDGs in this river basin with geographical water shortages and ecological vulnerability has become a crucial challenge in Northwest China, shared by other regions with similar issues worldwide.

1.2. Literature review

As a cross-cutting approach, nexus thinking can support the integration of SDGs by capturing the complex interlinkages among natural resources and providing comprehensive strategies spanning multiple systems rather than focusing on an isolated system. The importance of nexus planning in implementing SDG practices has been widely recognized following systems simulation and quantitative assessment methods [9−11]. Previously, several research works have been conducted exploring the interconnections of SDGs in a nexus, which involved formulating an index system and simulating the dynamics of various indicators. For example, Ioannou and Laspidou (2023) applied fuzzy cognitive maps to explore and quantify the interlinkages of the water−energy−food nexus in combination with the 17 SDGs, where the three key SDG indicators most influenced by the nexus were identified through a cause−effect relationship matrix [12]. Sarkodie et al. (2020), meanwhile, employed a machine learning technique to examine the relationships between energy consumption (SDG 7) and the climate (SDG 13) in an energy−climate−economy−population nexus; their results, specific to Kenya, showed that economic development could be expanded by enlarging the country's labor force and improving the energy structure [13]. As these examples demonstrate, nexus models are effective in cross-sectoral coordination and assessment; however, they do not serve to provide management guidance on a suitable resource allocation to achieve regional sustainable development.

A multi-objective programming (MOP) model has proven effective in overcoming this limitation and allowing practitioners to identify reliable resource allocation strategies for decision makers [14,15]. To that end, MOP models can resolve conflicts among different sectors and subsystems. From a sustainable development perspective, maximizing system efficiency when there are limited resources generates greater social wealth and satisfies human demands. Efficiency-oriented objectives are often presented as the ratios between outputs and inputs, such as the maximum water productivity and minimum carbon intensity [16,17]. In this context, the fractional programming (FP) can be integrated into the multi-objective framework to handle conflicting economic and environmental ratio objectives. Accordingly, several studies have focused on solving multi-objective fractional problems by incorporating the FP method into the MOP framework. For example, Yang et al. (2020) transformed the multi-objective fractional problem into a single-objective version under different aspiration levels by applying a linear goal programming procedure [18]. Meanwhile, Borza and Rambely (2021) proposed a solving algorithm for a multi-objective fractional model by integrating membership functions for the objectives using the max−min method [19]. Such approaches can address computational complexity and redundancy by translating multiple fractional objectives into a single linear objective version; however, they cannot avoid the assumptions associated with assigning weighting values. Here, the weighting value of each target is often subjective and highly volatile because it is based on the experience and information of diverse decision makers, which impacts the accuracy of efforts to determine the optimal solutions. Overcoming this hurdle, Meng and Wang (2014) first proposed a gray incidence multi-objective algorithm that can be used to determine objective weights by measuring the incidence degree based on gray theory [20]. Nevertheless, no research has adopted such an approach to address multi-objective fractional optimization problems in a nexus framework.

The Kaidu−Kongqi River Basin has attracted widespread attention due to its water crisis and ecological degradation. Previous studies mainly focused on assessing the influence of climate change on water and land resources in the KKRB [21−23], optimizing agricultural irrigation to alleviate the water shortage [24−26], or assessing the current water resources or eco-environmental status [7,21,27]. Meanwhile, as there have been insufficient data, few studies have been conducted on the water-related nexus system, focusing on allocating water among competitive users and subsystems. Likewise, few studies have analyzed the interrelationships among Sustainable Development Goals in the economy, ecology, and society [28]. Moreover, future population growth, energy use, and economic development driven by human activities will impact resource utilization practices in the area. As one of the means of gaining insights into the future socioeconomic trajectories of current generations, the Shared Socioeconomic Pathways (SSPs) offer a potential tool for improving the capacity for comprehensively assessing the water−energy−economy−carbon−ecology (WEECE) nexus in a complex environment. Previously, SSPs were employed for global change assessment and policy analysis [29,30]. However, there has been a lack of research on how to synthesize the sustainable management of the SDGs in a comprehensive nexus framework following the SSPs toward the future context they outline.

1.3. Research gap and objectives

Certain research gaps were identified when reviewing the previous studies. First, most SDG research studies have focused on quantifying the impacts of the SDGs on a water- or energy-related nexus. These studies have lacked a comprehensive modeling framework to fully capture the interactions between different subsystems and components and conduct collaborative management of the SDGs. Second, most MOP studies have ignored the need for system efficiencies in multiple dimensions (e.g., economic, social, and ecological); they have also been limited by the subjectivity of how weights have been determined for different targets during the solution process. Third, as one of the most prominent areas of water scarcity and ecological degradation, the Kaidu−Kongqi River Basin has attracted widespread attention from international scholars; however, there has been little research on the potential for collaborative management of its water-related nexus system amid changing social−economic pathways and policy interventions.

In response to the research gaps, in this study, we developed a gray fractional multi-objective programming-based water−energy−economy−carbon−ecology (GFMOP-WEECE) nexus model aimed at optimizing resource allocation to ensure sustainability under future socioeconomic pathways. The developed GFMOP-WEECE nexus model was applied to the selected arid river basin in Northwest China, where multiple scenarios were analyzed with a combination of socioeconomic development baselines and policy options related to the SDGs. The major contributions and novelty of this study can be summarized as follows: (1) proposing a water−energy−economy−carbon−ecology nexus concept framework to capture the interrelationships among resource utilization, economic activities, ecosystem requirements, and carbon emissions, as four subsystems; (2) developing a nexus model (the GFMOP-WEECE) to balance multiple ratio objectives with reduced subjectivity and optimal system efficiency by incorporating multi-objective programming, fractional programming, and gray incidence methods; and (3) identifying the trade-offs and synergies among different sustainable targets under future socioeconomic scenarios, as well as providing planning strategies for socioeconomic development and eco-environmental protection.

2. Material and methods

2.1. Study area and data

The Kaidu−Kongqi River Basin, located in the southern Tianshan Mountains of Northwest China, is a typical semiarid and arid region covering an area of 62 × 10^3 km^2 [31]. The basin includes the Kaidu River and the Kongqi River (Fig. 1), which serve as vital water sources for the counties of Kuerle, Yanqi, Hejing, Hoxud, Bohu, and Yuli and contribute about 75% of the water recharge for Bosten Lake, with the annual mean runoff of 35 × 10^8 m^3 [32,33]. Under the continental climate, characterized by little precipitation and excessive evaporation, water has become the main restrictive factor for maintaining socioeconomic development and environmental sustainability in the KKRB [34]. By the end of 2020, the population of the river basin exceeded one million, spread over six counties, and the gross industrial and agricultural output values had reached CNY (Chinese Yuan) 15 × 10^9 and CNY 17 × 10^9, respectively [27]. Intensive agriculture irrigation, industrial production, and energy generation have posed significant eco-environmental problems regarding water supply, carbon emissions, and ecological degradation. In detail, irrigation consumes over 70% of the water; it is necessary due to the arid climate, extensive cultivation of water-intensive crops, and low efficiency of practices in the field. This irrigation has led to a 9% annual increase in water demand and a significant reduction in available water (at the pace of 9 × 10^6 m^3) since 2000. Although the KKRB is rich in renewable energy resources, such as solar, wind, and hydropower, it is economically and socially underdeveloped. Its primary energy source is coal (representing as much as 65% of the regional energy structure), which involves the consumption of substantial water resources and the emission of large amounts of greenhouse gases. To achieve China's carbon neutrality goals, a shift to more efficient and cleaner energy technologies is desired for energy structure in the KKRB [35]. Moreover, over-exploitation of water resources has degraded natural habitats in the area. During 2002−2012, the level of Bosten Lake fell, with the shrinkage of its inflow severely impairing the ecological security of the downstream Tarim River. Moreover, from 1990 to 2018, the area of desert riparian forest was reduced by a significant 1.8 × 10^4 km^2 due to a combination of drought and economic development [33]. To achieve sustainability and harmony in the KKRB, there is a recognized need to work toward ensuring the synergistic management of its water utilization, energy generation, ecological restoration, and carbon emissions.

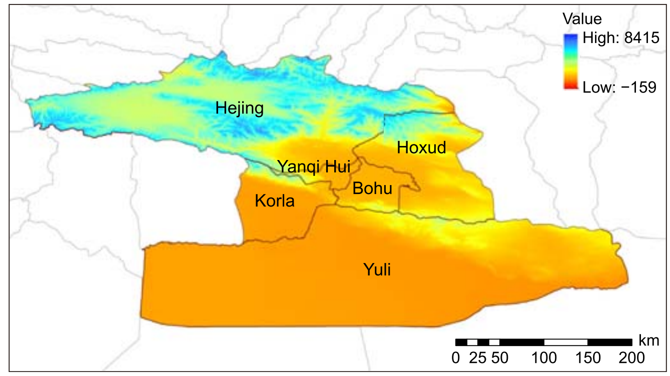


Fig. 1. The spatial pattern of the digital elevation model in the Kaidu-Kongqi River Basin, Northwest China.

Data for the model developed in this study were mainly obtained from the government statistical yearbooks, development plans, published references, and expert surveys. For example, the costs of energy generation and crop planting were derived from the Food and Agriculture Organization of the United Nations (FAOSTAT, www.fao.org); industrial water profits were calculated through a benefit-sharing coefficient method based on the Bayinguoleng Statistical Yearbook (2000−2020); the pollutant discharge and gas emissions of economic production were estimated via empirical emission coefficients while referring to Ba et al. (2020) [36] and Sun et al. (2020) [26]; the water consumption and carbon emission coefficients of energy exploitation, processing, and conversion were obtained from the IPCC 2006 Guidelines for the National Greenhouse Gas (GHG) Inventory and the related literature [37,38]; the water recycling rate and energy efficiency were ascertained from the 14th Five-Year Plan for Ecological Environment Protection in Xinjiang Uygur Zizhiqu and the Revolutionary Strategy of Energy

Production and Consumption (2016–2030); and representative costs and technical data on energy and agricultural production were drawn from the Electricity Statistical Yearbook of China, data collection in China's electric power industry, the 14th Five-Year Plan for Power Development, the China Water Resources Bulletin, and official government reports.

2.2. Development of the GFMOP-WEECE nexus model

In this study, a novel water–energy–economy–carbon–ecology nexus is proposed for coordinating SDGs by integrating four subsystems: water resources, the economy, energy, and ecology. Water security is the key factor constraining regional sustainable development for this arid river basin suffering from resource depletion and ecological degradation. Accordingly, the WEECE nexus has a water-centric perspective and focuses on motivating economic development, carbon emissions mitigation, ecosystem protection, and social equality through the conjunctive allocation of water and energy resources in an optimization framework. Managing the WEECE nexus is an intricate process when we consider the interactions between the four subsystems, coupled with different SDGs and the multiple sectors and stakeholders involved (Fig. 2). To account for these, based on the WEECE nexus framework, a GFMOP-WEECE nexus model is developed for planning resource allocation with sustainability as the goal in the future. This model includes four subsystems, three material flows, three water sources, nine water-use sectors, exploitation of three energy sources, three energy-processing technologies, thirteen energy conversion technologies, end uses for twelve energy sources, and a forty-year planning period. Regarding the specific interactions and material flows among various sectors, considering only the benefits or costs of different systems as a singular objective function would neglect the cooperative effects of subsystems and fail to uncover the potential for trade-offs between conflicting SDGs [39,40]. Four sustainable development objectives were examined in the economic, environmental, ecological, and social dimensions under thirty-two planning scenarios combining SSPs and sustainable strategy options to remedy this. The framework of this study is exhibited in Fig. 3. Next, the major equations of the GFMOP-WEECE nexus model will be provided below. For a better understanding of this model, the more detailed information on the GFMOP-WEECE nexus model is given in Appendices A and B, including the complete formulas and the physical meanings of the different parameters and variables involved.

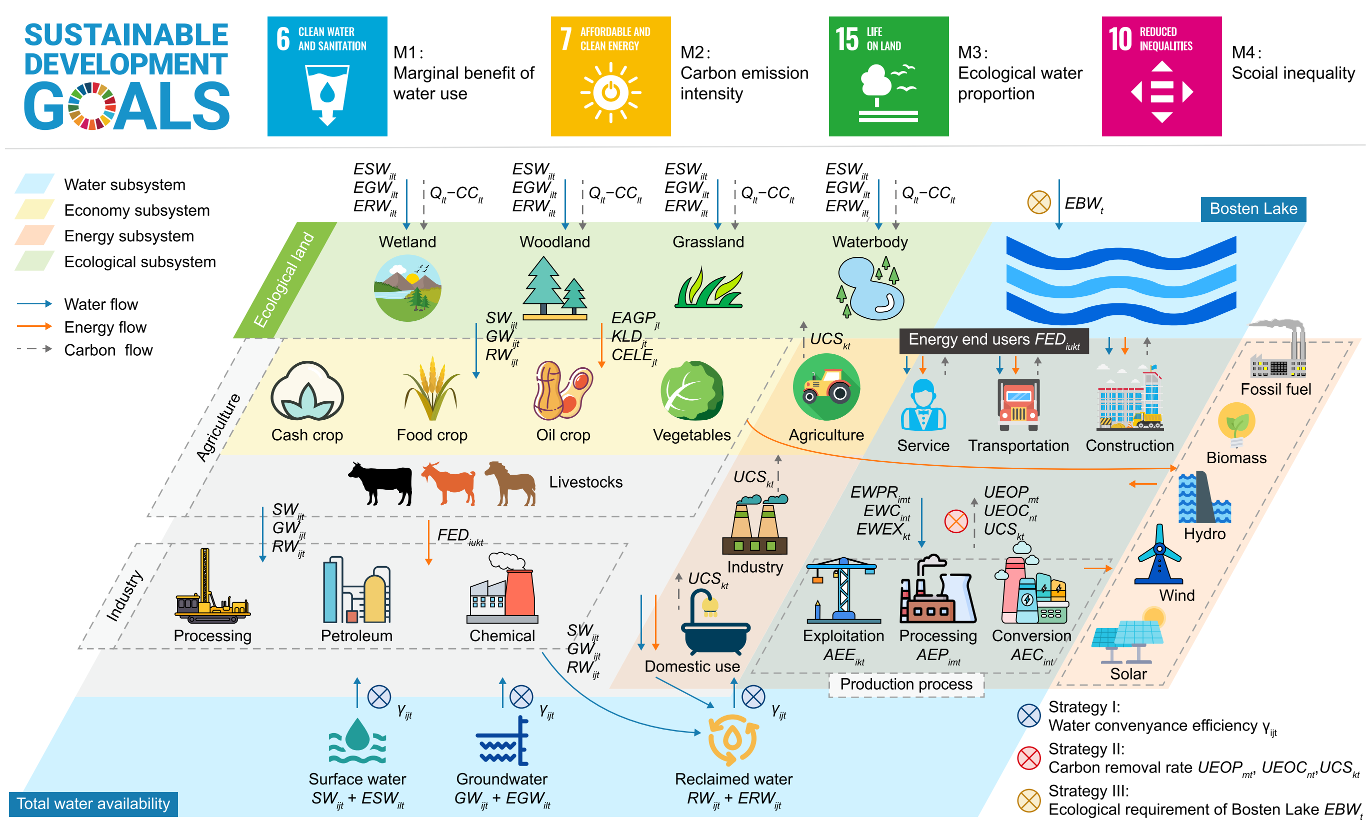


Fig. 2. Schematic diagram of the water–energy–economy–carbon–ecology (WEECE) nexus system. ESW_{ilt}: Surface water withdrawn for ecological sector l of county i in period t; EGW_{ilt}: Ground water withdrawn for ecological sector l of county i in period t; ERW_{ilt}: Reclaimed water withdrawn for ecological sector l of county i in period t; Q_{lt}: Carbon absorption of ecological sector l per ha; cc_{lt}: Carbon emission of ecological sector l per ha; EBW_t: Water inflow into Bosten Lake; SW_{ijt}: surface water withdrawn from Kaidu-Kongqi River for county i in period t; GW_{ijt}: ground water withdrawn for county i in period t; RW_{ijt}: Reclaimed water use from industry sector for county i in period t; UCS_{kt}: CO_2 emission factor of end-user for coal consumption during period t; $EAGP_{jt}$: Electricity consumption of agricultural products processing; KLD_{jt}: Diesel consumption of crop irrigation; $CELE_t$: Electricity consumption for drainage, drip and sprinkler irrigation; FED_{iukt}: Demand of energy k for end-user u during period t; γ_{ijt}: Water conveyance efficiency of user j; $EWPR_{mt}$: Amount of water required during energy processing in period t; EWC_{nt}: Amount of cooling water required during energy conversion in period t; $EWEX_{kt}$: Amount of water required during energy exploitation in period t; $UEOC_{nt}$: Emission factor of CO_2 for energy conversion technology n during period t; $UEOP_{mt}$: Emission factor of CO_2 by processing method m during period t; AEE_{ikt}: Amount of energy extraction for primary fossil fuel k during period t; AEP_{imt}: Amount of energy processing by processing method m during period t in county i; AEC_{int}: Amount of energy conversion for energy conversion technology n during period t in county i.

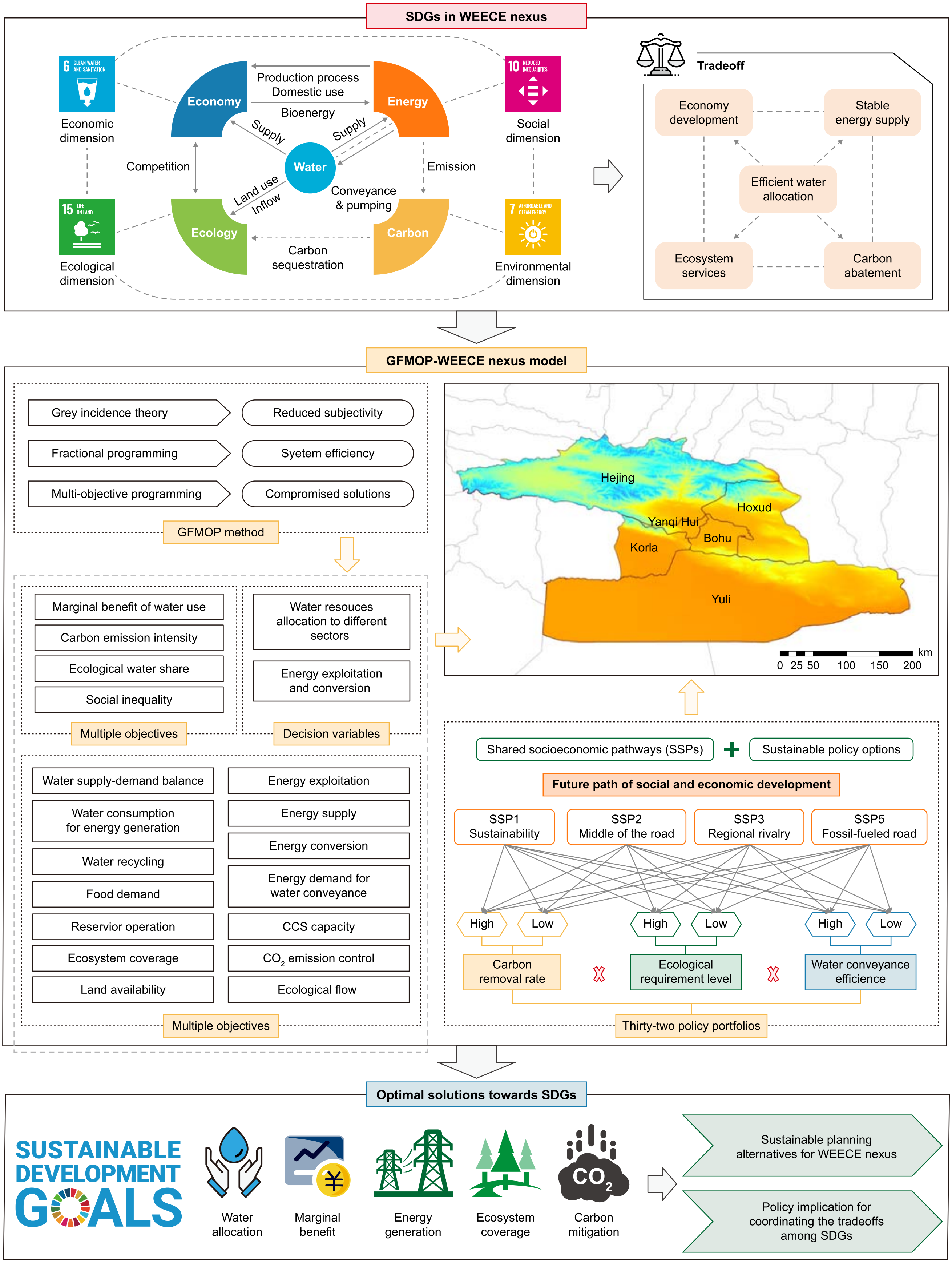


Fig. 3. Framework of this study. WEECE: water–energy–economy–carbon–ecology; GFMOP: Gray fractional multi-objective programming; SDGs: Sustainable development goals; CCS: Carbon capture and storage.

2.2.1. Objective function

(1) Economic dimension: Maximum marginal benefit of water use (MBW)

The marginal benefit reflects the water-use efficiency level (i.e., water productivity), which is a key concern when seeking to achieve sustainability in arid and semi-arid regions. Optimizing the marginal benefit means maximizing the system benefit per unit of water by optimally allocating the limited water resources to the agricultural, industry, domestic, energy, and ecological sectors. The profits of agricultural sectors are mainly derived from food production, which can be presented as the product of the crop price and yield. The agricultural costs include the costs of seeds, fertilizers, and pesticides, the costs of electricity for irrigation, drainage, and harvesting, the cost of diesel oil for farming machinery, and the cost of labor. The net profit of industry sectors can be calculated from the incomes from food processing, chemistry, and petroleum industrial activities, the extra benefit of water recycling, the costs of water pumping and conveyance, energy consumption, and fixed costs. The domestic profit equals the total revenue (including extra recycled water use) minus the water and energy consumption costs. The profits of the industrial and domestic sectors can be calculated via the benefit coefficient method. The net profits of the energy sector include the energy production revenue, energy export income, fuel exploitation cost, energy processing cost, energy conversion cost, pollutant control cost, water consumption cost, and carbon capture and storage (CCS) cost. The net profits of ecological sectors involve the ecosystem service values from instream environment flow and ecosystem land based on ten ecosystem service functions: the sediment transport value, climate regulation, sewage treatment, air pollutant absorption, biodiversity maintenance, organic matter production, carbon sequestration, oxygen release, water conservation, and soil retention. Thus, the objective function can be expressed as follows:

$$\text{Max } MBW = \frac{(PRO\_AGR + PRO\_DOM + PRO\_IND + PRO\_ECO + PRO\_ELE)}{WA} \tag{1}$$

where

$$\begin{aligned} PRO\_AGR = & \sum_{i}^{I}\sum_{j=1}^{5}\sum_{t}^{T} BW_{ijt} \times \frac{(SW_{ijt}+GW_{ijt}+DRW_{ijt})}{(1+LF_{ijt})} - \sum_{i}^{I}\sum_{j=1}^{5} \\ & \times \sum_{t}^{T} CE_{it} \times \left[\begin{array}{l} \frac{SW_{ijt}}{\gamma_{jt}} \times \frac{HK_{\mathrm{sur},it}}{102 \times 3.6 \times \mu_{\mathrm{sur},it}} + \frac{DRW_{ijt}}{\gamma_{jt}} \times \frac{HK_{\mathrm{sur},it}}{102 \times 3.6 \times \mu_{\mathrm{sur},it}} \\ + \frac{GW_{ijt}}{\gamma_{jt}} \times \frac{H_{\mathrm{lift},it} + H_{\mathrm{nop},it} + f_{\mathrm{loss},it}}{102 \times 3.6 \times \mu_{\mathrm{pump},it} \times \mu_{\mathrm{motor},it}} \end{array} \right] \\ & - \sum_{i}^{I}\sum_{j=1}^{5}\sum_{t}^{T} \frac{QF_{ijt} \times PF_{ijt} \times (SW_{ijt}+GW_{ijt}+DRW_{ijt})}{(1+LF_{ijt}) \times WPC_{ijt}} - \sum_{i}^{I}\sum_{j=1}^{4} \\ & \times \sum_{t}^{T} \frac{CE_{it} \times (SW_{ijt}+GW_{ijt}+DRW_{ijt}) \times \xi_{it} \times CELE_t}{(1+LF_{ijt}) \times WPC_{ijt}} - \sum_{i}^{I}\sum_{j=1}^{4} \\ & \times \sum_{t}^{T} \frac{CE_{it} \times YA_{ijt} \times (SW_{ijt}+GW_{ijt}+DRW_{ijt}) \times EAGP_{jt}}{(1+LF_{ijt}) \times WPC_{ijt}} - \sum_{i}^{I}\sum_{j=1}^{4} \\ & \times \sum_{t}^{T} \frac{(SW_{ijt}+GW_{ijt}+DRW_{ijt}) \times KLD_{jt} \times CKL_t}{(1+LF_{ijt}) \times WPC_{ijt}} - \sum_{i}^{I}\sum_{j=1}^{5} \\ & \times \sum_{t}^{T} \frac{FC_{ijt} \times (SW_{ijt}+GW_{ijt}+DRW_{ijt})}{(1+LF_{ijt}) \times WPC_{ijt}} \end{aligned} \tag{2}$$

$$\begin{aligned} PRO\_IND = & \sum_{i}^{I}\sum_{t}^{T}\sum_{j=6}^{8} BW_{ijt} \times (SW_{ijt}+GW_{ijt}+IRW_{ijt}+DRW_{ijt}) \\ & + \sum_{i}^{I}\sum_{t}^{T}\sum_{j=6}^{8} \alpha_{ijt} \times (SW_{ijt}+GW_{ijt}+IRW_{ijt}+DRW_{ijt}) \\ & \times (BR_{ijt} - TIC_{ijt}) - \sum_{i}^{I}\sum_{t}^{T}\sum_{j=6}^{8} CE_{it} \\ & \times \left[\begin{array}{l} \frac{SW_{ijt}+IRW_{ijt}+DRW_{ijt}}{\gamma_{jt}} \times \frac{HK_{\mathrm{sur},it}}{102 \times 3.6 \times \mu_{\mathrm{sur},it}} + \\ \frac{GW_{ijt}}{\gamma_{jt}} \times \frac{H_{\mathrm{lift},it} + H_{\mathrm{nop},it} + f_{\mathrm{loss},it}}{102 \times 3.6 \times \mu_{\mathrm{pump},it} \times \mu_{\mathrm{motor},it}} \end{array} \right] \end{aligned} \tag{3}$$

$$\begin{aligned} PRO\_DOM = & \sum_{i}^{I}\sum_{t}^{T} BW_{i9t} \times (SW_{i9t}+GW_{i9t}+DRW_{ijt}) + \sum_{i}^{I} \\ & \times \sum_{t}^{T}\sum_{j=9} \beta_{ijt} \times (SW_{ijt}+GW_{ijt}+DRW_{ijt}) \times (BR_{ijt} - TDC_{ijt}) - \sum_{i}^{I} \\ & \times \sum_{t}^{T} CE_{it} \times \left[\frac{SW_{i9t}}{\gamma_{9t}} \times \frac{HK_{\mathrm{sur},it}}{102 \times 3.6 \times \mu_{\mathrm{sur},it}} + \frac{GW_{i9t}}{\gamma_{9t}} \times \frac{H_{\mathrm{lift},it} + H_{\mathrm{nop},it} + f_{\mathrm{loss},it}}{102 \times 3.6 \times \mu_{\mathrm{pump},it} \times \mu_{\mathrm{motor},it}} \right] \end{aligned} \tag{4}$$

$$\begin{aligned} PRO\_ECO = & \sum_{t}^{T}\sum_{i}^{I}\sum_{l}^{L} \left\{ \begin{array}{l} \frac{ESW_{ilt}+EGW_{ilt}+ERW_{ilt}}{GWD_{lt}} \times \\ \left[\begin{array}{l} \sum_{k=1}^{2} (\beta_{lkt} \times VP_{kt} \times VPB_{kt}) + WP_{lt} \times TC_t + \\ V_t + ZP_{lt} \times \sum_{q=1}^{2} \sigma_q \times PI_{qt} \times I_q + RP_{lt} \times RC_t \\ + RP_{lt} \times RO_t \times RCI_t + TCI_t \times TP_{lt} \\ + LCI_t - (KCI_{lt} + ICI_{lt}) \end{array} \right] \end{array} \right\} \\ & - \sum_{t}^{T}\sum_{l}^{L} \\ & \times \sum_{i}^{I} CE_{lt} \times \left[\begin{array}{l} \frac{ESW_{ilt}}{\gamma_{it}} \times \frac{HK_{\mathrm{sur},it}}{102 \times 3.6 \times \mu_{\mathrm{sur},it}} + \frac{ERW_{ilt}}{\gamma_{it}} \times \frac{HK_{\mathrm{sur},it}}{102 \times 3.6 \times \mu_{\mathrm{sur},it}} \\ + \frac{EGW_{ilt}}{\gamma_{it}} \times \frac{H_{\mathrm{lift},it} + H_{\mathrm{nop},it} + f_{\mathrm{loss},it}}{102 \times 3.6 \times \mu_{\mathrm{pump},it} \times \mu_{\mathrm{motor},it}} \end{array} \right] \end{aligned} \tag{5}$$

$$
\begin{aligned}
PRO\_ENE = & \sum_{i=1}^{I}\sum_{j=1}^{J}\sum_{k=1}^{12}\sum_{t=1}^{T} RED_{kt}\times FED_{iukt} \\
& + \sum_{i=1}^{I}\sum_{k=1}^{12}\sum_{t=1}^{T} REX_{kt}\times AEX_{ikt} - \sum_{i=1}^{I}\sum_{k=1}^{3}\sum_{t=1}^{T} CEE_{kt}\times AEE_{ikt} \\
& - \sum_{i=1}^{I}\sum_{k=1}^{12}\sum_{t=1}^{T} CEI_{kt}\times AEI_{ikt} - \sum_{i=1}^{I}\sum_{m=1}^{3}\sum_{t=1}^{T} CEP_{mt}\times AEP_{imt} \\
& - \sum_{i=1}^{I}\sum_{n=1}^{11}\sum_{t=1}^{T} FCEC_{nt}\times CEC_{int} + VCEC_{nt}\times AEC_{int} + VCCC_{nt}\times ECC_{int} \\
& + \sum_{i=1}^{I}\sum_{n=5}^{8}\sum_{t=1}^{T} BCLP_{nt}\times AEC_{int} - \sum_{t=1}^{T} BCLP_{11,t}\times AEC_{i,11,t} \\
& - \sum_{i=1}^{I}\sum_{m=1}^{3}\sum_{t=1}^{T} AEP_{imt}\times UEOP_{mt}\times ROM_{t}\times COM_{t} \\
& - \sum_{i=1}^{I}\sum_{n=1}^{11}\sum_{t=1}^{T} AEC_{int}\times UEOC_{nt}\times ROM_{t}\times COM_{t} \\
& - \sum_{i=1}^{I}\sum_{q=1}^{3}\sum_{m=1}^{3}\sum_{t=1}^{T} AEP_{imt}\times UESP_{qmt}\times RSM_{qt}\times CSM_{qt} \\
& - \sum_{i=1}^{I}\sum_{q=1}^{3}\sum_{n=1}^{11}\sum_{t=1}^{T} AEC_{int}\times UESC_{qnt}\times RSM_{qt}\times CSM_{qt}
\end{aligned}
\tag{6}
$$

$$
\begin{aligned}
WA = & \sum_{t=1}^{T}\sum_{j=1}^{J}\sum_{i=1}^{I}(SW_{ijt}+GW_{ijt}) \\
& + \sum_{t=1}^{T}\sum_{j=1}^{J}\sum_{i=1}^{I}(ESW_{ilt}+EGW_{ilt}) \\
& + \sum_{k=1}^{3}\sum_{t=1}^{T} EWEX_{kt}\times AEE_{ikt} \\
& + \sum_{m=1}^{3}\sum_{t=1}^{T} EWPR_{mt}\times AEP_{imt} \\
& + \sum_{n=1}^{4}\sum_{t=1}^{T} EWC_{nt}\times AEC_{int} + \sum_{t=1}^{T} EWW_{t}\times AEC_{5t} \\
& + \sum_{n=1}^{11}\sum_{t=1}^{T} EWO_{nt}\times AEC_{int}
\end{aligned}
\tag{7}
$$

(2) Environmental dimension: Minimum carbon emission intensity (CEI)

Promoting the control of carbon emissions during water allocation and economic production processes is one of the key ways to achieve an emissions peak and carbon neutrality in the future [41]. The net carbon emissions of the WEECE nexus system mainly include the carbon emissions of energy sectors restricted by water allocation and the carbon absorption derived from ecosystem coverage subject to ecological water use. Hence, the second objective is to minimize the carbon emissions per unit of water use in the WEECE nexus system, which can be expressed as follows:

$$
\mathrm{Min}\,CEI = \frac{\begin{aligned} & \sum_{t}^{T}\sum_{i}^{I}\sum_{m=1}^{3}\sigma_t\times AEP_{imt}\times UEOP_{mt}\times(1-ROM_t)+ \\ & \sum_{t}^{T}\sum_{i}^{I}\sum_{n=1}^{11}\sigma_t\times AEC_{int}\times UEOC_{nt}\times(1-ROM_t)+ \\ & \sum_{t}^{T}\sum_{k}^{K}\sum_{i}^{I}\sum_{j}^{J}\sigma_t\times FED_{iukt}\times CSC_k\times UCS_{k,t}\times(1-ROME_{ukt})+\sum_{m}^{M}\frac{IC_{mt}}{L_{mt}}\times\sigma_t-\sum_{m}^{M}IC_{mt}\times r_t-\sum_{t}^{T}\sum_{l}^{L}\sum_{i}^{I}\frac{ESW_{ilt}+EGW_{ilt}+ERW_{ilt}}{GWD_{lt}}\times cc_{lt}\end{aligned}}{\sum_{t=1}^{T}\sum_{j=1}^{J}\sum_{i=1}^{I}(SW_{ijt}+GW_{ijt})+\sum_{t=1}^{T}\sum_{j=1}^{J}\sum_{i=1}^{I}(ESW_{ilt}+EGW_{ilt})+\sum_{k=1}^{3}\sum_{t=1}^{T}EWEX_{kt}\times AEE_{ikt}+\sum_{m=1}^{3}\sum_{t=1}^{T}EWPR_{mt}\times AEP_{imt}+\sum_{n=1}^{4}\sum_{t=1}^{T}EWC_{nt}\times AEC_{int}+\sum_{t=1}^{T}EWW_t\times AEC_{5t}+\sum_{n=1}^{11}\sum_{t=1}^{T}EWO_{nt}\times AEC_{int}}
\tag{8}
$$

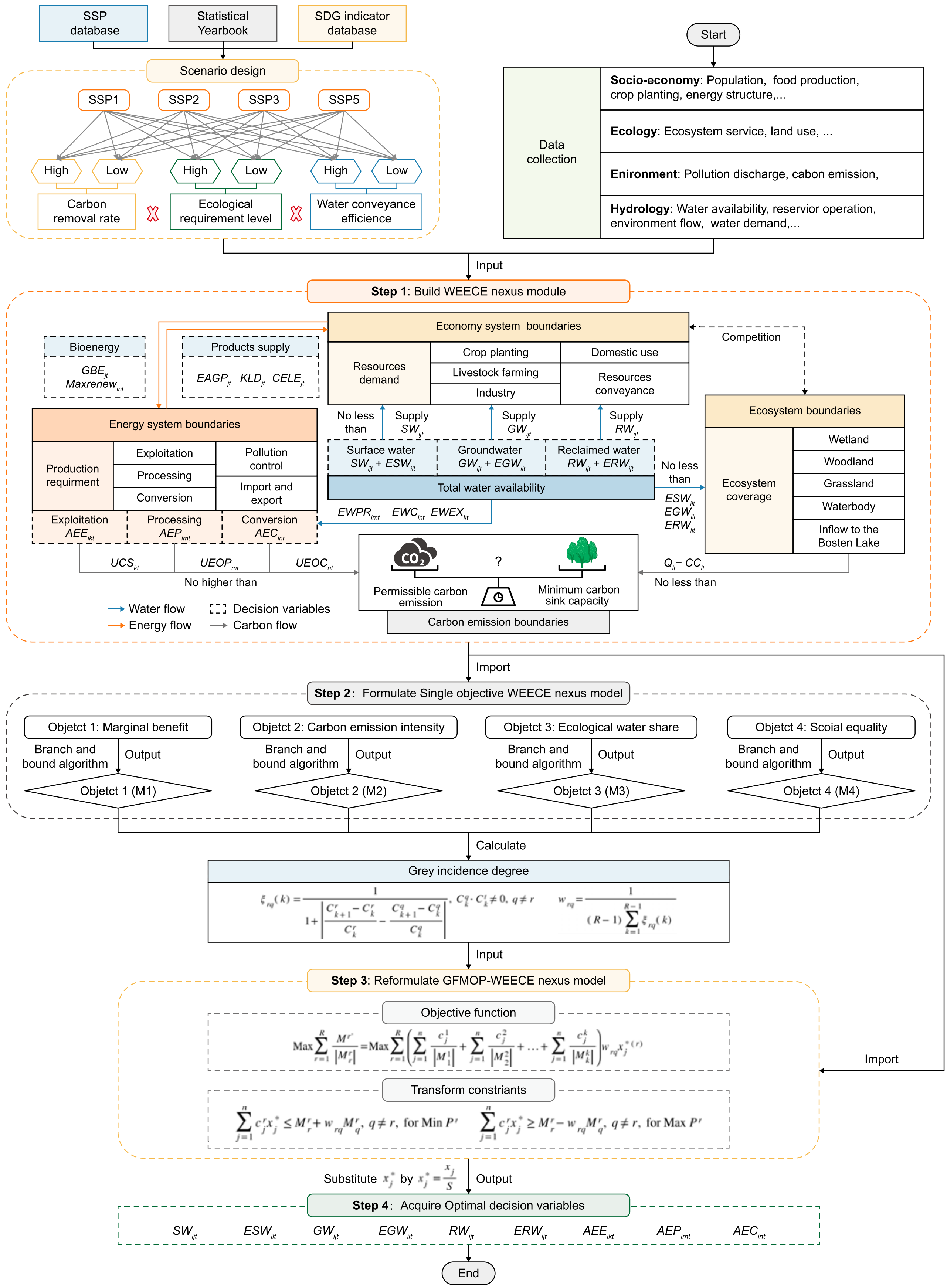
Table 1
Scenario matrix.

Scenario	Socioeconomic baseline	Sustainable options		
		Carbon removal rate (α)	Ecological requirement Level (β)	Water conveyance efficiency (γ)
$S_{1\text{-HHH}}$	SSP1	High	High	High
$S_{1\text{-HLH}}$		High	Low	High
$S_{1\text{-HHL}}$		High	High	Low
$S_{1\text{-LHH}}$		Low	High	High
$S_{1\text{-LLH}}$		Low	Low	High
$S_{1\text{-LHL}}$		Low	High	Low
$S_{1\text{-LHL}}$		Low	High	Low
$S_{1\text{-HLL}}$		High	Low	Low
$S_{1\text{-LLL}}$		Low	Low	Low
$S_{2\text{-HHH}}$	SSP2	High	High	High
$S_{2\text{-HLH}}$		High	Low	High
$S_{2\text{-HHL}}$		High	High	Low
$S_{2\text{-LHH}}$		Low	High	High
$S_{2\text{-LLH}}$		Low	Low	High
$S_{2\text{-LHL}}$		Low	High	Low
$S_{2\text{-LHL}}$		Low	High	Low
$S_{2\text{-HLL}}$		High	Low	Low
$S_{2\text{-LLL}}$		Low	Low	Low
$S_{3\text{-HHH}}$	SSP3	High	High	High
$S_{3\text{-HLH}}$		High	Low	High
$S_{3\text{-HHL}}$		High	High	Low
$S_{3\text{-LHH}}$		Low	High	High
$S_{3\text{-LLH}}$		Low	Low	High
$S_{3\text{-LHL}}$		Low	High	Low
$S_{3\text{-LHL}}$		Low	High	Low
$S_{3\text{-HLL}}$		High	Low	Low
$S_{3\text{-LLL}}$		Low	Low	Low
$S_{5\text{-HHH}}$	SSP5	High	High	High
$S_{5\text{-HLH}}$		High	Low	High
$S_{5\text{-HHL}}$		High	High	Low
$S_{5\text{-LHH}}$		Low	High	High
$S_{5\text{-LLH}}$		Low	Low	High
$S_{5\text{-LHL}}$		Low	High	Low
$S_{5\text{-LHL}}$		Low	High	Low
$S_{5\text{-HLL}}$		High	Low	Low
$S_{5\text{-LLL}}$		Low	Low	Low

(3) Ecological dimension: Maximum ecological water proportion (*EWP*)

Ecological crisis is a significant concern in the KKRB due to high evaporation rates and low precipitation. Perennial shortages in the ecological water supply in the KKRB have resulted in a constant decline in the water level of Bosten Lake and the large-scale degradation of grasslands. When models prioritize economic ratio objectives (e.g., the marginal benefit), agricultural and industrial activities are often prioritized in water allocation owing to their high benefits per unit of water, though this will raise the water requirements placed on the local ecosystems [26,42]. In 2019, the ecological water allocation in Xinjiang Uygur Zizhiqu only accounted for 2.83% of the total water allocation, significantly lower than the national average of 5.70% [6]. As the important indicator for restoring the downstream ecological corridor of the Kaidu−Kongqi River Basin, the third objective function is to maximize the comprehensive ecological water proportion (including meeting the water demand of ecological land and the necessary inflow into Bosten Lake), as follows:

$$\text{Max } EWP = \frac{\sum_{t}^{T}\sum_{i}^{I}\sum_{l}^{L}\frac{ESW_{ilt}+ERW_{ilt}}{\gamma_{lt}} + \sum_{t}^{T}\sum_{i}^{I}\sum_{l}^{L}\frac{EGW_{ilt}}{\gamma_{lt}} + TSW_t - \sum_{i}^{I}\sum_{j}^{J}\frac{SW_{ijt}}{\gamma_{ijt}} - \sum_{t}^{T}\sum_{i}^{I}\sum_{l}^{L}\frac{ESW_{ilt}}{\gamma_{lt}}}{\sum_{t=1}^{T}\sum_{j=1}^{J}\sum_{i=1}^{I}(SW_{ijt}+GW_{ijt}) + \sum_{t=1}^{T}\sum_{j=1}^{J}\sum_{i=1}^{I}(ESW_{ilt}+EGW_{ilt}) + \sum_{k=1}^{3}\sum_{t=1}^{T}EWEX_{kt}\times AEE_{ikt} + \sum_{m=1}^{3}\sum_{t=1}^{T}EWPR_{mt}\times AEP_{imt} + \sum_{n=1}^{4}\sum_{t=1}^{T}EWC_{nt}\times AEC_{int} + \sum_{t=1}^{T}EWW_t\times AEC_{5t} + \sum_{n=1}^{11}\sum_{t=1}^{T}EWO_{nt}\times AEC_{int}} \tag{9}$$



SSP database
Statistical Yearbook
SDG indicator database
Scenario design
SSP1
SSP2
SSP3
SSP5
High
Low
Carbon removal rate
Ecological requirement level
Water conveyance efficiency
Start
Data collection
Socio-economy: Population, food production, crop planting, energy structure,...
Ecology: Ecosystem service, land use, ...
Enironment: Pollution discharge, cabon emission,
Hydrology: Water availability, reservior operation, environment flow, water demand,...
Input
Step 1: Build WEECE nexus module
Economy system boundaries
Competition
Bioenergy
GBE
Maxrenew
Products supply
EAGP KLD CELE
Resources demand
Crop planting
Livestock farming
Industry
Domestic use
Resources conveyance
Energy system boundaries
Production requirment
Exploitation
Processing
Conversion
Pollution control
Import and export
Exploitation AEE
Processing AEP
Conversion AEC
No less than
Supply SW
Supply GW
Supply RW
Surface water SW + ESW
Groundwater GW + EGW
Reclaimed water RW + ERW
Total water availability
EWPR EWC EWEX
No less than
ESW EGW ERW
Ecosystem boundaries
Ecosystem coverage
Wetland
Woodland
Grassland
Waterbody
Inflow to the Bosten Lake
UCS UEOP UEOC
No higher than
Permissible carbon emission
?
Minimum carbon sink capacity
Carbon emission boundaries
Q − CC
No less than
Water flow
Energy flow
Decision variables
Carbon flow
Import
Step 2: Formulate Single objective WEECE nexus model
Objetct 1: Marginal benefit
Objetct 2: Carbon emission intensity
Objetct 3: Ecological water share
Objetct 4: Scoial equality
Branch and bound algorithm
Output
Objetct 1 (M1)
Objetct 2 (M2)
Objetct 3 (M3)
Objetct 4 (M4)
Calculate
Grey incidence degree
Input
Step 3: Reformulate GFMOP-WEECE nexus model
Objective function
Transform constriants
Import
Substitute x_j^* by $x_j^* = \frac{x_j}{S}$
Output
Step 4: Acquire Optimal decision variables
SW ESW GW EGW RW ERW AEE AEP AEC
End

Fig. 4. Flowchart of model composition and computational procedure. ESW_{ilt}: Surface water withdrawn for ecological sector l of county i in period t; EGW_{ilt}: Ground water withdrawn for ecological sector l of county i in period t; ERW_{ilt}: Reclaimed water withdrawn for ecological sector l of county i in period t; Q_{lt}: Carbon absorption of ecological sector l per ha; cc_{lt}: Carbon emission of ecological sector l per ha; EBW_t: Water inflow into Bosten Lake; SW_{ijt}: surface water withdrawn from Kaidu-Kongqi River for county i in period t; GW_{ijt}: ground water withdrawn for county i in period t; RW_{ijt}: Reclaimed water use from industry sector for county i in period t; UCS_{kt}: CO_2 emission factor of end-user for coal consumption during period t; $EAGP_{jt}$: Electricity consumption of agricultural products processing; KLD_{jt}: Diesel consumption of crop irrigation; $CELE_t$: Electricity consumption for drainage, drip and sprinkler irrigation; $EWPR_{mt}$: Amount of water required during energy processing in period t; EWC_{nt}: Amount of cooling water required during energy conversion in period t; $EWEX_{kt}$: Amount of water required during energy exploitation in period t; $UEOC_{nt}$: Emission factor of CO_2 for energy conversion technology n during period t; $UEOP_{mt}$: Emission factor of CO_2 by processing method m during period t; AEE_{ikt}: Amount of energy extraction for primary fossil fuel k during period t; AEP_{imt}: Amount of energy processing by processing method m during period t in county i; AEC_{int}: Amount of energy conversion for energy conversion technology n during period t in county i. GBE_{jt}: Conversion coefficient of biomass energy per unit yield of crops; $MAXrenew_{int}$: The availability of renewable energy n during period t in county i; SSP: Shared socioeconomic pathway; SSP1: The road of sustainability; SSP2: The road of medium challenges; SSP3: The road of regional rivalry; SSP5: The road of fossil-fueled development.

(4) Social dimension: Minimum social inequality of the WEECE nexus (SI)

Sustainable management of the WEECE nexus requires considering the fairness and rationality of resource allocation, which can help ensure social stability. Here, the Pietra–Ricci index describes the fairness of resource allocation among sub-regions [43]. The value range of the Pietra–Ricci index is 0–0.5, where a smaller value indicates a more balanced distribution of the WEECE nexus. Therefore, the objective function of the social dimension is to minimize the Pietra–Ricci index, which can be expressed as follows:

$$\mathrm{Min}\,SI=\frac{\dfrac{\sum_{i=1}^{I}\left|\begin{array}{l}\sum_{t=1}^{T}\sum_{j=1}^{J}SW_{ijt}+GW_{ijt}+\sum_{t=1}^{T}\sum_{l=1}^{L}ESW_{ilt}+EGW_{ilt}+\sum_{k=1}^{3}\sum_{t=1}^{T}EWEX_{kt}\times AEE_{ikt}\\+\sum_{m=1}^{3}\sum_{t=1}^{T}EWPR_{mt}\times AEP_{imt}+\sum_{n=1}^{4}\sum_{t=1}^{T}EWC_{nt}\times AEC_{int}+\sum_{t=1}^{T}EWW_t\times AEC_{5t}\\+\sum_{n=1}^{11}\sum_{t=1}^{T}EWO_{nt}\times AEC_{int}-\sum_{t=1}^{T}PO_{it}\end{array}\right|}{\sum_{t=1}^{T}\sum_{i=1}^{I}PO_{it}}}{2\times\left[\begin{array}{l}\sum_{t=1}^{T}\sum_{j=1}^{J}\sum_{i=1}^{I}(SW_{ijt}+GW_{ijt})+\sum_{t=1}^{T}\sum_{j=1}^{J}\sum_{i=1}^{I}(ESW_{ilt}+EGW_{ilt})+\\\sum_{k=1}^{3}\sum_{t=1}^{T}EWEX_{kt}\times AEE_{ikt}+\sum_{m=1}^{3}\sum_{t=1}^{T}EWPR_{mt}\times AEP_{imt}+\\\sum_{n=1}^{4}\sum_{t=1}^{T}EWC_{nt}\times AEC_{int}+\sum_{t=1}^{T}EWW_t\times AEC_{5t}+\\\sum_{n=1}^{11}\sum_{t=1}^{T}EWO_{nt}\times AEC_{int}\end{array}\right]} \tag{10}$$

2.2.2. Constraints

(1) Constraints of water availability

$$\begin{aligned}&TSW_t+TGW_t+\sum_{i}^{I}\sum_{t}^{T}\sum_{j=6}^{8}\alpha_{ijt}\times(SW_{ijt}+GW_{ijt}+DRW_{ijt}+IRW_{ijt})\\&+\sum_{i}^{I}\sum_{t}^{T}\sum_{j=9}\beta_{ijt}\times(SW_{ijt}+GW_{ijt}+DRW_{ijt})\geq\sum_{i}^{I}\sum_{j}^{J}\frac{SW_{ijt}+GW_{ijt}}{\gamma_{jt}}\\&+\sum_{t}^{T}\sum_{i}^{I}\sum_{l}^{L}\frac{ESW_{ilt}+EGW_{ilt}+ERW_{ilt}}{\gamma_{lt}}\\&+\sum_{k=1}^{3}\sum_{t=1}^{T}EWEX_{kt}\times AEE_{ikt}+\sum_{m=1}^{3}\sum_{t=1}^{T}EWPR_{mt}\times AEP_{imt}\\&+\sum_{n=1}^{4}\sum_{t=1}^{T}EWC_{nt}\times AEC_{int}+\sum_{t=1}^{T}EWW_t\times AEC_{5t}\\&+\sum_{n=1}^{11}\sum_{t=1}^{T}EWO_{nt}\times AEC_{int},\ \forall t\end{aligned} \tag{11}$$

$$\sum_{i}^{I}\sum_{j}^{J}\frac{GW_{ijt}}{\gamma_{jt}}\leq TGW_t\times PGE_t,\ \forall t \tag{12}$$

$$\begin{aligned}&\sum_{i}^{I}\sum_{t}^{T}\sum_{j=6}^{8}\alpha_{ijt}\times(SW_{ijt}+GW_{ijt}+DRW_{ijt}+IRW_{ijt})\leq CIM_{it\ \max}\\&+\sum_{i}^{I}\sum_{t}^{T}\sum_{j=9}\beta_{ijt}\times(SW_{ijt}+GW_{ijt}+DRW_{ijt})\leq CDM_{it\ \max}\end{aligned} \tag{13}$$

$$\begin{aligned}&\sum_{i}^{I}\sum_{j}^{J}DRW_{ijt}+\sum_{i}^{I}\sum_{j}^{J}IRW_{ijt}+\sum_{i}^{I}\sum_{l}^{L}ERW_{ilt}\leq\\&\sum_{i}^{I}\sum_{t}^{T}\sum_{j=6}^{8}\alpha_{ijt}\times(SW_{ijt}+GW_{ijt}+DRW_{ijt}+IRW_{ijt})+\\&\sum_{i}^{I}\sum_{t}^{T}\sum_{j=9}\beta_{ijt}\times(SW_{ijt}+GW_{ijt}+DRW_{ijt}),\ \forall t\end{aligned} \tag{14}$$

$$DRW_{ijt}+IRW_{ijt}=RW_{ijt},\ \forall i,j,t \tag{15}$$

(2) Constraints of water demands

$$SW_{ijt}+GW_{ijt}+DRW_{ijt}\geq DW_{ijt},\ \forall i,t,j=1,\ldots,5 \tag{16}$$

$$SW_{ijt}+GW_{ijt}+DRW_{ijt}+IRW_{ijt}\geq DW_{ijt},\ \forall i,t,j=6,\ldots,8 \tag{17}$$

$$SW_{ijt}+GW_{ijt}+DRW_{ijt}\geq DW_{ijt},\ \forall i,t,j=9 \tag{18}$$

(3) Constraint of land availability

$$A_{\min,it}\leq\sum_{j=1}^{4}\frac{SW_{ijt}+GW_{ijt}+DRW_{ijt}}{(1+LF_{ijt})\times WPC_{ijt}}\leq A_{\max,it},\ \forall i,t,j=1,\ldots,4 \tag{19}$$

(4) Constraint of water reuse rate

$$\frac{\sum_{i}^{I}\sum_{j}^{J}DRW_{ijt}+\sum_{i}^{I}\sum_{j}^{J}IRW_{ijt}+\sum_{i}^{I}\sum_{l}^{L}ERW_{ilt}}{\sum_{i}^{I}\sum_{j}^{J}(SW_{ijt}+GW_{ijt})}\geq PWR_t,\ \forall t \tag{20}$$

(5) Constraint of food demand

Table 2
Scenario assumption and data sources.

Scenario description		Level	Assumption	Key drivers	Scale	Data sources
Socioeconomic baseline (SSP)		SSP1	Sustainability, low emission and adaption challenge	GDP Population Industrial structure Crop land CO_2 emission	County	SSP Public database (https://tntcat.iiasa.ac.at/SspDb/) Gridded datasets for population and economy under Shared Socioeconomic Pathways (https://doi.org/10.57760/sciencedb.01683) Pan et al. (2020) [49] Zhang et al. (2021a) [50] Jing et al. (2022) [51]
		SSP2	Middle of the road, intermediate emission and adaptation challenge			
		SSP3	Regional rivalry, medium-to-high emission and adaption challenge			
		SSP5	Fossil-fueled development, high emission and low adaption challenge			
Sustainable options	Carbon removal rate (α)	High	Upper limit of CCUS potential of China in 2060	Carbon capture efficiency during energy processing, conversion and consumption	Basin	ACCA (2021) [52]
		Low	Lower bound of CCUS potential of China in 2060			
	Ecological requirement level (β)	High	Ecological water supply from Kaidu River to Bosten Lake under different runoff frequency of 25 %	Ecological flow into Bosten Lake	Basin	Wu (2019) [56] Ji et al. (2021) [57]
		Low	Ecological water supply from Kaidu River to Bosten Lake under different runoff frequency of 75 %			
	Water conveyance efficiency (γ)	High	By 2060, reach the highest level of water conveyance efficiency of provinces in China during 2003–2019	Water conveyance efficiency	Water user	Huang (2019) [54] Xu et al. (2021) [55] Guo (2013) [65]
		Low	By 2060, reach the average level of water conveyance efficiency during 2003–2019			

$$\sum_{i}^{I}\sum_{j=2}^{2}\frac{YA_{ijt}\times\left(SW_{ijt}+GW_{ijt}+DRW_{ijt}\right)}{\left(1+LF_{ijt}\right)\times WPC_{ijt}}\geq\sum_{i}^{I}FD_{it}\times PO_{it},\ \forall t \tag{21}$$

(6) Constraint of electricity consumption for agricultural production

$$\sum_{i}^{I}\sum_{j}^{J}\frac{\left(SW_{ijt}+GW_{ijt}+DRW_{ijt}\right)\times\xi_{it}\times CELE_{t}}{\left(1+LF_{ijt}\right)\times WPC_{ijt}}+\sum_{i}^{I}\sum_{j}^{J}\frac{YA_{ijt}\times\left(SW_{ijt}+GW_{ijt}+DRW_{ijt}\right)\times EAGP_{jt}}{\left(1+LF_{ijt}\right)\times WPC_{ijt}}\leq\sum_{u=1}FED_{iukt},\ \forall i,t,k=11,j=1,\ldots,4 \tag{22}$$

(7) Constraint of diesel oil for agricultural machinery

$$\sum_{i}^{I}\sum_{j=1}^{4}\frac{\left(SW_{ijt}+GW_{ijt}+DRW_{ijt}\right)\times KLD_{jt}}{\left(1+LF_{ijt}\right)\times WPC_{ijt}}\leq\sum_{i}^{I}\sum_{u=1}\sum_{k}^{K}FED_{iukt}\times\varsigma_{\mathrm{fe},t},\ \forall t,k=8 \tag{23}$$

(8) Constraint of bioenergy production from crop planting

$$\sum_{i}^{I}\sum_{j}^{J}\frac{YA_{ijt}\times\left(SW_{ijt}+GW_{ijt}+DRW_{ijt}\right)\times GBE_{jt}}{\left(1+LF_{ijt}\right)\times WPC_{ijt}}\geq MAXrenew_{int},\ \forall t,n=8,j=1,\ldots,4 \tag{24}$$

(9) Constraint of ecological flow into Bosten Lake

$$TSW_{t}-\sum_{i}^{I}\sum_{j}^{J}\frac{SW_{ijt}}{\gamma_{jt}}+\sum_{t}^{T}\sum_{i}^{I}\sum_{l}^{L}\frac{ESW_{ilt}}{\gamma_{lt}}+\sum_{k=1}^{3}\sum_{t=1}^{T}EWEX_{kt}\times AEE_{ikt}+\sum_{m=1}^{3}\sum_{t=1}^{T}EWPR_{mt}\times AEP_{imt}+\sum_{n=1}^{4}\sum_{t=1}^{T}EWC_{nt}\times AEC_{int}+\sum_{t=1}^{T}EWW_{t}\times AEC_{5t}+\sum_{n=1}^{11}\sum_{t=1}^{T}EWO_{nt}\times AEC_{int}-WKL_{t}\geq EBW_{t},\forall t \tag{25}$$

(10) Constraint of ecosystem land coverage

$$\sum_{i}^{I}\sum_{l}^{L}\frac{ESW_{ilt}+EGW_{ilt}+DRE_{ilt}}{GWD_{lt}}\geq TDE_{t},\ \forall t \tag{26}$$

(11) Constraint of energy exploitation

$$AEE_{i,k,t}\leq MAXAEE_{ikt},\ k=1,2,3,\ \forall i,t \tag{27}$$

(12) Constraint of water consumption for energy generation

$$\sum_{k=1}^{3}\sum_{t=1}^{T}EWEX_{kt}\times AEE_{ikt}+\sum_{m=1}^{3}\sum_{t=1}^{T}EWPR_{mt}\times AEP_{imt}+\sum_{n=1}^{4}\sum_{t=1}^{T}EWC_{nt}\times AEC_{int}+\sum_{t=1}^{T}EWW_{t}\times AEC_{5t}+\sum_{n=1}^{11}\sum_{t=1}^{T}EWO_{nt}\times AEC_{int}\leq TWE_{it},\ \forall i,t \tag{28}$$

(13) Constraints of supply and demand for raw coal, crude oil, and natural gas

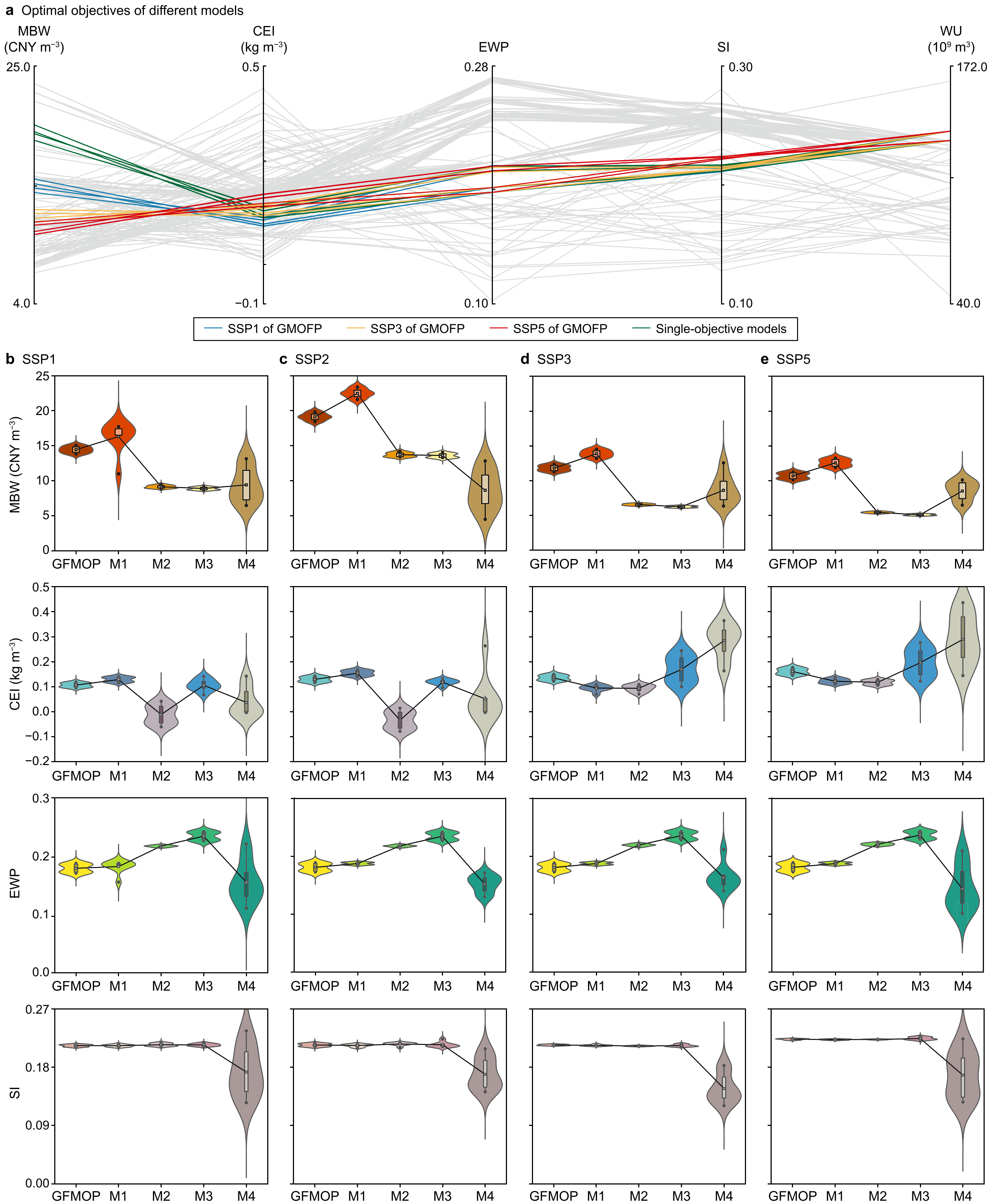


Fig. 5. Optimal objectives under multi-and single-objective models. **a**, Optimal objectives from the multi-objective model. **b**–**e**, Specific distributions of objectives from multi-and single-objective models under SSP1 (**b**), SSP2 (**c**), SSP3 (**d**), and SSP5 (**e**). SSP: Shared socioeconomic pathway; GFMOP: Gray fractional multi-objective programming; MBW: Marginal benefit of water use; CEI: Carbon emission intensity; EWP: Ecological water proportion; SI: Social inequality; M1:The single-objective optimization model targeting the marginal benefit of water use; M2: The single-objective optimization model targeting carbon emissions intensity; M3: The single-objective optimization model targeting proportion of ecological water use; M4: The single-objective optimization model targeting social inequality.

$$AEE_{ikt} + AEI_{ikt} - AEX_{ikt} - AEP_{i1t} \times UECP_{i1t} - \sum_{n=1}^{2} AEC_{int} \times UECC_{int} - AEC_{i9t} \times UECC_{i9t} - LR_{ikt} \geq \sum_{u=1}^{U} FED_{iukt}, k = 1, \forall i, t \tag{29}$$

$$AEE_{ikt} + AEI_{ikt} - AEX_{ikt} - AEP_{i3t} \times UECP_{3t} - LR_{ikt} \geq \sum_{u=1}^{U} FED_{iukt}, k = 2, \forall i, t \tag{30}$$

$$AEE_{ikt} + AEI_{ikt} - AEX_{ikt} - AEP_{i4t} \times UECP_{4t} + \sum_{n=3}^{4} AEC_{int} \times UECC_{nt} - AEC_{i10t} \times UECC_{10t} - LR_{ikt} \geq \sum_{u=1}^{U} FED_{iukt}, k = 3, \forall i, t \tag{31}$$

(14) Constraints of supply and demand for coal products (cleaned coal and coke)

$$AEI_{ikt} - AEX_{ikt} + AEP_{i1t} - AEP_{i2t} \times UECP_{2t} - LR_{ikt} \geq \sum_{u=1}^{U} FED_{iukt}, k = 4, \forall i, t \tag{32}$$

$$AEI_{ikt} - AEX_{ikt} + AEP_{i2t} - LR_{ikt} \geq \sum_{u=1}^{U} FED_{iukt}, k = 5, \forall i, t \tag{33}$$

(15) Constraints of supply and demand for oil products (gasoline, kerosene, diesel oil, and fuel oil)

$$AEI_{ikt} - AEX_{ikt} + 0.2 \times AEP_{i3t} - LR_{ikt} \geq \sum_{u=1}^{U} FED_{iukt}, k = 6, \forall i, t \tag{34}$$

$$AEI_{ikt} - AEX_{ikt} + 0.06 \times AEP_{i3t} - LR_{ikt} \geq \sum_{u=1}^{U} FED_{iukt}, k = 7, \forall i, t \tag{35}$$

$$AEI_{ikt} - AEX_{ikt} + 0.37 \times AEP_{i3t} - LR_{ikt} \geq \sum_{u=1}^{U} FED_{iukt}, k = 8, \forall i, t \tag{36}$$

$$AEI_{ikt} - AEX_{ikt} + 0.07 \times AEP_{i3t} - LR_{ikt} \geq \sum_{u=1}^{U} FED_{iukt}, k = 9, \forall i, t \tag{37}$$

$$AEI_{ikt} - AEX_{ikt} + AEP_{i4t} - LR_{ikt} \geq \sum_{u=1}^{U} FED_{iukt}, k = 10, \forall i, t \tag{38}$$

(16) Constraints of supply and demand for electricity and heat

$$\sum_{n=1}^{8} AEC_{int} \times (1 - LE_t) \geq \sum_{u=1}^{U} FED_{iukt}, k = 11, \forall i, t \tag{39}$$

$$(AEC_{i2t} + AEC_{i4t}) \times RHE_t + \sum_{n=9}^{11} AEC_{int} - LR_t \geq \sum_{u=1}^{U} FED_{iukt}, k = 12, \forall i, t \tag{40}$$

(17) Constraint of energy conversion

$$CEC_{int} \times OT_{nt} \geq AEC_{int}, \forall i, n, t \tag{41}$$

(18) Constraint of pollutant reduction for energy generation

$$\sum_{q=1}^{3} \sum_{m=1}^{3} \sum_{t=1}^{T} AEP_{imt} \times UESP_{qmt} \times RSM_{qt} + \sum_{q=1}^{3} \sum_{n=1}^{11} \times \sum_{t=1}^{T} AEC_{int} \times UESC_{qnt} \times RSM_{qt} + \sum_{q=1}^{3} \sum_{u=1}^{U} \sum_{k=1}^{12} \times \sum_{t=1}^{T} FED_{iukt} \times CSC_{ukt} \times UPS_{it} \times RSME_{it} \leq TLP_{iqt}, \forall t \tag{42}$$

(19) Constraint of CCS capacity

$$\sum_{m}^{M} IC_{mt} \leq \sum_{m}^{M} \left(\frac{IC_{mt}}{L_{mt}} \times \sigma_t \right) + \sum_{t}^{T} \sum_{i}^{I} \sum_{m=1}^{3} \sigma_t \times AEP_{imt} \times UEOP_{mt} \times (1 - ROM_t) + \sum_{t}^{T} \sum_{i}^{I} \sum_{n=1}^{11} \sigma_t \times AEC_{int} \times UEOC_{nt} \times (1 - ROM_t) + \sum_{t}^{T} \sum_{k}^{K} \sum_{i}^{I} \sum_{u}^{U} \times \sigma_t \times FED_{iukt} \times CSC_{ukt} \times UCS_{kt} \times (1 - ROME_{ukt}), \forall t \tag{43}$$

(20) Constraint of CO_2 emissions

$$\sum_{t}^{T} \sum_{i}^{I} \sum_{n=1}^{11} \sigma_t \times AEC_{int} \times UEOC_{nt} \times (1 - ROM_t) + \sum_{t}^{T} \sum_{k}^{K} \sum_{i}^{I} \sum_{j}^{J} \sigma_t \times FED_{ijkt} \times CSC_{ukt} \times UCS_{kt} \times \left(1 - ROME_{jkt}\right) + \sum_{m}^{M} \left(\frac{IC_{mt}}{L_{mt}} \times \sigma_t \right) - \sum_{m}^{M} IC_{mt} \times r_t - \sum_{t}^{T} \sum_{l}^{L} \times \sum_{i}^{I} \frac{ESW_{ilt} + EGW_{ilt} + ERW_{ilt}}{GWD_{lt}} \times cc_{lt} \leq \sum_{i}^{I} TLC_{it}, \forall t \tag{44}$$

2.2.3. Assumptions and limitations

Certain basic assumptions were made to clarify the limitations

Table 3
The interactive effects of different objectives under the GFMOP-WEECE nexus model.

Variables	Indexes	MBW	CEI	EWP	SI
MBW	Pearson correlation	1	−0.775[a]	0.846[a]	−0.818[a]
	Sig. (two-tailed)	-	0.000	0.000	0.000
	N	32	32	32	32
CEI	Pearson correlation	−0.775[a]	1	−0.551[a]	0.871[a]
	Sig. (two-tailed)	0.000	-	0.001	0.000
	N	32	32	32	32
EWP	Pearson correlation	0.846[a]	−0.551[a]	1	−0.658[a]
	Sig. (two-tailed)	0.000	0.001	-	0.000
	N	32	32	32	32
SI	Pearson correlation	−0.818[a]	0.871[a]	−0.658[a]	1
	Sig. (two-tailed)	0.000	0.000	0.000	-
	N	32	32	32	32

[a] Correlation is significant at the 0.05 level (two-tailed).

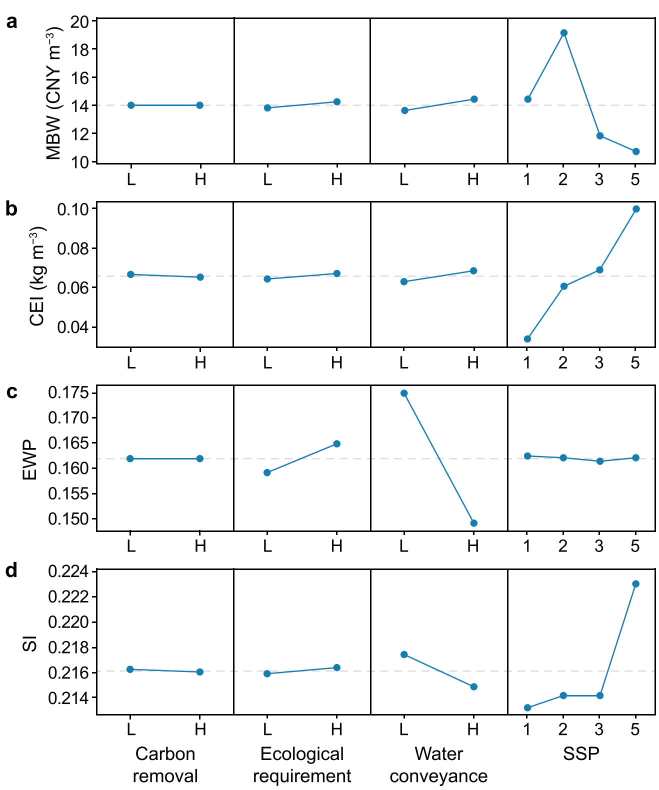


Fig. 6. The effects of different scenarios on marginal benefit of water use (**a**), carbon emissions intensity (**b**), proportion of ecological water use (**c**), and social inequality (**d**) under the GFMOP model. L: Low level; H: High level; MBW: Marginal benefit of water use; CEI: Carbon emission intensity; EWP: Ecological water proportion; SI: Social inequality.

of the model concerning the actual conditions of the WEECE nexus system.

(1) The model framework assumes that all available water resources (including surface water, groundwater, and reclaimed water) can be freely allocated to any user as long as all constraints are satisfied. This assumption ensures equalized access to water resources among all users to achieve the optimal water use efficiency throughout the river basin.
(2) The model is developed to plan water and energy resource allocation with a top-down perspective. The large-scale facility demolition and renewal and the lifespan of industrial facilities are not considered specifically since the WEECE nexus mainly depicts the water, energy, and carbon flows among different system components. In this study, the depreciation costs of all fixed assets are simplified into the unit water benefit and fixed cost (i.e., BW_{ijt} and TIC_{ijt}) in the model.
(3) The minimum ecological flow into Bosten Lake is considered in the constraint for water resource allocation; the instream flows (WKL_t) and the inflow to Bosten Lake (EBW_t) are guaranteed first, and then water resources can be allocated to different water use sectors and regions, which is a conventional approach in practice [44]. The ecological water demands of Bosten Lake, mainly arising from the Kaidu River, other tributaries, and groundwater recharge, are not considered in this model.
(4) A long-term horizon is highlighted in the developed model, assuming that the trajectory of future runoff is known with certainty based on historical records. The assumption of available resources provides a conservative lower-bound benchmark for estimating impacts and flexible support for the current institutions, which can be used to better account for relative values and changes amid limited water resources.
(5) Although the developed model is applied to the KKRB in Northwest China in this study, it is also applicable to efforts aimed at the synergistic management of SDGs in other arid/semi-arid river basins, which requires substituting the data inputs based on regional characteristics.

2.2.4. Solution method

The key to solving the optimization model is to transform the nonlinear, multi-objective programming model into a linear, single-objective programming model. Two steps are needed in this transformation: the application of the gray incidence multi-objective algorithm proposed by Meng and Wang (2014) and the application of the branch and bound algorithm [20,45]. First, the general fractional, multi-objective programming model can be transformed into a linear form by using the branch and bound algorithm through the auxiliary variable method, as follows:

$$\text{Max } f^r = P^r\left(x_j^*\right), if\ r \in I, Q\left(x_j^*\right), \text{if } \ r \in I^c, r = 1, 2, \ldots, R \tag{44a}$$

subject to

$$\sum_{j=1}^{n} a_{ij}\left(x_j^*\right) \le b_i \times s, i = 1, 2, \ldots m, j = 1, \ldots, n \tag{44b}$$

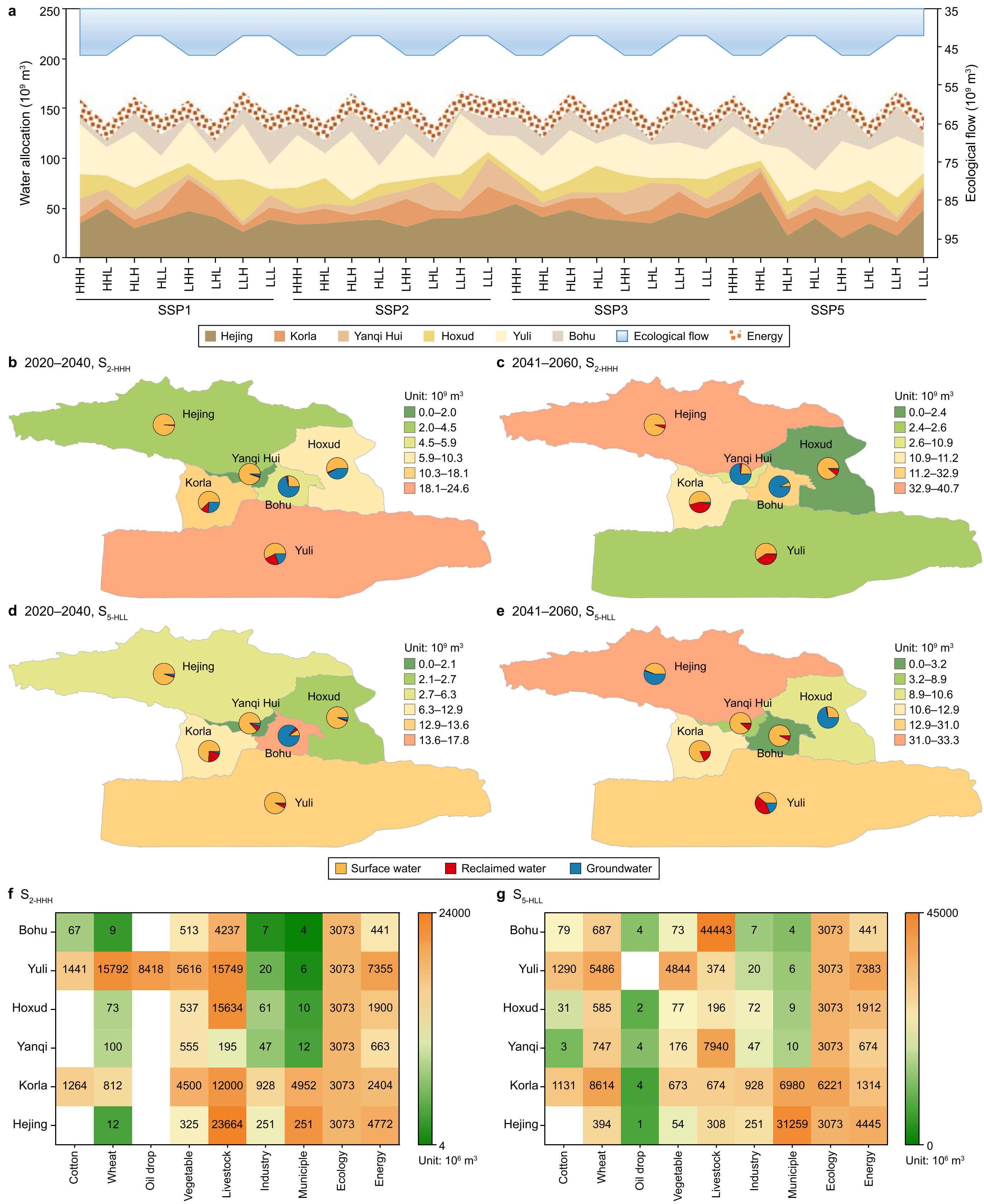


Fig. 7. Water allocation structures in different regions. **a,** Water allocation amounts under different scenarios. **b**–**c,** Regional water allocation and supply structure of different water sources under $S_{2\text{-HHH}}$ during 2020–2040 (**b**) and 2041–2060 (**c**). **d**–**e,** Regional water allocation and supply structure of different water sources under $S_{5\text{-HLL}}$ during 2020–2040 (**d**) and 2041–2060 (**e**). **e**–**f,** Water allocation of different sectors under $S_{2\text{-HHH}}$ (**e**) and $S_{5\text{-HLL}}$ (**f**). $S_{5\text{-HLL}}$: Scenario of high carbon removal rate, low ecological requirement, and low water conveyance efficiency under SSP5 (the road of fossil-fueled development); $S_{2\text{-HHH}}$: Scenario of high carbon removal rate, low ecological requirement, and low water conveyance efficiency under SSP2 (the road of medium challenges).

$$P^r\left(x_j^*\right)=1, if\ r\in I, -Q\left(x_j^*\right)=1, \text{if } r\in I^c; s>0, x_j^*>0, j=1,2,\ldots,n \tag{44c}$$

where $x_j^* = x_j \times s$, $s = \frac{1}{\sum_{j=1}^{n} d_j x_j + \beta}$, and the constraint set is a convex set with feasible points. Then, the incidence degree based on gray theory is introduced to characterize the relationships among objective functions and convert multiple objectives into one. Constraint conditions are constructed for new single-objective programming. The solution to the original multi-objective optimization problem can be obtained without excessive computation or judgment subjectivity in determining weights. The optimal values $C^r X^{(r)}$ of each objective and decision variables $X^{(r)}$ can be acquired by solving each objective function individually with all constraints $p_r^r = C^r X^{(r)}$. Assuming the desired solution is $X^{(0)} = (X_1, X_2, \ldots, X_n)$, the optimal objective can be $p^{r'} = C^r X^{(0)}$. According to Meng and Wang (2014), the multi-objective model can be transformed as follows:

$$\text{Max} \sum_{r=1}^{R} \frac{p^{r'}}{|p_r^r|} = \text{Max} \sum_{r=1}^{R} \left(\sum_{j=1}^{n} \frac{c_j^1}{|p_1^1|} + \sum_{j=1}^{n} \frac{c_j^2}{|p_2^2|} + \ldots + \sum_{j=1}^{n} \frac{c_j^k}{\left|p_k^k\right|} \right) w_{rq} x_j^{*(r)} \tag{45a}$$

subject to

$$\sum_{j=1}^{n} c_j^r x_j^* \geq p_r^r - w_{rq} p_q^r, q \neq r, \text{for Max } P^r \tag{45b}$$

$$\sum_{j=1}^{n} c_j^r x_j^* \leq p_r^r + w_{rq} p_q^r, q \neq r, \text{for Min } P^r \tag{45c}$$

$$\sum_{j=1}^{n} a_{ij} \left(x_j^*\right) \leq b_i \times s, i = 1, 2, \ldots m, j = 1, \ldots, n \tag{45d}$$

$$w_{rq} = \frac{1}{(R-1) \times \sum_{k=1}^{R-1} \left[1 + \left| \frac{C_{k+1}^r - C_k^r}{C_k^r} - \frac{C_{k+1}^q - C_k^q}{C_k^q} \right| \right]}, C_k^q \times C_k^t \neq 0, k = 1, 2, \ldots, R-1 \tag{45e}$$

where w_{rq} is the similitude degree of incidence. By substituting x_j^* with $x_j^* = \frac{x_j}{s}$, the GFMOP can be solved. Details of the solution algorithms for the GFMOP method can be found by referring to the Supplementary Materials.

2.3. Scenario design

As shown in Table 1, thirty-two scenarios were analyzed by combining four socioeconomic development baselines (i.e., the shared socioeconomic pathways: SSP1, SSP2, SSP3, and SSP5) and eight sustainable strategy options (including two carbon removal rates of energy production, two conveyance efficiencies of water resources, and two ecological requirement levels of Bosten Lake). Combining sustainable strategies with SSPs and comprehensively evaluating the impacts of socioeconomic and environmental policies on the WEECE nexus, has practical significance for the sustainable use of water, energy, and land resources and identifying the best management alternatives for the KKRB.

The SSPs provide baselines for future socioeconomic development in terms of multiple factors such as population, technological, and economic growth. SSP1 describes a sustainability-focused path (i.e., the Green Road) that achieves development goals with lower resource intensity, less fossil fuel utilization, and lower regional inequality. SSP2 represents an intermediate path (i.e., the Middle of the Road) in which social, economic, and technological trends do not shift markedly from historical patterns. SSP3 envisions a regional rivalry path (i.e., the Rocky Road) where economic development is slow, consumption is material intensive, and inequalities persist over time. SSP4 charts an imbalanced path (i.e., the Divided Road) with ever-increasing inequalities and stratification both across and within countries. SSP5 indicates a fossil-fueled development path (i.e., the Highway) where resource-intensive, fossil-fuel-based production practices will drive economic and social development. SSP1 and SSP5 envision relatively optimistic trends for economic development with opposite paths. SSP2, meanwhile, assumes moderate progress in achieving the Sustainable Development Goals. SSP3 and SSP4 share many elements, and SSP3 is relatively more representative in providing a pessimistic pathway considering national competition. Therefore, SSP1, SSP2, SSP3, and SSP5, widely used in previous studies [29,46,47], were selected to reflect rational and typical conditions for future socioeconomic development.

Economic, demographic, industrial, and ecological data were first predicted to forecast future resource allocation patterns under different SSPs. The population, industrial mix, and gross domestic product (GDP) were determined from the gridded SSP population and economic data from 2021 to 2100, based on the Population–Development–Environment (PDE) model and the Cobb–Douglas production model [48]. The land-use patterns, energy structure, and carbon emissions were derived from the related literature and government statistical data. All the inputs for the SSP scenarios were processed with data assimilation. In detail, SSP grid data were classified and aggregated to obtain county-level population and industrial structure data during 2021–2060 based on geographical locations. According to the carbon emission prediction trends in Xinjiang Uygur Zizhiqu provided by Pan et al. (2020) [49], county-level carbon emission data were calculated based on the proportions of the population and the GDP in the Kaidu–Kongqi River Basin. Additionally, based on the prediction trends for land use and the energy structure published by Zhang et al. (2021a) [50] and Jing et al. (2022) [51], future energy production structures for each county were determined according to the historical and current data of the Bayingolin Mongol Autonomous Prefecture. These data were modified based on the Xinjiang Production & Construction Group Statistical Yearbook, the Bulletin of Ecological Environment Protection of the Bayangol Mongol Autonomous Prefecture in 2021, and related studies by multiplying the proportion and growth rate.

Although the SSPs have a range of possible business-as-usual features, they do not explicitly include any commitments to enacting sustainable strategies. To remedy this, sustainable strategy options were combined with the SSPs to evaluate the impacts of different policy scenarios on the WEECE nexus about achieving sustainability in the future. In detail, the carbon removal rate of energy production was determined based on the status report of carbon capture, utilization and storage (CCUS) progress in China [52] and the Big Earth Data in Support of the Sustainable Development Goals [53]. The water conveyance efficiency was selected to control the water loss amid limited water availability. Relevant data were extracted from historical records from the Bayinguoleng Statistical Yearbook and prediction results from Huang (2019) [54] and Xu et al. (2021) [55]. As China's largest freshwater lake inland, Bosten Lake of the KKRB should be guaranteed an ecological flow to

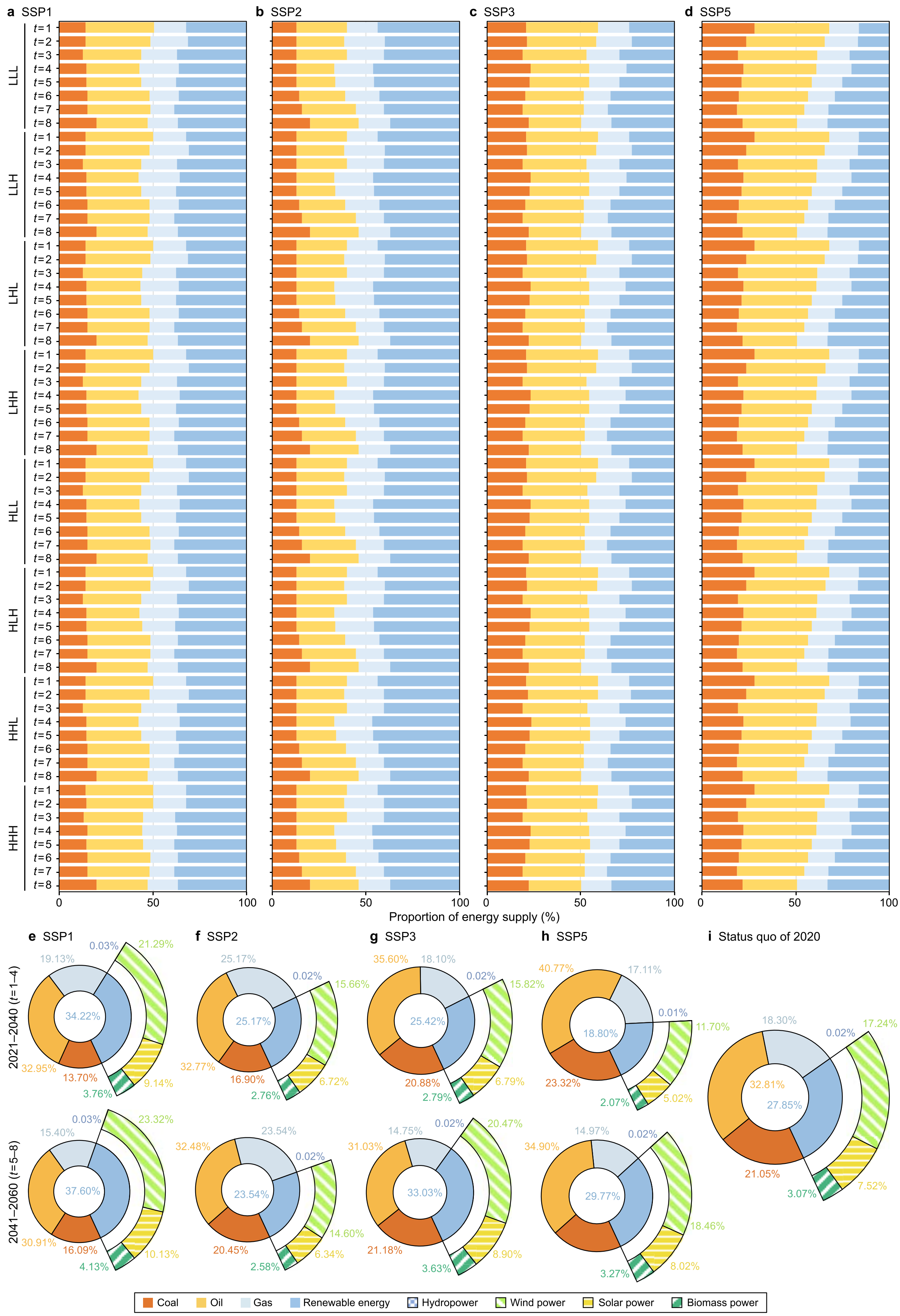

a SSP1
b SSP2
c SSP3
d SSP5
LLL
LLH
LHL
LHH
HLL
HLH
HHL
HHH
t=1
t=2
t=3
t=4
t=5
t=6
t=7
t=8
0
50
100
Proportion of energy supply (%)
e SSP1
f SSP2
g SSP3
h SSP5
i Status quo of 2020
2021–2040 (t=1–4)
2041–2060 (t=5–8)
19.13%
0.03%
21.29%
34.22%
32.95%
13.70%
3.76%
9.14%
25.17%
0.02%
15.66%
25.17%
32.77%
16.90%
2.76%
6.72%
35.60%
18.10%
0.02%
15.82%
25.42%
20.88%
2.79%
6.79%
40.77%
17.11%
0.01%
11.70%
18.80%
23.32%
2.07%
5.02%
18.30%
0.02%
17.24%
32.81%
27.85%
21.05%
3.07%
7.52%
0.03%
23.32%
15.40%
37.60%
30.91%
16.09%
4.13%
10.13%
32.48%
23.54%
0.02%
23.54%
14.60%
20.45%
2.58%
6.34%
31.03%
14.75%
0.02%
20.47%
33.03%
21.18%
3.63%
8.90%
34.90%
14.97%
0.02%
29.77%
18.46%
3.27%
8.02%
Coal
Oil
Gas
Renewable energy
Hydropower
Wind power
Solar power
Biomass power

Fig. 8. Energy supply patterns over the planning horizon (2021–2060). **a–d,** Energy structure over planning periods under SSP1 (**a**), SSP2 (**b**), SSP3 (**c**), and SSP5 (**d**). **e–f,** Specific energy supply proportions of scenarios with high-level of carbon removal rate, high-level ecological requirement, and high level of water conveyance efficiency under SSP1 (**e**), SSP2 (**f**), SSP3 (**g**), and SSP5 (**h**). L: Low level; H: High level; SSP: Shared socioeconomic pathway; SSP1: The road of sustainability; SSP2: The road of medium challenges; SSP3: The road of regional rivalry; SSP5: The road of fossil-fueled development.

maintain ecosystem health. Taking the historical observations of the Dashankou Hydrological Station from 1970 to 2018 as a data series, the runoffs of the Kaidu River into Bosten Lake were divided into wet and dry conditions using the frequency analysis method [56,57]. Two levels of ecological requirements for Bosten Lake were investigated, corresponding to the hydrologic frequencies of 25% and 75%, respectively.

Fig. 4 presents a flowchart for developing the GFMOP-WEECE nexus model and its computational logic. The first step was to collect data and design the scenarios of SSP baselines and sustainable strategy options for the river basin; the second step was to formulate the WEECE nexus model and define the system boundaries, operational logic, decision variables, resources, and carbon flows; the third step was to formulate single objective models for the WEECE nexus and obtain solutions by using the branch and bound algorithm; the fourth step was to calculate a similitude degree of incidence for each objective function and reformulate the new objective function, expressed as a minimization of deviation based on the gray incidence degree. The fifth step was to solve the transformed linear model and generate optimal results under thirty-two scenarios for SSP baselines and sustainable strategy options. The scenario matrix and data sources are listed in Tables 1 and 2. The subscripts of the scenario names represent different combinations of SSPs and sustainable options. For example, $S_{1\text{-HLH}}$ denotes the scenario under SSP1, a high carbon removal rate, a low ecological requirement, and a high water conveyance efficiency. The core input data for the different scenarios are given in the Supplementary Materials.

3. Results analysis

3.1. Synergy and trade-offs of multiple objectives

The WEECE nexus includes four subsystems (i.e., water, energy, ecology, and economy), three Sustainable Development Goals, and three main material flows (water, energy, and carbon) (Fig. 3). Different objectives and system components are interconnected, and any change in one subsystem can influence the others, resulting in variations in different objectives. For instance, increasing the ecological water proportion will restrict economic and energy production resource use, affecting the marginal benefit and carbon emission intensity. Conversely, reducing the carbon emission intensity will drive changes in both the energy and economic structures toward a decreased energy consumption, potentially enhancing the proportion of ecological water allocation for carbon sinks. To illustrate the interrelationships and interactions among multi-dimensional SDGs, a parallel coordinate plot is introduced to depict the variations in the optimal objectives under different scenarios. Fig. 5 shows the selection of socioeconomic pathways, demonstrating a trade-off among sustainability goals. Generally, a multi-objective model's sustainability performance follows the SSP2 > SSP1 > SSP3 > SSP5 trend. Under the intermediate development pathway (SSP2), the marginal benefit reaches its peak value (CNY 19.8 m^{-3}, under $S_{2\text{-HHH}}$) across all shared socioeconomic pathways. This shows a reduction in carbon intensity, an increase in the ecological water proportion, and a slight improvement in social inequality compared to the fossil-fueled development path (SSP5). With the over-exploitation of fossil fuels and resource-intensive lifestyles, SSP5 leads to higher water withdrawal, massive water loss, and lower marginal effectiveness of resource allocation (averaging a 44.2% decline compared to SSP2). On the other hand, the sustainable path (SSP1) with the lowest resource and energy consumption may reduce the economic benefit of the nexus system. Therefore, the WEECE nexus plans under the intermediate path (SSP2) are optimal and can be adopted. As shown in Table 3, the correlation analysis results illustrate that the carbon intensity and social inequality are negatively correlated with the marginal benefit, indicating that promoting the economic efficiency of water use will yield synergistic benefits in the environmental and social dimensions. Additionally, the carbon intensity related to the energy subsystem exhibits a strong positive correlation with social inequality, implying that high-intensity energy production will further exacerbate social inequality in the KKRB.

Based on the results of the multi-factorial experiment, the variation in SSPs has greater impacts on the model objectives than the variation in the sustainable strategy options (Fig. 6). The SSP baseline settings involve a series of model parameters, including the population, GDP, land use, and energy structure. Compared with sustainable options related to individual parameters, selecting SSP baselines more significantly alters the model inputs, leading to substantial changes in system components and objectives. The results illustrate that enhancing the water conveyance efficiency (γ) will increase by 6.07% in the marginal benefit and 10.41% in the carbon intensity. Conversely, the ecological water proportion and social inequality show a decreasing trend in their γ levels. Although a high efficiency of water conveyance allows great economic growth to be achieved, it may cause a reduction in the water allocation to maintain ecosystem services. The carbon-sink capacity of the ecosystem will decrease, inducing more carbon emissions from the nexus system.

Meanwhile, social inequality will, on average, decline by 1.19% since more water resources can be saved and allocated to regions with high population densities. The overall gap in per capita water availability can thus be reduced throughout the river basin, and the fairness in the resource distribution can be improved for the WEECE nexus. A high level of ecological flow into Bosten Lake (β) corresponds to a high carbon intensity (rising by 4.23%) and high social inequality (increasing by 0.25%) since it restricts the water availability for ecosystem land use related to carbon sequestration and economic activities for regional development. Moreover, improvements in the carbon removal rate (α) will contribute to reductions in both carbon intensity and social inequality. Considering the negative impact of water-saving strategies on carbon abatement, a two-pronged strategy that considers both carbon emissions control for energy production and facility upgrades for the water conveyance system is suggested to implement sustainable practices in the future.

The performance of the proposed GFMOP-WEECE nexus model was evaluated through a comparison with four single-objective optimization models that were coded and solved with the same constraints. The results of both the single- and multi-objective models are presented in Fig. 5. M1, M2, M3, and M4 represent the single-objective optimization models targeting the marginal benefit, carbon emissions intensity, proportion of ecological water use, and social inequality, respectively. In the parallel coordinates plot, the objectives of the proposed model (colored lines) will vary within the range of maximum and minimum values obtained from the single-objective models (gray lines). Taking M3 as an example, the proportion of ecological water will reach its optimal value

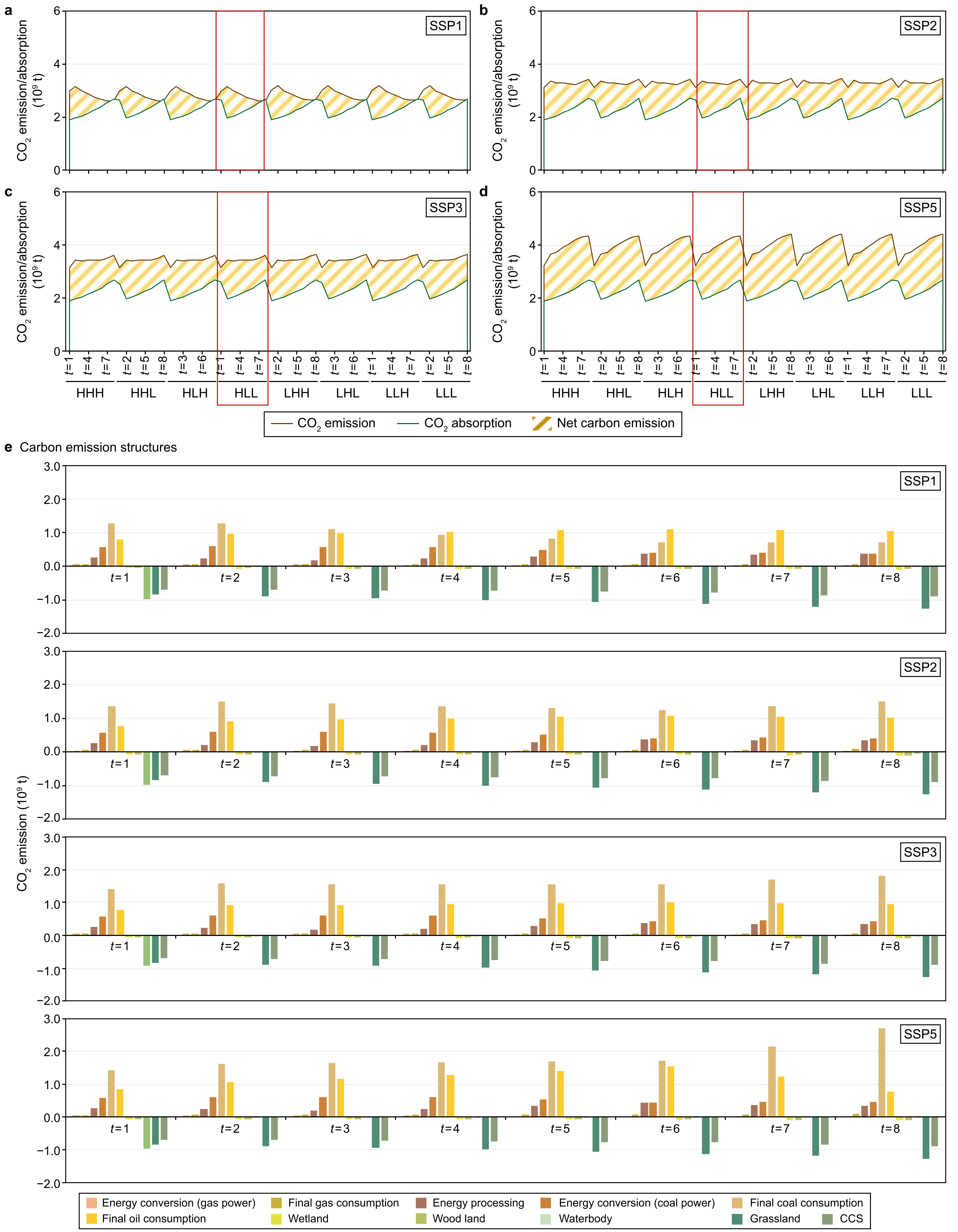

a
b
c
d
SSP1
SSP2
SSP3
SSP5
CO_2 emission/absorption (10^9 t)
HHH
HHL
HLH
HLL
LHH
LHL
LLH
LLL
CO_2 emission
CO_2 absorption
Net carbon emission
e Carbon emission structures
CO_2 emission (10^9 t)
Energy conversion (gas power)
Final gas consumption
Energy processing
Energy conversion (coal power)
Final coal consumption
Final oil consumption
Wetland
Wood land
Waterbody
Grassland
CCS

Fig. 9. Carbon emission structure under different scenarios. **a**–**d**, Total amounts of carbon emissions and absorptions under SSP1 (**a**), SSP2 (**b**), SSP3 (**c**), and SSP5 (**d**). **e,** Carbon emission structures during the whole process of energy supply and carbon sinks of ecosystems. L: Low level; H: High level; SSP: Shared socioeconomic pathway; SSP1: The road of sustainability; SSP2: The road of medium challenges; SSP3: The road of regional rivalry; SSP5: The road of fossil-fueled development; CCS: Carbon capture and storage.

under SSP5, where the lowest marginal benefit and highest intensity of carbon emissions will simultaneously occur (Fig. 5e). M4 performs weakly on all objectives except for social inequality, which exhibits the widest range in the objective variation. Focusing on one dimension alone may lead to significant negative consequences in other dimensions. M1 achieves the closest results to the proposed model among the four single-objective models. Compared to M1, the proposed model will bring about a reduction of 47.56% in unit carbon emissions and an improvement of 0.22% in social inequality despite a decline of 6.53% in ecological water allocation and a slight decrease of 0.04% in the system benefit (Fig. 5c). Overall, the proposed multi-objective model outperforms the other models in identifying coordinated alternatives in a water–energy–economy–carbon–ecology nexus directed toward sustainability.

3.2. Improvement in the marginal benefit and optimal water allocation

Fig. 7a illustrates the water resource allocation under different scenarios. A high resource-intensive development path, such as SSP5, will pressure the regional water supply. The highest water allocation across the river basin is 167.30×10^9 m^3 under $S_{5\text{-LLH}}$, and the lowest allocation is 133.42×10^9 m^3 under $S_{2\text{-LHL}}$. A low carbon removal rate, low ecological requirements for Bosten Lake, and low water conveyance efficiency will contribute to higher water consumption in the WEECE nexus. A low ecological requirement for the downstream lake will expand the water availability of upstream regions, and a low water conveyance efficiency will exacerbate water stress amidst growing socioeconomic demands. Compared to scenarios of high α levels, the regional water use (including the agricultural, industrial, municipal, and ecological sectors) under a low carbon removal rate will increase by 1.25% with the decreased energy water consumption. This is because a higher carbon removal rate corresponds to a lower carbon emission intensity, where fossil energy production (i.e., oil, coal, and natural gas) will be restricted, reducing water consumption during energy exploitation and conversion. More water resources can be allocated to regions for regional economic activities, and different sustainable options will impact water distribution patterns among regions. With the improvement in the water conveyance efficiency, the share of water allocation to Yuli County, with the largest population and land area, will increase by 13.28%, and the shares to Yanqi and Korla will decrease by 3.14% and 1.97%, respectively. Meanwhile, Bohu is the county closest to Bosten Lake, meaning its water allocation is significantly dependent on the ecological requirement level; that allocation will decrease by 22.77% with an increased level of ecological flow into the lake.

Fig. 7b–e displays the utilization patterns of different water sources in different regions. $S_{2\text{-HHH}}$ (with the highest marginal benefit) and $S_{5\text{-HLL}}$ (with the lowest marginal benefit) were selected for a comparative analysis. As the marginal benefit increases by 95.50% (i.e., from $S_{5\text{-HLL}}$ to $S_{2\text{-HHH}}$), 5.18×10^9 m^3 of water consumption of the KKRB can be avoided, and the fairness of water allocation across six counties will be enhanced (i.e., social inequality is decreased by 11.76%). These results imply that enhancing water-use efficiency will curb regional inequalities and facilitate water-saving practices. In detail, the shares of water use in different regions follow a decreasing order over the planning periods, as follows: Yuli > Hejing > Korla > Hoxud > Bohu > Yanqi. Hejing exhibits the most significant temporal changes among the six counties. Meanwhile, Korla and Bohu will experience decreases in their water distribution over time (reducing by 38.10% and 59.40%, respectively). Three types of water sources (i.e., surface water, groundwater, and reclaimed water) will vary differently within the planning horizon. Although the amount of surface water ranks first among the different kinds of water sources, its share will significantly decrease from 2021 to 2060. Compared to the early stage, the share of reclaimed water used in Hejing will rise by 61.13%, and the share of groundwater in Yuli will increase by 12.64% during the late stage (under $S_{2\text{-HHH}}$). Compared to the scenario with the highest marginal benefit, the total share of groundwater under $S_{5\text{-HLL}}$ will decrease by 4.29%, and the share of surface water will rise by 2.86%; meanwhile, the share of reclaimed water for the WEECE nexus will increase by 1.43%, especially in Bohu and Yanqi. The low ecological requirement level under $S_{5\text{-HLL}}$ corresponds to more available surface water for economic activities, compensating for the massive water loss resulting from a low water conveyance efficiency. Moreover, reclaimed water will be promoted to satisfy the surging water demand under the fossil-fueled development pathway.

Fig. 7f and g set out the detailed structure of water allocation among different sectors. Generally, the agricultural water allocation in $S_{2\text{-HHH}}$ is significantly higher than in $S_{5\text{-HLL}}$ (rising by 41.39%), particularly for oil crop planting and livestock farming. Cotton cultivation will remarkably expand with the water allocation (increased by 9.37%) under the intermediate development pathway. The high-water productivity of the cotton crop may be conducive to enhancing the marginal benefit in the WEECE nexus, which will increase from CNY 10.14–19.82 m^{-3} from SSP5 to SSP2. Moreover, a shift in the food production structure will occur under different scenarios. Yuli County is a major supplier of cereal products (i.e., wheat) among the six counties. Under the intensified food supply pressure resulting from the highest population growth under SSP5, Korla, and Yuli will share the burden of maintaining the wheat supply throughout the river basin. Furthermore, the cleaner energy production structure in $S_{2\text{-HHH}}$ enables more water resources to be assigned to the energy sector (rising by 8.45% compared to SSP5). Although the municipal sector possesses a relatively low economic benefit per unit of water allocation, it receives greater water resources under SSP5 than in SSP2 (with an increase of 2.00×10^9 m^3). To sustainably fulfill the water requirements of various sectors, reclaimed water, primarily derived from domestic wastewater, is encouraged as a supplementary water source. Furthermore, certain sacrifices in economic returns are required to mitigate the risk of resource shortage with optimal utilization efficiency.

3.3. Transition to a clean and low-carbon energy structure

The overall energy structure (calculated by calorific value) in descending order is as follows: SSP1 > SSP2 > SSP5 > SSP3. From SSP1 to SSP5, the proportion of clean energy (i.e., renewable energy and natural gas) will decline by 32.32%. The total shares of coal and oil will increase by 19.46%, which corresponds to an increase in the carbon emission intensity of energy production (Fig. 8). This may be driven by the socioeconomic development pathway's sustainable direction, which focuses on low population growth and a clean energy structure. Under SSP1 and SSP2, the supply of high-polluting energy (i.e., coal and oil) exhibits a slight growth with the increased shares of natural gas and renewable energy over time, indicating a high potential for carbon emissions reduction. Generally, energy supply patterns under the sustainable and intermediate development pathways have similar trends with high renewable energy shares. For example, there are notable increases in wind and solar power generation over time under SSP1 and SSP2 (rising by 68.08% and 67.78%, respectively), leading to both reduced overall carbon emissions and more efficient energy generation than in the SSP3 and SSP5 scenarios. In comparison, the sustainable strategy options show no significant effects on the energy supply, implying that energy demand-side management affected by different socioeconomic pathways will play a prominent role in planning energy production to become cleaner and more sustainable.

The proportion of fossil energy power in the KKRB would be 53.1–60.4% over the planning horizon. Compared to the status quo of the energy structure in 2020, the proportion of fossil energy during 2041–2060 will decline by 6.86%, and the renewable energy share will increase by 9.76% under SSP1. From 2021 to 2060, the proportions of coal and oil under the SSP1 and SSP2 scenarios will decrease and then increase. This may be attributed to the improvements in carbon capture techniques and energy conversion efficiency in the long term. Under the SSP3 and SSP5 scenarios, the percentages of coal and oil will constantly reduce over time, indicating that tight restrictions on the use of high-polluting energy will be effective for achieving future carbon peaking and carbon neutrality goals. Taking $S_{1\text{-HLH}}$ as an example, the proportions of oil and natural gas will slightly lower over the planning horizon, and renewable energy will increase, with the percentage of wind power rising to 23.32% by the end of the planning period (Fig. 8). Under SSP5, fossil energy will decrease, and the total share of renewable energy will significantly increase to 29.95%, with the growth rates from largest to smallest as follows: wind > solar > biomass > hydro. The results indicate that oil and natural gas should first be restricted amid the surging energy demand. Given its immense power generation potential, wind power should be prioritized for development in the future.

3.4. Strategy to achieve carbon neutrality goal

Fig. 9 illustrates the CO_2 emission patterns throughout the planning horizon. Accompanied by energy structure adjustment, the net CO_2 emissions of the WEECE nexus system exhibit a trend of SSP5 > SSP3 > SSP2 > SSP1. Specifically, a high water conveyance efficiency will lead to higher carbon emissions than those with a lower water conveyance efficiency. This is because a high efficiency of water use will stimulate economic growth but squeeze the share of ecosystem water allocation, thereby impeding the carbon sequestration capacity of the ecosystem lands. The increases in the ecological requirement and carbon removal rate (i.e., from low to high) will increase CO_2 emissions of 0.67% and 0.24%, respectively. This is because a high water inflow to Bosten Lake will provide the water resources available for economic and energy purposes, consequently reducing the overall carbon emissions throughout the river basin; in addition, promoting carbon capture techniques during energy processing and conversion will also be conducive to reducing the unit carbon emissions. In general, SSP1, SSP2, and SSP3 are projected to achieve peak CO_2 emissions in 2026–2030 ($t = 2$), with 1.21×10^9, 1.41×10^9, and 1.47×10^9 tons, respectively. In contrast, the carbon-peaking time of SSP5 is relatively delayed, occurring during 2046–2050 ($t = 6$). Furthermore, negative carbon emissions will not be achieved until 2055–2060 ($t = 8$) under the SSP1 scenario, implying that SSP1 may be the potential scenario of choice among the four development pathways for achieving the dual goals of carbon peaking and carbon neutrality.

The lowest unit carbon emissions will occur under the option of a combination of a high carbon removal rate, low ecological requirement, and high-water conveyance efficiency (i.e., $S_{1\text{-HLH}}$, $S_{2\text{-HLH}}$, $S_{3\text{-HLH}}$, and $S_{5\text{-HLH}}$), reaching 22.63×10^9–31.40×10^9 tons across different SSPs (Fig. 9). The detailed carbon emission and absorption structures are provided in Fig. 9e. From 2021 to 2060, total carbon emissions will fall, and the total carbon absorptions will rise. Final oil and coal consumption will produce the main proportion of carbon emissions while using carbon capture and storage (i.e., CCS) and grassland carbon sinks will contribute most of the carbon absorption. Great importance should be attached to the energy conversion process for carbon emissions management, though its share declines by 36.7–26.5% from 2021 to 2060. Under the $S_{1\text{-HHL}}$ scenario, carbon emissions from final gas and oil consumption will increase by 37.0% and 31.2%, and carbon emissions from final coal consumption will decrease by 43.5%. Under the SSP2, SSP3, and SSP5 scenarios, carbon emissions from final coal consumption will increase, and coal will rank first among the different emission sources by the end of the planning period. The major contributors to carbon absorption are CCS and grassland, ranging from 26.85% to 37.65% during 2021–2025 to 31.70% and 53.04% in 2056–2060, respectively. To reduce the total carbon emissions and achieve China's 2060 carbon neutrality goal, a series of measures should be adopted in combination with the WEECE nexus system, such as strict management of consumer-end emissions, expansion of grassland coverage, promotion of carbon capture techniques, and raising the ecological red line for Bosten Lake.

4. Discussion

4.1. Comparison with other studies

The results obtained in this study demonstrate that variations in the shared socioeconomic pathway, water conveyance efficiency, ecological requirement, and carbon removal rate affect resource allocation patterns and the achievement of the Sustainable Development Goals. Previous research works exploring the pursuit of the SDGs in a water-related nexus system also indicated that improving the water-use efficiency (i.e., marginal benefit) will restrict fossil energy power generation and thus generate the co-benefit of reducing the carbon emission intensity, aligning closely with our findings [58,59]. Furthermore, we compared our study with others in the literature on resource management in arid watersheds with similar environmental and geographical characteristics. For example, Li et al. (2021) proposed a multi-dimensional optimization approach for agricultural systems by considering the correlation between water and land resources, and they found that among the different SSPs, taking a middling path (e.g., SSP2) will be the best option to balance different sustainability goals in an arid river basin [60]. Meanwhile, Sun et al. (2020) proposed a water–food–energy nexus model for the KKRB, where the proportion of fossil energy power was optimized at 53.1–60.4% in adaption to water and environmental constraints, consistent with the results from our GMFOP-WEECE nexus model (i.e., 46.5–60.8%) [26]. Such consistency further validates the applicability of the GMFOP-WEECE nexus model in exploring the trade-offs among different SDGs and identifying options for the synergistic management of water and energy resources. Compared to the above studies, our study has three advantages: (1) these studies focused solely on the water-related nexus of an agricultural system in an arid basin, while we have proposed a more comprehensive nexus framework to depict the complex interactions among water, energy, economy, ecological, and carbon subsystems; (2) no previous study attempted to balance conflicting SDGs in the economic, environmental, ecological, and social dimensions without a weight determination process, whereas our study strikes a trade-off among SDGs with reduced subjectivity and enhanced efficiency through the GFMOP method; (3) our study is the first attempt at integrating the GFMOP method into the WEECE nexus for efficient and collaborative management schemes in the KKRB under changing policies, which represented a gap in the previous literature. Therefore, our study provides new insights into the options for the synergistic management of the SDGs in compound water—energy—economy—carbon—ecology nexus system, building on the previous research efforts.

4.2. Policy implications

Based on the results analysis, we surmise that regional water allocation should be adapted in response to changes as part of sustainable strategy options. For instance, under poor canal conditions with a low water conveyance efficiency, the water allocation to Yuli County should be primarily restricted to ensure the water supply throughout the Kaidu—Kongqi River Basin. When enhancing the ecological flow for the downstream lake, the government can offer specific financial subsidies to Bohu County as ecological compensation, which is appropriate given its sensitivity to changes in the γ level. In the long term, managers should phase down surface water use and appropriately enhance groundwater exploitation and reclaimed water utilization to replenish the limited water resources. To improve the recovery rate of wastewater and purify it to a high quality suitable for reuse, optimization of the water circulation network and advancement of the wastewater techniques used should be explored for industrial water systems. This could involve installing sensors and control systems, reverse osmosis, membrane bioreactors, and advanced oxidation processes. Moreover, as it offers an important supplemental water source, utilizing urban domestic reclaimed water will ensure access to an adequate and reliable water supply for the agricultural, industrial, ecological, and energy sectors. Beyond this, with special attention paid to the behaviors and efficiency of domestic water usage, improvements relating to urban water-saving and upgrades of sewage treatment plants (e.g., rainwater collection, decentralized treatment infrastructure, and disinfection systems) could be critical to ensuring there is an adequate and reliable water supply and mitigating the ecological impact in the future. In addition, appropriate economic incentives, such as wastewater treatment fees and water price subsidies, will be essential for regions with relatively great water demands and low economic growth, such as Yanqi and Bohu.

Considering the impacts of the energy consumption structure and resource utilization intensity under different shared socioeconomic pathways, demand-side management will play a prominent role in planning energy production that is cleaner and more sustainable. Among the four shared socioeconomic pathways, SSP1 is the most promising option for achieving the goals of carbon peaking and carbon neutrality since it is projected to result in negative carbon emissions during 2056—2060. To balance the growing energy demand, the KKRB should phase up the proportion of renewable energy (accounting for [20.92%, 32.86%] till 2056—2060); in particular, wind and solar energy should be vigorously developed. However, since electricity generated from renewable energy is inherently unstable due to natural constraints, the KKRB should retain a certain coal and oil supply (accounting for [46.48%, 47.42%] over 2021—2060) to ensure a continuous, safe, and stable supply of electricity. In general, SSP1 is projected to achieve peak CO_2 emissions in 2026—2030, which is far ahead of SSP5, with the emissions amount decreasing by 0.64×10^9 tons. Peaking early in carbon emissions will win us time and increase the likelihood of us achieving carbon neutrality at a low cost while making room for carbon reductions in other regions.

Apart from an energy structure transition, carbon removal technologies and ecological carbon sinks are the other keys to achieving carbon neutrality. As coal and oil are the major sources of carbon emissions, the application of CCS in coal-fired thermal power and oilfield gas processing will be major forces of carbon reduction. Throughout the planning horizon, CCS techniques and grassland planting will contribute 39.52% and 49.13% of CO_2 absorption, respectively. During 2056—2060, CCS will reduce CO_2 emissions by 0.90×10^9 tons, and grassland carbon sinks could facilitate a reduction of 1.27×10^9 tons of CO_2 emissions. Considering the importance of a high CCS installation rate in achieving our carbon goals, it is recommended that policymakers introduce incentives and subsidy policies to facilitate early CCS deployment, as well as promote innovative carbon capture technology, such as bioenergy with carbon capture and storage (BECCS) projects. In addition, improving water conveyance efficiency, with a strict red line for the ecological flow, will also be conducive to reducing carbon emissions. A series of measures can be adopted in combination with the WEECE nexus system, such as the strict management of consumer-end emissions, enlargement of the grassland coverage, promotion of carbon capture techniques, and raising the ecological red line for the inflow to Bosten Lake.

4.3. Limitations and future directions

Compared to other research works, our study has made progress in the following three areas: (1) a comprehensive WEECE nexus framework was formulated by considering resource allocation, economic production, energy generation, carbon abatement, and ecosystem requirements over a long-term horizon; (2) the developed GFMOP-WEECE nexus can balance multi-dimensional SDGs with reduced subjectivity and enhanced efficiency, as well as generate alternatives based on compromise, through analyses of trade-offs and synergies of the SDGs; (3) different SSP baselines and sustainable strategy options were examined in the developed model, providing useful insights in terms of policy selection to achieve the holistic planning of socioeconomic development and eco-environmental protection.

Despite the above progress, certain limitations remained to be addressed. The quantitative modeling of the WEECE nexus framework requires an enormous computational load and long run time, along with the collection of extensive datasets. Furthermore, limited by the data availability, this study focused solely on a typical arid river basin in Northwest China, suffering a resource crisis and ecological degradation. Given China's vast and diverse territory, the GFMOP-WEECE nexus model can be improved and extended to other regions with varying characteristics by incorporating input—output analysis and water footprint assessment into an optimized model framework [61,62]. Moreover, WEECE nexus planning is highly complex, involving multiple factors and processes in decision-making. These processes/factors and their interactions constitute nonlinear and uncertain features. So far, the GFMOP method has limitations in addressing the nonlinear dependencies between variables and the vagueness of parameters in the planning process. To strengthen the flexibility and robustness of the optimization schemes, other uncertainty analysis techniques may be introduced to address multiple uncertain variables in future research, such as interval and stochastic programming methods [63,64].

5. Conclusions

In this study, a gray fractional multi-objective optimization model was developed for planning the water—energy—economy—carbon—ecology nexus toward sustainable development in river basins. By incorporating multi-objective programming, fractional programming, and the gray incidence method in one framework, the developed model has the following advantages: (1) the complex interactions among SDGs can be captured in water–energy–economy–carbon–ecology nexus based on a comprehensive optimization framework; (2) the model can balance multiple objectives and optimize system efficiency without assuming subjective weights; and (3) synergistic alternatives for resource allocation, economic production, and ecosystem protection can be identified by coordinating trade-offs among different SDGs in response to future socioeconomic changes.

The applicability and practicality of the GFMOP-WEECE nexus model were verified in a real-world case in the Kaidu–Kongqi River Basin, an arid region of Northeast China. Thirty-two scenarios were designed with the combination of four socioeconomic development baselines, two CO_2 removal rates, two water conveyance efficiencies, and two ecological requirement levels. We made several key findings: (1) the carbon intensity and social inequality are negatively correlated with the marginal benefit, indicating that promoting the economic efficiency of water utilization will yield synergistic benefits in from the environment and social dimensions; (2) an intermediate pathway (SSP2) may be the best choice to achieve a compromise between different sustainable objectives, with the highest marginal benefit of CNY 19.8 m^{-3} and a relatively low carbon intensity across different SSPs; (3) surface water ranks first among the three kinds of water sources with a decreasing trend over time, but from 2021 to 2060, the share of reclaimed water used in Hejing County will significantly rise by 61.13%, and the share of groundwater in Yuli County will increase by 12.64% over this time; (4) oil and natural gas should be restricted first amid the surging energy demand in the river basin, and given its immense power generation potential, wind power should be prioritized for development in the future (with the percentage rising to 23.32% during 2041–2060); (5) SSP1 is projected to achieve peak CO_2 emissions in 2026–2030, which is far ahead of SSP5, with a decrease value of 0.6×10^9 tons, and it is also a promising option for achieving negative carbon emissions during 2055–2060 in future development pathways; and (6) CCS and grassland planting stand as the main potential contributors to CO_2 absorption, accounting for 39.52% and 49.13% of absorption in the planning horizon, respectively.

Accordingly, several policy suggestions have emerged. For example, improvements to urban waste saving and upgrades to sewage treatment plants seem critical to ensure an adequate and reliable water supply for the ecological system and social economy in the future. Moreover, to balance the growing energy demand and the carbon neutrality goal, efforts should be made to phase up the proportion of renewable energy, especially for wind and solar power, in the Kaidu-Kongqi River Basin. Additionally, a series of measures can be adopted in combination to control the carbon emissions from the WEECE nexus system, such as strict management of consumer-end emissions, expansion of grassland coverage, promotion of carbon capture techniques, and raising the ecological red line for the inflow to Bosten Lake.

This study is a new attempt at sustainable resource management from a novel water–economy–energy–carbon–ecology nexus perspective. Compared with traditional single-objective models, the proposed GFMOP model exhibits a superiority in uncovering potential trade-offs among multiple SDGs and identifying compromised alternatives for planning WEECE nexus towards harmony and sustainability. The model framework and solving method are also portable to similar regions elsewhere suffering resource crises and ecological degradation. However, due to a lack of regional data sources, certain simplifications had to be made in this study. In the future, more robust techniques such as fuzzy and stochastic programming methods should be incorporated to handle the dynamics of complex components and uncertainties in the nexus system. In addition, by introducing footprint theory and input–output analysis, the real demands and consumption of natural resources may be measured. All the above concerns should be addressed in further research to enhance the flexibility and applicability of the introduced modeling framework.

CRediT authorship contribution statement

Yufei Zhang: Writing - Review & Editing, Writing - Original Draft, Visualization, Software, Methodology, Investigation, Data Curation, Conceptualization. **Yongping Li:** Writing - Review & Editing, Supervision, Resources, Project Administration, Funding Acquisition, Conceptualization. **Guohe Huang:** Writing - Review & Editing, Funding Acquisition, Data Curation. **Yuan Ma:** Supervision, Investigation, Formal Analysis, Data Curation. **Yanxiao Zhou:** Writing - Review & Editing, Formal Analysis, Data Curation.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix C. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.ese.2024.100481.

Appendix A. Nomenclature for variables and parameters

Subscripts

MBW	Marginal benefit of water use, CNY m^{-3}
CEI	Carbon emission intensity, kg m^{-3}
EWP	Ecological water proportion
SI	Social inequality of WEECE nexus
i	Counties of the river basin, $i = 1, \ldots, 6$, with $i = 1$ for Hejing, $i = 2$ for Korla, $i = 3$ for Yanqi, $i = 4$ for Hoxud, $i = 5$ for Yuli, $i = 6$ for Bohu
j	Water user of the river basin, $j = 1, \ldots, 9$, with $j = 1$ for cotton, $j = 2$ for wheat, $j = 3$ for oil crop, $j = 4$ for vegetable, $j = 5$ for livestock, $j = 6$ for products processing industry, $j = 7$ for petroleum industry, $j = 8$ for chemical industry, $j = 9$ for domestic use
u	Energy consumers of the river basin, $u = 1, \ldots, 7$, with $u = 1$ for agriculture, $u = 2$ for industry, $u = 3$ for construction, $u = 4$ for transportation, $u = 5$ for service industry, $j = 6$ for domestic use, $j = 7$ for others
l	Ecological lands of the river basin, $l = 1,2,3,4$, with $l = 1$ for wetland, $l = 2$ for grassland, $l = 3$ for woodland, $l = 4$ for waterbody
t	The planning periods, $t = 1, \ldots, 8$, $t = 1$ for period 1 (2021–2025), $t = 2$ for period 2 (2026–2030), $t = 3$ for period 3 (2031–2035), $t = 4$ for period 4 (2036–2040), $t = 5$ for period 5 (2041–2045), $t = 6$ for period 6

(2046–2050), $t = 7$ for period 7 (2051–2055), $t = 8$ for period 8 (2056–2060)

k Energy carriers, $k = 1, \ldots, 12$, with $k = 1$ for raw coal, $k = 2$ for crude oil; $k = 3$ for nature gas, $k = 4$ for cleaned coal, $k = 5$ for coke, $k = 6$ for gasoline, $k = 7$ for kerosene, $k = 8$ for diesel oil, $k = 9$ for fuel oil, $k = 10$ for LNG, $k = 11$ for electricity, $k = 12$ for heat

m Energy processing types, $m = 1,2,3,4$, $m = 1$ for coal washing, $m = 2$ for coking, $m = 3$ for gas liquefaction, $m = 4$ for oil refining

n Energy conversion technologies, $n = 1, \ldots, 12$, with $n = 1$ for coal-fired power plant, $n = 2$ for coal-fired combined heat and power plant, $n = 3$ for gas-fired power plant, $n = 4$ for gas-fired combined heat and power plant, $n = 5$ for nuclear power plant, $n = 6$ for hydropower plant, $n = 7$ for wind power plant, $n = 8$ for solar power plant, $n = 9$ for biomass power plant, $n = 10$ for coal-fired heating station, $n = 11$ for gas-fired heating station, $n = 12$ for geothermal heating station

q The air pollutants, $q = 1,2,3$, with $q = 1$ for sulfur dioxide (SO_2), $q = 1$ for nitrogen dioxide (NO_x), $q = 3$ for particle matters (PM)

Parameters and variables

BW_{ijt} Water allocation benefit for county i in period t, m^3
SW_{ijt} Surface water withdrawn from Kaidu-Kongqi River for county i in period t, m^3
GW_{ijt} Ground water withdrawn for county i in period t, m^3
RW_{ijt} Reclaimed water use for county i in period t, m^3
IRW_{ijt} Reclaimed water use from industry sector for county i in period t, m^3
DRW_{ijt} Reclaimed water use from domestic sector for county i in period t, m^3
$HK_{\mathrm{sur},it}$ The elevation head of surface water for county i in period t, m
$H_{\mathrm{lift},it}$ The lifting head of groundwater for county i in period t, m
$H_{\mathrm{nop},it}$ The pressure head of groundwater for county i in period t, m
$f_{\mathrm{loss},it}$ The head loss of groundwater for county i in period t, m
$\mu_{\mathrm{pump},it}$ Pumping efficiency of groundwater for county i in period t, m
$\mu_{\mathrm{motor},it}$ Power efficiency of pumping machine for county i in period t, m
$\mu_{\mathrm{sur},it}$ Pumping efficiency of surface water for county i in period t, m
LF_{ijt} Leaching fraction for crop j in county i under period t
CE_{it} Electricity utilization cost for water allocation and delivery in period t, CNY kWh^{-}
YA_{ijt} Crop yield per area in county i for each period, kg ha^{-1}
PF_{ijt} Cost of fertilizer application for crop j in county i under period t, CNY kg^{-1}
WPC_{ijt} Water requirement for crop j in county i under period t, m^3 ha^{-1}
FC_{ijt} Fixed cost of crop irrigation, CNY ha^{-1}
DW_{ijt} Water demand for user j in county i under period t, m^3
$EAGP_{jt}$ Electricity consumption of agricultural products processing, kWh kg^{-1}
KLD_{jt} Diesel consumption of crop irrigation, kg kg^{-1}
$CELE_t$ Electricity consumption for drainage, drip and sprinkler irrigation, kWh ha^{-1}
EBW_t Water inflow into Bosten Lake, m^3
BR_{ijt} Benefit of water reuse, CNY m^{-3}
α_{ijt} Reuse rate of industrial wastewater, %
γ_{jt} Water conveyance efficiency of user j, %
TIC_{ijt} Fixed cost of industrial production, CNY m^{-3}
β_{ijt} Reuse rate of domestic wastewater, %
TDC_{ijt} Cost of domestic wastewater treatment, CNY m^{-3}
ESW_{ilt} Surface water withdrawn for ecological sector l of county i in period t, m^3
EGW_{ilt} Ground water withdrawn for ecological sector l of county i in period t, m^3
EBW_t Ground water withdrawn for ecological sector l of county i in period t, m^3
ERW_{ilt} Domestic reclaimed water for ecological sector l of county i in period t, m^3
GWD_{lt} Water demand per area of ecological sector l in each period, m^3 ha^{-1}
EBW_t Ecological requirement of Bosten Lake in period t, m^3
β_{lkt} Percentage of vegetation k coverage in ecological sector l under period t, %
VP_{kt} Yield of vegetation k per ha in period t, CNY ha^{-1}
VPB_{kt} Price of vegetation k in period t, CNY ha^{-1}
WP_{lt} Water purification ability of ecological sector l per ha, CNY ha^{-1}
TC_t Treatment cost of wastewater in period t, CNY h^{-1}
V_t Price of vegetation k in period t, CNY h^{-1}
ZP_{lt} Soil erosion index of ecological sector l per ha
σ_q Percentage of eutrophication material q per ha, %
RP_{lt} Water conservation of ecological sector l per ha, m^3
RC_t Cost of reservoir construction, CNY ha^{-1}
RO_t Rainfall runoff coefficient of ecological sector l
RCI_t Water price, CNY m^{-3}
TCI_t Tourism value of ecological sector l per ha, CNY ha^{-1}
LCI_t Scientific research value of ecological sector l per ha, CNY ha^{-1}
KCI_{lt} Maintenance and fix cost of ecological sector l per ha, CNY ha^{-1}
cc_{lt} Carbon emission of ecological sector l per ha, kg ha^{-1}
Q_t Carbon absorption of ecological sector l per ha, kg ha^{-1}
TSW_t Surface water availability in period t, m^3
TGW_t Ground water availability in period t, m^3
TRW_t Reclaimed water availability in period t, m^3
PGE_t Ground water exploitation coefficient
$CIM_{it\ \max}$ Treatment capacity of industrial wastewater, m^3
$CDM_{it\ \max}$ Treatment capacity of domestic wastewater, m^3
$A_{\max,it}$ Maximum arable area for each period, ha
$A_{\min,it}$ Minimum arable area for each period, ha
ξ_{it} Installation rate of drip irrigation, sprinkler irrigation
FD_{it} Food demand in county i for each period, kg
PO_{it} Population in county i for each period, capita
$\varsigma_{\mathrm{fe},t}$ Allowable proportion of agricultural consumption in diesel production, %
GBE_{jt} Conversion coefficient of biomass energy per unit yield of crops
$MAXrenew_{int}$ The availability of renewable energy n during period t in county I, kWh
QF_{ijt} Quantity of fertilizer applied to for crop j in county i under period t, kg ha^{-1}
AMF_{jt} Quantity of fertilizer applied to for crop j in county i under period t, kg ha^{-1}
AMM_{jt} Quantity of pesticide applied to for crop j in county i under period t, kg ha^{-1}
ADM_{jt} Quantity of plastic film applied to for crop j in county i under period t, kg ha^{-1}
CEF_{jt} Fertilizer residue rate for crop j, %
CEM_{jt} Pesticide residue rate for crop j, %
CDM_{jt} Plastic film residue rate for crop j, %
TLW_{it} Allowable water allocation for crop leaching, m^3
$PN_{\mathrm{mf},t}$ Nitrogen content in fertilizers

$PN_{\mathrm{mm},t}$	Nitrogen content in pesticides
$PN_{\mathrm{dm},t}$	Nitrogen content in plastic films
MNO_t	Allowable nitrogen emission in the field, kg
$PP_{\mathrm{mf},t}$	Phosphorus content in fertilizers
$PP_{\mathrm{mm},t}$	Phosphorus content in pesticides
$PP_{\mathrm{dm},t}$	Phosphorus content in plastic films
MPO_t	Phosphorus nitrogen emission in the field, kg
$\delta_{\mathrm{oil},t}$	Conversion coefficient of diesel-to-standard oil
CNO_t	Concentration of NO_x emission per unit consumption of oil consumption, kg kg $^{-1}$
CPM_t	Concentration of PM emission per unit consumption of oil consumption, kg kg $^{-1}$
CSO_t	Concentration of SO_2 emission per unit consumption of oil consumption, kg kg $^{-1}$
CCO_t	Concentration of CO_2 emission per unit consumption of oil consumption, kg kg $^{-1}$
TNO_t	Permissible NO_x emission in the field, kg
TPM_t	Permissible PM emission in the field, kg
TSO_t	Permissible SO_2 emission in the field, kg
TCO_t	Permissible CO_2 emission in the field, kg
IC_{mt}	Carbon reduction capacity of CCS techniques, kg
r_t	CO_2 capture rate
L_{mt}	CO_2 emission of CCS techniques, kg
σ_t	Emission factor
μ_i'	Power generation efficiency of power plants with CCS techniques
μ_i	Power generation efficiency of power plants without CCS techniques
REX_{kt}	Export benefit of energy k to other regions during period t in county i, CNY kg^{-1} or CNY kJ^{-1} or CNY kWh^{-1} or CNY m^{-3}
RED_{kt}	Local benefit of energy k during period t in county i, CNY kg^{-1} or CNY kJ^{-1} or CNY kWh^{-1} or CNY m^{-3}
AEX_{ikt}	Export amount for energy k to other regions during period t in county i, kg or kJ or kWh or m^3
CEE_{kt}	Cost of energy extraction for primary fossil fuel k during period t, CNY kg^{-1} or CNY kJ^{-1} or CNY kWh^{-1} or CNY m^{-3}
AEE_{ikt}	Amount of energy extraction for primary fossil fuel k during period t, kg or kJ or kWh or m^3
CEI_{kt}	Import cost of energy k during period t, CNY kg^{-1} or CNY kJ^{-1} or CNY kWh^{-1} or CNY m^{-3}
AEI_{ikt}	Import amount for energy k from other regions during period t in county i, kg or kJ or kWh or m^3
CEP_{mt}	Cost of energy processing by processing method m during period, CNY kg^{-1}
AEP_{imt}	Amount of energy processing by processing method m during period t in county i, kg
$FCEC_{nt}$	Fixed cost of electricity generation for energy conversion technology n during period t, CNY kg^{-1} or CNY kJ^{-1} or CNY kWh^{-1} or CNY m^{-3}
CEC_{int}	Capacity of energy conversion technology n during period t in county i, kg or kJ or kWh or m^3
$VCEC_{nt}$	Flexible cost of electricity generation for energy conversion technology n during period t, CNY kg^{-1} or CNY kJ^{-1} or CNY kWh^{-1} or CNY m^{-3}
AEC_{int}	Amount of energy conversion for energy conversion technology n during period t in county i, kg or kJ or kWh or m^3
$VCCC_{nt}$	Cost of capacity expansion for energy conversion technology n during period t, CNY kg^{-1} or CNY kJ^{-1} or CNY kWh^{-1} or CNY m^{-3}
ECC_{int}	Expanded capacity of energy conversion technology n during period t in county i, kg or kJ or kWh or m^3
$BCLP_{nt}$	Revenue of renewable energy n, kWh
$UEOP_{mt}$	Emission factor of CO_2 by processing method m during period t, kg kg^{-1}
ROM_t	Reduction rate of CO_2 during period t, %
COM_t	The cost of CO_2 capture during period t, CNY kg^{-1}
$CPMM_{imt}$	Removal rate of CO_2 by carbon capture technique during energy processing, %
CPN_{int}	Removal rate of CO_2 by carbon capture technique during energy conversion, %
$UEOC_{nt}$	Emission factor of CO_2 for energy conversion technology n during period t, kg kg^{-1} or kg kJ^{-1} or kg kWh^{-1} or kg m^{-3}
FED_{iukt}	Demand of energy k for end-user u during period t, kg or kJ or kWh or m^3
CSC_{ukt}	Conversion factor of energy k
UCS_{kt}	CO_2 emission factor of end-user for coal consumption during period t, kg kg^{-1} or kg kJ^{-1} or kg kWh^{-1} or kg m^{-3}
$ROME_{ukt}$	Reduction rate of CO_2 during period t, %
$UESP_{qmt}$	Emission factor of air pollutant q by processing method m during period t, kg kg^{-1}
RSM_{qt}	Reduction rate of air pollutant q for energy processing and conversion during period t, %
CSM_{qt}	Reduction cost of air pollutant q for energy processing and conversion during period t, CNY kg^{-1}
$UESC_{qnt}$	Emission factor of air pollutant q for energy conversion technology n during period t, kg kg^{-1} or kg kJ^{-1} or kg kWh^{-1} or kg m^{-3}
UPS_{qkt}	Pollutant emission factor of end-user for energy k consumption during period t, kg kg^{-1} or kg kJ^{-1} or kg kWh^{-1} or kg m^{-3}
$RSME_{qukt}$	Reduction rate of air pollutant q of end-user during period t, %
$EWEX_{kt}$	Amount of water required during energy exploitation in period t, m^3 kg^{-1} or m^3 kJ^{-1} or m^3 kWh^{-1} or m^3 m^{-3}
$EWPR_{mt}$	Amount of water required during energy processing in period t, m^3 kg^{-1}
EWC_{nt}	Amount of cooling water required during energy conversion in period t, m^3 kg^{-1} or m^3 kJ^{-1} or m^3 kWh^{-1} or m^3 m^{-3}
EWW_t	Amount of water consumption during hydropower generation in period t, m^3 kWh^{-1}
EWO_{nt}	Amount of other type water required during energy conversion in period t
$MAXAEE_{ikt}$	Upper limit amount of energy extraction for primary fossil fuel k during period t in region r
$MAXEI_{ikt}$	Upper limit of import amount for energy k from other regions during period t
$MAXEX_{ikt}$	Upper limit of import amount for energy k from other regions during period t
TWE_{it}	Upper limit of water consumption during energy exploitation, processing and conversion, m^3
$UECP_{imt}$	Energy processing coefficient for energy processing technology m during period t
$UECC_{int}$	Energy conversion coefficient for energy conversion technology n during period t
LR_{ikt}	Loss rate of energy transportation during period t, %
LE_t	Loss rate of electricity transportation during period t, %
RHE_t	Thermoelectric conversion coefficient
RCP_{imt}	Upper limit of energy processing by processing method m during period t, kg
TY_{int}	Retired capacity of energy conversion measure k during period t, kg or kJ or kWh or m^3
OT_{nt}	Operating time for energy conversion technology n during period t, h

TLC_{it} Permissible CO_2 emission for energy generation during period t, kg
TLP_{iqt} Permissible air pollutant emission for energy generation during period t, kg

Appendix B. GFMOP-WEECE nexus model

A gray fractional multi-objective programming method (GFMOP) is developed for planning WEECE nexus towards sustainability in the future. The GFMOP-WEECE nexus model includes four subsystems, three material flows, three kinds of water sources, nine water-use sectors, exploitation of three energy sources, three energy processing technologies, thirteen energy conversion technologies, end use for twelve energy sources and forty-year planning period. Four sustainable development objectives from economic, environmental, ecological and social dimensions are examined under 32 planning scenarios.

B.1 Objectives

(1) Economic dimension: maximum marginal benefit of water use (MBW)

Marginal benefit reflects water-use efficiency level (i.e., water productivity) which is a key concern for reaching sustainability of arid and semi-arid regions. Optimizing marginal benefit means maximizing system benefit per unit water through allocating limited water resources to agriculture, industry, domestic, energy and ecological sectors. The objective function can be expressed as:

$$\text{Max } MBW = \frac{\begin{pmatrix} PRO\_AGR + PRO\_DOM + PRO\_IND \\ +PRO\_ECO + PRO\_ELE \end{pmatrix}}{WA} \tag{B.1}$$

where

$$\begin{aligned} PRO\_AGR = & \sum_i^I \sum_{j=1}^5 \sum_t^T BW_{ijt} \times \frac{(SW_{ijt} + GW_{ijt} + DRW_{ijt})}{(1 + LF_{ijt})} - \sum_i^I \sum_{j=1}^5 \\ & \times \sum_t^T CE_{it} \times \begin{bmatrix} \frac{SW_{ijt}}{\gamma_{jt}} \times \frac{HK_{\text{sur},it}}{102 \times 3.6 \times \mu_{\text{sur},it}} + \frac{DRW_{ijt}}{\gamma_{jt}} \times \frac{HK_{\text{sur},it}}{102 \times 3.6 \times \mu_{\text{sur},it}} \\ + \frac{GW_{ijt}}{\gamma_{jt}} \times \frac{H_{\text{lift},it} + H_{\text{nop},it} + f_{\text{loss},it}}{102 \times 3.6 \times \mu_{\text{pump},it} \times \mu_{\text{motor},it}} \end{bmatrix} \\ & - \sum_i^I \sum_{j=1}^5 \sum_t^T \frac{QF_{ijt} \times PF_{ijt} \times (SW_{ijt} + GW_{ijt} + DRW_{ijt})}{(1 + LF_{ijt}) \times WPC_{ijt}} - \sum_i^I \sum_{j=1}^4 \\ & \times \sum_t^T \frac{CE_{it} \times (SW_{ijt} + GW_{ijt} + DRW_{ijt}) \times \xi_{it} \times CELE_t}{(1 + LF_{ijt}) \times WPC_{ijt}} - \sum_i^I \sum_{j=1}^4 \\ & \times \sum_t^T \frac{CE_{it} \times YA_{ijt} \times (SW_{ijt} + GW_{ijt} + DRW_{ijt}) \times EAGP_{jt}}{(1 + LF_{ijt}) \times WPC_{ijt}} - \sum_i^I \sum_{j=1}^4 \\ & \times \sum_t^T \frac{(SW_{ijt} + GW_{ijt} + DRW_{ijt}) \times KLD_{jt} \times CKL_t}{(1 + LF_{ijt}) \times WPC_{ijt}} - \sum_i^I \sum_{j=1}^5 \\ & \times \sum_t^T \frac{FC_{ijt} \times (SW_{ijt} + GW_{ijt} + DRW_{ijt})}{(1 + LF_{ijt}) \times WPC_{ijt}} \end{aligned} \tag{B.2}$$

$$\begin{aligned} PRO\_IND = & \sum_i^I \sum_t^T \\ & \times \sum_{j=6}^8 BW_{ijt} \times (SW_{ijt} + GW_{ijt} + IRW_{ijt} + DRW_{ijt}) + \sum_i^I \sum_t^T \\ & \times \sum_{j=6}^8 \alpha_{ijt} \times (SW_{ijt} + GW_{ijt} + IRW_{ijt} + DRW_{ijt}) \times (BR_{ijt} - TIC_{ijt}) \\ & - \sum_i^I \sum_t^T \\ & \times \sum_{j=6}^8 CE_{it} \times \begin{bmatrix} \frac{SW_{ijt} + IRW_{ijt} + DRW_{ijt}}{\gamma_{jt}} \times \frac{HK_{\text{sur},it}}{102 \times 3.6 \times \mu_{\text{sur},it}} + \\ \frac{GW_{ijt}}{\gamma_{jt}} \times \frac{H_{\text{lift},it} + H_{\text{nop},it} + f_{\text{loss},it}}{102 \times 3.6 \times \mu_{\text{pump},it} \times \mu_{\text{motor},it}} \end{bmatrix} \end{aligned} \tag{B.3}$$

$$\begin{aligned} PRO\_DOM = & \sum_i^I \sum_t^T BW_{i9t} \times (SW_{i9t} + GW_{i9t} + DRW_{ijt}) + \sum_i^I \\ & \times \sum_t^T \sum_{j=9} \beta_{ijt} \times (SW_{ijt} + GW_{ijt} + DRW_{ijt}) \times (BR_{ijt} - TDC_{ijt}) - \sum_i^I \\ & \times \sum_t^T CE_{it} \times \left[\frac{SW_{i9t}}{\gamma_{9t}} \times \frac{HK_{\text{sur},it}}{102 \times 3.6 \times \mu_{\text{sur},it}} + \frac{GW_{i9t}}{\gamma_{9t}} \times \frac{H_{\text{lift},it} + H_{\text{nop},it} + f_{\text{loss},it}}{102 \times 3.6 \times \mu_{\text{pump},it} \times \mu_{\text{motor},it}} \right] \end{aligned} \tag{B.4}$$

$$\begin{aligned} PRO\_ECO = & \sum_t^T \sum_i^I \sum_l^L \left\{ \begin{aligned} & \frac{ESW_{ilt} + EGW_{ilt} + ERW_{ilt}}{GWD_{lt}} \times \\ & \begin{bmatrix} \sum_{k=1}^2 (\beta_{lkt} \times VP_{kt} \times VPB_{kt}) + WP_{lt} \times TC_t + \\ V_t + ZP_{lt} \times \sum_{q=1}^2 \sigma_q \times PI_{qt} \times I_q + RP_{lt} \times RC_t \\ + RP_{lt} \times RO_t \times RCI_t + TCI_t \times TP_{lt} \\ + LCI_t - (KCI_{lt} + ICI_{lt}) \end{bmatrix} \end{aligned} \right\} \\ & - \sum_t^T \sum_l^L \\ & \times \sum_i^I CE_{lt} \times \begin{bmatrix} \frac{ESW_{ilt}}{\gamma_{it}} \times \frac{HK_{\text{sur},it}}{102 \times 3.6 \times \mu_{\text{sur},it}} + \frac{DRE_{ilt}}{\gamma_{it}} \times \frac{HK_{\text{sur},it}}{102 \times 3.6 \times \mu_{\text{sur},it}} \\ + \frac{EGW_{ilt}}{\gamma_{it}} \times \frac{H_{\text{lift},it} + H_{\text{nop},it} + f_{\text{loss},it}}{102 \times 3.6 \times \mu_{\text{pump},it} \times \mu_{\text{motor},it}} \end{bmatrix} \end{aligned} \tag{B.5}$$

$$
\begin{aligned}
PRO\_ENE = & \sum_{i=1}^{I}\sum_{j=1}^{J}\sum_{k=1}^{12}\sum_{t=1}^{T} RED_{kt} \times FED_{iiukt} + \sum_{i=1}^{I}\sum_{k=1}^{12} \\
& \times \sum_{t=1}^{T} REX_{kt} \times AEX_{ikt} - \sum_{i=1}^{I}\sum_{k=1}^{3}\sum_{t=1}^{T} CEE_{kt} \times AEE_{ikt} - \sum_{i=1}^{I}\sum_{k=1}^{12} \\
& \times \sum_{t=1}^{T} CEI_{kt} \times AEI_{ikt} - \sum_{i=1}^{I}\sum_{m=1}^{3}\sum_{t=1}^{T} CEP_{mt} \times AEP_{imt} - \sum_{i=1}^{I}\sum_{n=1}^{11} \\
& \times \sum_{t=1}^{T} FCEC_{nt} \times CEC_{int} + VCEC_{nt} \times AEC_{int} + VCCC_{nt} \times ECC_{int} + \sum_{i=1}^{I} \\
& \times \sum_{n=5}^{8}\sum_{t=1}^{T} BCLP_{nt} \times AEC_{int} - \sum_{t=1}^{T} BCLP_{11t} \times AEC_{i11t} - \sum_{i=1}^{I}\sum_{m=1}^{3} \\
& \times \sum_{t=1}^{T} AEP_{imt} \times UEOP_{mt} \times ROM_t \times COM_t - \sum_{i=1}^{I}\sum_{n=1}^{11} \\
& \times \sum_{t=1}^{T} AEC_{int} \times UEOC_{nt} \times ROM_t \times COM_t - \sum_{i=1}^{I}\sum_{q=1}^{3}\sum_{m=1}^{3} \\
& \times \sum_{t=1}^{T} AEP_{imt} \times UESP_{qmt} \times RSM_{qt} \times CSM_{qt} - \sum_{i=1}^{I}\sum_{q=1}^{3}\sum_{n=1}^{11} \\
& \times \sum_{t=1}^{T} AEC_{int} \times UESC_{qnt} \times RSM_{qt} \times CSM_{qt}
\end{aligned} \tag{B.6}
$$

$$
\begin{aligned}
WA = & \sum_{t=1}^{T}\sum_{j=1}^{J}\sum_{i=1}^{I}(SW_{ijt} + GW_{ijt}) + \sum_{t=1}^{T}\sum_{j=1}^{J} \\
& \times \sum_{i=1}^{I}(ESW_{ilt} + EGW_{ilt}) + \sum_{k=1}^{3}\sum_{t=1}^{T} EWEX_{kt} \times AEE_{ikt} + \sum_{m=1}^{3} \\
& \times \sum_{t=1}^{T} EWPR_{mt} \times AEP_{imt} + \sum_{n=1}^{4} \\
& \times \sum_{t=1}^{T} EWC_{nt} \times AEC_{int} + \sum_{t=1}^{T} EWW_t \times AEC_{5t} + \sum_{n=1}^{11} \\
& \times \sum_{t=1}^{T} EWO_{nt} \times AEC_{int}
\end{aligned} \tag{B.7}
$$

(2) Environmental dimension: minimum carbon emission intensity (*CEI*)

Promoting control of carbon emission during water allocation and economic production processes is one of key fields to achieve emission peak and carbon neutrality in the future. Net carbon emission of WEECE nexus system mainly includes CO_2 emissions of energy sectors restricted by water allocation, and CO_2 absorption derived from ecosystem coverage subject to ecological water use. Hence, the second objective is to minimum carbon emission per unit of water use in the WEECE nexus system, which can be expressed as:

$$
\text{Min } CEI = \frac{\begin{array}{l}\sum_{t}^{T}\sum_{i}^{I}\sum_{m=1}^{3}\sigma_t \times AEP_{imt} \times UEOP_{mt} \times (1 - ROM_t) + \\ \sum_{t}^{T}\sum_{i}^{I}\sum_{n=1}^{11}\sigma_t \times AEC_{int} \times UEOC_{nt} \times (1 - ROM_t) + \\ \sum_{t}^{T}\sum_{k}^{K}\sum_{i}^{I}\sum_{j}^{J}\sigma_t \times FED_{iukt} \times CSC_k \times UCS_{k,t} \times (1 - ROME_{ukt}) + \sum_{m}^{M}\frac{IC_{mt}}{L_{mt}} \times \sigma_t - \sum_{m}^{M} IC_{mt} \times r_t - \sum_{t}^{T}\sum_{l}^{L}\sum_{i}^{I}\frac{ESW_{ilt} + EGW_{ilt} + ERW_{ilt}}{GWD_{lt}} \times cc_{lt}\end{array}}{\sum_{t=1}^{T}\sum_{j=1}^{J}\sum_{i=1}^{I}(SW_{ijt} + GW_{ijt}) + \sum_{t=1}^{T}\sum_{j=1}^{J}\sum_{i=1}^{I}(ESW_{ilt} + EGW_{ilt}) + \sum_{k=1}^{3}\sum_{t=1}^{T} EWEX_{kt} \times AEE_{ikt} + \sum_{m=1}^{3}\sum_{t=1}^{T} EWPR_{mt} \times AEP_{imt} + \sum_{n=1}^{4}\sum_{t=1}^{T} EWC_{nt} \times AEC_{int} + \sum_{t=1}^{T} EWW_t \times AEC_{5t} + \sum_{n=1}^{11}\sum_{t=1}^{T} EWO_{nt} \times AEC_{int}} \tag{B.8}
$$

(3) Ecological dimension: maximum ecological water proportion (EWP)

The proportion of ecological water use is an important indicator for guaranteeing the restoration of the fragile environment and sustainable development of water-stressed regions.

Thus, the third objective function is to maximize the comprehensive ecological water proportion as:

$$\text{Max } EWP = \frac{\sum_{t}^{T}\sum_{i}^{I}\sum_{l}^{L}\frac{ESW_{ilt}+EGW_{ilt}+ERW_{ilt}}{\gamma_{lt}} + TSW_t - \sum_{i}^{I}\sum_{j}^{J}\frac{SW_{ijt}}{\gamma_{ijt}} - \sum_{t}^{T}\sum_{i}^{I}\sum_{l}^{L}\frac{ESW_{ilt}}{\gamma_{lt}}}{\begin{array}{l}\sum_{t=1}^{T}\sum_{j=1}^{J}\sum_{i=1}^{I}(SW_{ijt}+GW_{ijt}) + \sum_{t=1}^{T}\sum_{j=1}^{J}\sum_{i=1}^{I}(ESW_{ilt}+EGW_{ilt}) + \\ \sum_{k=1}^{3}\sum_{t=1}^{T}EWEX_{kt}\times AEE_{ikt} + \sum_{m=1}^{3}\sum_{t=1}^{T}EWPR_{mt}\times AEP_{imt} + \\ \sum_{n=1}^{4}\sum_{t=1}^{T}EWC_{nt}\times AEC_{int} + \sum_{t=1}^{T}EWW_t\times AEC_{5t} + \sum_{n=1}^{11}\sum_{t=1}^{T}EWO_{nt}\times AEC_{int}\end{array}} \tag{B.9}$$

(4) Social dimension: minimum social inequality of WEECE nexus (SI)

Sustainable management of WEECE nexus needs to consider the fairness and rationality of resources allocation, which can help ensure social stability. Pietra-Ricci index is employed to describe the fairness of resources allocation among sub-regions. The value range of the Pietra-Ricci index is 0−0.5, and smaller value of Pietra-Ricci index indicates more balanced distribution of WEECE nexus. Therefore, the objective function of the social dimension is to minimize Pietra-Ricci index which can be expressed as follows:

$$\text{Min}\, SI = \frac{\dfrac{\sum_{i=1}^{I}\left|\begin{array}{l}\sum_{t=1}^{T}\sum_{j=1}^{J}SW_{ijt}+GW_{ijt}+\sum_{t=1}^{T}\sum_{l=1}^{L}ESW_{ilt}+EGW_{ilt}+\sum_{k=1}^{3}\sum_{t=1}^{T}EWEX_{kt}\times AEE_{ikt} \\ +\sum_{m=1}^{3}\sum_{t=1}^{T}EWPR_{m,t}\times AEP_{imt}+\sum_{n=1}^{4}\sum_{t=1}^{T}EWC_{nt}\times AEC_{int}+\sum_{t=1}^{T}EWW_t\times AEC_{5t} \\ +\sum_{n=1}^{11}\sum_{t=1}^{T}EWO_{nt}\times AEC_{int}-\sum_{t=1}^{T}PO_{it}\end{array}\right|}{\sum_{t=1}^{T}\sum_{i=1}^{I}PO_{it}}}{2\times\left[\begin{array}{l}\sum_{t=1}^{T}\sum_{j=1}^{J}\sum_{i=1}^{I}(SW_{ijt}+GW_{ijt})+\sum_{t=1}^{T}\sum_{j=1}^{J}\sum_{i=1}^{I}(ESW_{ilt}+EGW_{ilt})+ \\ \sum_{k=1}^{3}\sum_{t=1}^{T}EWEX_{kt}\times AEE_{ikt}+\sum_{m=1}^{3}\sum_{t=1}^{T}EWPR_{mt}\times AEP_{imt}+ \\ \sum_{n=1}^{4}\sum_{t=1}^{T}EWC_{nt}\times AEC_{int}+\sum_{t=1}^{T}EWW_t\times AEC_{5t}+ \\ \sum_{n=1}^{11}\sum_{t=1}^{T}EWO_{nt}\times AEC_{int}\end{array}\right]} \tag{B.10}$$

B.2 Constraints

(1) Constraints of water availability

$$\begin{array}{l}TSW_t + TGW_t + \sum_{i}^{I}\sum_{t}^{T}\sum_{j=6}^{8}\alpha_{ijt}\times(SW_{ijt}+GW_{ijt}+DRW_{ijt}+IRW_{ijt}) + \sum_{i}^{I} \\ \times\sum_{t}^{T}\sum_{j=9}\beta_{ijt}\times(SW_{ijt}+GW_{ijt}+DRW_{ijt}) \geq \sum_{i}^{I}\sum_{j}^{J}\frac{SW_{ijt}+GW_{ijt}}{\gamma_{jt}} + \sum_{t}^{T} \\ \times\sum_{i}^{I}\sum_{l}^{L}\frac{ESW_{ilt}+EGW_{ilt}+ERW_{ilt}}{\gamma_{lt}} + \sum_{k=1}^{3}\sum_{t=1}^{T}EWEX_{kt}\times AEE_{ikt} + \sum_{m=1}^{3} \\ \times\sum_{t=1}^{T}EWPR_{mt}\times AEP_{imt} + \sum_{n=1}^{4} \\ \times\sum_{t=1}^{T}EWC_{nt}\times AEC_{int} + \sum_{t=1}^{T}EWW_t\times AEC_{5t} + \sum_{n=1}^{11} \\ \times\sum_{t=1}^{T}EWO_{nt}\times AEC_{int},\ \forall t\end{array} \tag{B.11}$$

$$\sum_{i}^{I}\sum_{j}^{J}\frac{GW_{ijt}}{\gamma_{jt}} \leq TGW_t \times PGE_t,\ \forall t \tag{B.12}$$

$$\begin{array}{l}\sum_{i}^{I}\sum_{t}^{T} \\ \times\sum_{j=6}^{8}\alpha_{ijt}\times(SW_{ijt}+GW_{ijt}+DRW_{ijt}+IRW_{ijt}) \leq CIM_{it\ \max} + \sum_{i}^{I} \\ \times\sum_{t}^{T}\sum_{j=9}\beta_{ijt}\times(SW_{ijt}+GW_{ijt}+DRW_{ijt}) \leq CDM_{it\ \max}\end{array} \tag{B.13}$$

$$\begin{array}{l}\sum_{i}^{I}\sum_{j}^{J}DRW_{ijt} + \sum_{i}^{I}\sum_{j}^{J}IRW_{ijt} + \sum_{i}^{I}\sum_{l}^{L}ERW_{ilt} \leq \\ \sum_{i}^{I}\sum_{t}^{T}\sum_{j=6}^{8}\alpha_{ijt}\times(SW_{ijt}+GW_{ijt}+DRW_{ijt}+IRW_{ijt}) + \\ \sum_{i}^{I}\sum_{t}^{T}\sum_{j=9}\beta_{ijt}\times(SW_{ijt}+GW_{ijt}+DRW_{ijt})\quad \forall t\end{array} \tag{B.14}$$

$$DRW_{ijt} + IRW_{ijt} = RW_{ijt},\ \forall i,j,t \tag{B.15}$$

(2) Constraints of water demands

$$SW_{ijt} + GW_{ijt} + DRW_{ijt} \geq DW_{ijt},\ \forall i,t,j = 1,\ldots,5 \tag{B.16}$$

$$SW_{ijt} + GW_{ijt} + DRW_{ijt} + IRW_{ijt} \geq DW_{ijt},\ \forall i,t,j = 6,\ldots,8 \tag{B.17}$$

$$SW_{ijt} + GW_{ijt} + DRW_{ijt} \geq DW_{ijt},\ \forall i,t,j = 9 \tag{B.18}$$

(3) Constraints of electricity requirement during water pump and conveyance

$$\sum_{j}^{J}\sum_{i}^{I}\frac{SW_{ijt}}{\gamma_{jt}}\times\frac{HK_{\mathrm{sur},it}}{102\times3.6\times\mu_{\mathrm{sur},it}}+\sum_{j}^{J}\times\sum_{i}^{I}\frac{DRW_{ijt}}{\gamma_{jt}}\times\frac{HK_{\mathrm{sur},it}}{102\times3.6\times\mu_{\mathrm{sur},it}}+\sum_{i=1}^{I}\times\sum_{j=1}^{J}\frac{GW_{ijt}}{\gamma_{jt}}\times\frac{H_{\mathrm{lift},it}+H_{\mathrm{nop},it}+f_{\mathrm{loss},it}}{102\times3.6\times\mu_{\mathrm{pump},it}\times\mu_{\mathrm{motor},it}}\leq\sum_{n=1}^{8}AEC_{int}\times(1-LE_t)-\sum_{u=1}FED_{iukt},\ \forall i,j,t \tag{B.19}$$

(4) Constraint of reservoir water balance

$$TRW_t-(1+10\%)\times WKL_t-RHS_t-\sum_{i=1}^{I}\sum_{t=1}^{T}EWW_t\times AEC_{5t}\geq\sum_{i}^{I}\sum_{j}^{J}\frac{SW_{ijt}}{\gamma_{jt}}+\sum_{t}^{T}\sum_{i}^{I}\sum_{l}^{L}\frac{ESW_{ilt}}{\gamma_{lt}}+\sum_{k=1}^{3}\sum_{t=1}^{T}EWEX_{kt}\times AEE_{ikt}+\sum_{m=1}^{3}\sum_{t=1}^{T}EWPR_{mt}\times AEP_{imt}+\sum_{n=1}^{4}\sum_{t=1}^{T}EWC_{nt}\times AEC_{int}+\sum_{n=1}^{11}\times\sum_{t=1}^{T}EWO_{nt}\times AEC_{int} \tag{B.20}$$

(5) Constraints of reservoir water supply

$$\sum_{i=1}^{I}\sum_{t=1}^{T}EWW_t\times AEC_{5t}\leq\left[\begin{array}{l}\sum_{i}^{I}\sum_{j}^{J}\frac{SW_{ijt}+GW_{ijt}+DRW_{ijt}}{\gamma_{jt}}+\sum_{t}^{T}\sum_{i}^{I}\sum_{l}^{L}\frac{ESW_{ijt}+EGW_{ijt}+DRE_{ijt}}{\gamma_{lt}}\\+\sum_{k=1}^{3}\sum_{t=1}^{T}EWEX_{kt}\times AEE_{ikt}+\sum_{m=1}^{3}\sum_{t=1}^{T}EWPR_{mt}\times AEP_{imt}\\+\sum_{n=1}^{4}\sum_{t=1}^{T}EWC_{nt}\times AEC_{int}+\sum_{t=1}^{T}EWW_t\times AEC_{5t}\\+\sum_{n=1}^{11}\sum_{t=1}^{T}EWO_{nt}\times AEC_{int}\end{array}\right]\times PEN_t,\ \forall t \tag{B.21}$$

$$\sum_{i}^{I}\sum_{j=1}^{4}\frac{SW_{ijt}+GW_{ijt}+DRW_{ijt}}{\gamma_{jt}}\leq\left[\begin{array}{l}\sum_{i}^{I}\sum_{j}^{J}\frac{SW_{ijt}+GW_{ijt}+DRW_{ijt}}{\gamma_{jt}}+\sum_{t}^{T}\sum_{i}^{I}\sum_{l}^{L}\frac{ESW_{ijt}+EGW_{ijt}+DRE_{ijt}}{\gamma_{lt}}\\+\sum_{k=1}^{3}\sum_{t=1}^{T}EWEX_{kt}\times AEE_{ikt}+\sum_{m=1}^{3}\sum_{t=1}^{T}EWPR_{mt}\times AEP_{imt}\\+\sum_{n=1}^{4}\sum_{t=1}^{T}EWC_{nt}\times AEC_{int}+\sum_{t=1}^{T}EWW_t\times AEC_{5t}\\+\sum_{n=1}^{11}\sum_{t=1}^{T}EWO_{nt}\times AEC_{int}\end{array}\right]\times PIN_t,\ \forall t \tag{B.22}$$

(6) Constraint of land availability

$$A_{\mathrm{min},it}\leq\sum_{j=1}^{4}\frac{SW_{ijt}+GW_{ijt}+DRW_{ijt}}{(1+LF_{ijt})\times WPC_{ijt}}\leq A_{\mathrm{max},it},\ \forall i,t,j=1,\ldots,4 \tag{B.23}$$

(7) Constraint of water reuse rate

$$\frac{\sum_{i}^{I}\sum_{j}^{J}DRW_{ijt}+\sum_{i}^{I}\sum_{j}^{J}IRW_{ijt}+\sum_{i}^{I}\sum_{l}^{L}ERW_{ilt}}{\sum_{i}^{I}\sum_{j}^{J}(SW_{ijt}+GW_{ijt})}\geq PWR_t,\ \forall t \tag{B.24}$$

(8) Constraint of soil salinity control

$$\sum_{j=1}^{4}LF_{ijt}\times\frac{SW_{ijt}+GW_{ijt}+DRW_{ijt}}{1+LF_{ijt}}\leq TLW_{it},\ \forall i,t \tag{B.25}$$

(9) Constraint of food demand

$$\sum_{i}^{I}\sum_{j=2}^{2}\frac{YA_{ijt}\times(SW_{ijt}+GW_{ijt}+DRW_{ijt})}{(1+LF_{ijt})\times WPC_{ijt}}\geq\sum_{i}^{I}FD_{it}\times PO_{it},\ \forall t \tag{B.26}$$

(10) Constraint of electricity consumption for agricultural production

$$\sum_{i}^{I}\sum_{j}^{J}\frac{(SW_{ijt}+GW_{ijt}+DRW_{ijt})\times\xi_{it}\times CELE_t}{(1+LF_{ijt})\times WPC_{ijt}}+\sum_{i}^{I}\sum_{j}^{J}\frac{YA_{ijt}\times(SW_{ijt}+GW_{ijt}+DRW_{ijt})\times EAGP_{jt}}{(1+LF_{ijt})\times WPC_{ijt}}\leq\sum_{u=1}FED_{iukt},\ \forall i,t,k=11,j=1,\ldots,4 \tag{B.27}$$

(11) Constraint of diesel oil for agricultural machinery

$$\sum_{i}^{I}\sum_{j=1}^{4}\frac{(SW_{ijt}+GW_{ijt}+DRW_{ijt})\times KLD_{jt}}{(1+LF_{ijt})\times WPC_{ijt}}\leq\sum_{i}^{I}\sum_{u=1}\sum_{k}^{K}FED_{iukt}\times\varsigma_{\mathrm{fe},t},\ \forall t,k=8 \tag{B.28}$$

(12) Constraint of bioenergy production from crop planting

$$\sum_{i}^{I}\sum_{j}^{J}\frac{YA_{ijt}\times(SW_{ijt}+GW_{ijt}+DRW_{ijt})\times GBE_{jt}}{(1+LF_{ijt})\times WPC_{ijt}}\geq MAXrenew_{int},\ \forall t,n=8,j=1,\ldots,4 \tag{B.29}$$

(13) Constraints of field contaminants discharge (i.e., total phosphorus and total nitrogen)

$$\sum_{i}^{I}\sum_{j}^{J}\frac{SW_{ijt}+GW_{ijt}+DRW_{ijt}}{(1+LF_{ijt})\times WPC_{ijt}}\times\begin{pmatrix}AMF_{jt}\times CEF_{jt}\times PN_{\mathrm{mf},t}+\\AMM_{jt}\times CEM_{jt}\times PN_{\mathrm{mm},t}+\\ADM_{jt}\times CDM_{jt}\times PN_{\mathrm{dm},t}\end{pmatrix}\leq MNO_t,\ \forall t,j=1,\ldots,4 \tag{B.30}$$

$$\sum_{i}^{I}\sum_{j}^{J}\frac{SW_{ijt}+GW_{ijt}+DRW_{ijt}}{(1+LF_{ijt})\times WPC_{ijt}}\times\begin{pmatrix}AMF_{jt}\times CEF_{jt}\times PP_{\mathrm{mf},t}+\\AMM_{jt}\times CEM_{jt}\times PP_{\mathrm{mm},t}+\\ADM_{jt}\times CDM_{jt}\times PP_{\mathrm{dm},t}\end{pmatrix}\leq MPO_t,\ \forall t,j=1,\ldots,4 \tag{B.31}$$

(14) Constraints of field gases emissions (NO_x, PM_{10}, SO_2, CO_2)

$$\sum_{i}^{I}\sum_{j}^{J}\frac{SW_{ijt}+GW_{ijt}+DRW_{ijt}}{(1+LF_{ijt})\times WPC_{ijt}}\times KLD_{jt}\times\delta_{\mathrm{oil},t}\times CNO_t\leq TNO_t,\ \forall t,j=1,\ldots,4 \tag{B.32}$$

$$\sum_{i}^{I}\sum_{j}^{J}\frac{SW_{ijt}+GW_{ijt}+DRW_{ijt}}{(1+LF_{ijt})\times WPC_{ijt}}\times KLD_{jt}\times\delta_{\mathrm{oil},t}\times CPM_t\leq TPM_t,\ \forall t,j=1,\ldots,4 \tag{B.33}$$

$$\sum_{i}^{I}\sum_{j}^{J}\frac{SW_{ijt}+GW_{ijt}+DRW_{ijt}}{(1+LF_{ijt})\times WPC_{ijt}}\times KLD_{jt}\times\delta_{\mathrm{oil},t}\times CSO_t\leq TSO_t,\ \forall t,j=1,\ldots,4 \tag{B.34}$$

$$\sum_{i}^{I}\sum_{j}^{J}\frac{SW_{ijt}+GW_{ijt}+DRW_{ijt}}{(1+LF_{ijt})\times WPC_{ijt}}\times KLD_{jt}\times\delta_{\mathrm{oil},t}\times CCO_t\leq TCO_t,\ \forall t,j=1,\ldots,4 \tag{B.35}$$

(15) Constraint of ecological flow into Bosten Lake

$$TSW_t-\sum_{i}^{I}\sum_{j}^{J}\frac{SW_{ijt}}{\gamma_{jt}}+\sum_{t}^{T}\sum_{i}^{I}\sum_{l}^{L}\frac{ESW_{ilt}}{\gamma_{lt}}+\sum_{k=1}^{3}\sum_{t=1}^{T}EWEX_{kt}\times AEE_{ikt}+\sum_{m=1}^{3}\sum_{t=1}^{T}EWPR_{mt}\times AEP_{imt}+\sum_{n=1}^{4}\sum_{t=1}^{T}EWC_{nt}\times AEC_{int}+\sum_{t=1}^{T}EWW_t\times AEC_{5t}+\sum_{n=1}^{11}\sum_{t=1}^{T}EWO_{nt}\times AEC_{int}-WKL_t\geq EBW_t,\ \forall t \tag{B.36}$$

(16) Constraint of ecosystem land coverage

$$\sum_{i}^{I}\sum_{l}^{L}\frac{ESW_{ilt}+EGW_{ilt}+ERW_{ilt}}{GWD_{lt}}\geq TDE_t,\ \forall t \tag{B.37}$$

(17) Constraint of CO_2 emissions

$$\sum_{t}^{T}\sum_{i}^{I}\sum_{n=1}^{11}\sigma_t\times AEC_{int}\times UEOC_{nt}\times(1-ROM_t)+\sum_{t}^{T}\sum_{k}^{K}\sum_{i}^{I}\sum_{u}^{U}\sigma_t\times FED_{iukt}\times CSC_k\times UCS_{kt}\times\left(1-ROME_{jkt}\right)+\sum_{m}^{M}\frac{IC_{mt}}{L_{mt}}\times\sigma_t-\sum_{m}^{M}IC_{mt}\times r_t-\sum_{t}^{T}\sum_{l}^{L}\times\sum_{i}^{I}\frac{ESW_{ilt}+EGW_{ilt}+ERW_{ilt}}{GWD_{lt}}\times cc_{lt}\leq\sum_{i}^{I}TLC_{it} \tag{B.38}$$

(18) Constraint of energy exploitation

$$AEE_{ikt}\leq MAXAEE_{ikt},\ k=1,2,3,\ \forall i,t \tag{B.39}$$

(19) Constraints of energy import and export

$$AEI_{ikt}\leq MAXEI_{ikt},\ \forall i,k,t \tag{B.40}$$

$$AEX_{ikt}\leq MAXEX_{ikt},\ \forall i,k,t \tag{B.41}$$

(20) Constraint of renewable energy

$$CEC_{int}\leq MAXrenew_{int},\ n=5,6,7,8,\ \forall i,t \tag{B.42}$$

(21) Constraint of water consumption for energy generation

$$\sum_{k=1}^{3}\sum_{t=1}^{T}EWEX_{kt}\times AEE_{ikt}+\sum_{m=1}^{3}\sum_{t=1}^{T}EWPR_{mt}\times AEP_{imt}+\sum_{n=1}^{4}\times\sum_{t=1}^{T}EWC_{nt}\times AEC_{int}+\sum_{t=1}^{T}EWW_{t}\times AEC_{5t}+\sum_{n=1}^{11}\times\sum_{t=1}^{T}EWO_{nt}\times AEC_{int}\leq TWE_{it} \tag{B.43}$$

(22) Constraints of supply and demand for raw coal, crude oil and nature gas

$$AEE_{ikt}+AEI_{ikt}-AEX_{ikt}-AEP_{i1t}\times UECP_{i1t}-\sum_{n=1}^{2}AEC_{int}\times UECC_{int}-AEC_{i9t}\times UECC_{i9t}-LR_{ikt}\geq\sum_{u=1}^{U}FED_{iukt},k=1,\forall i,t \tag{B.44}$$

$$AEE_{ikt}+AEI_{ikt}-AEX_{ikt}-AEP_{i3t}\times UECP_{3t}-LR_{ikt}\geq\sum_{u=1}^{U}FED_{iukt},k=2,\forall i,t \tag{B.45}$$

$$AEE_{ikt}+AEI_{ikt}-AEX_{ikt}-AEP_{i4t}\times UECP_{4t}+\sum_{n=3}^{4}AEC_{int}\times UECC_{nt}-AEC_{i10t}\times UECC_{10t}-LR_{ikt}\geq\sum_{u=1}^{U}FED_{iukt},k=3,\forall i,t \tag{B.46}$$

(23) Constraints of supply and demand for coal products (cleaned coal and coke)

$$AEI_{ikt}-AEX_{ikt}+AEP_{i1t}-AEP_{i2t}\times UECP_{2t}-LR_{ikt}\geq\sum_{u=1}^{U}FED_{iukt},k=4,\forall i,t \tag{B.47}$$

$$AEI_{ikt}-AEX_{ikt}+AEP_{i2t}-LR_{ikt}\geq\sum_{u=1}^{U}FED_{iukt},k=5,\forall i,t \tag{B.48}$$

(24) Constraints of supply and demand for oil products (gasoline, kerosene, diesel oil and fuel oil)

$$AEI_{ikt}-AEX_{ikt}+0.2\times AEP_{i3t}-LR_{ikt}\geq\sum_{u=1}^{U}FED_{iukt},k=6,\forall i,t \tag{B.49}$$

$$AEI_{ikt}-AEX_{ikt}+0.06\times AEP_{i3t}-LR_{ikt}\geq\sum_{u=1}^{U}FED_{iukt},k=7,\forall i,t \tag{B.50}$$

$$AEI_{ikt}-AEX_{i,k,t}+0.37\times AEP_{i3t}-LR_{ikt}\geq\sum_{u=1}^{U}FED_{iukt},k=8,\forall i,t \tag{B.51}$$

$$AEI_{ikt}-AEX_{ikt}+0.07\times AEP_{i3t}-LR_{ikt}\geq\sum_{u=1}^{U}FED_{iukt},k=9,\forall i,t \tag{B.52}$$

$$AEI_{ikt}-AEX_{ikt}+AEP_{i4t}-LR_{ikt}\geq\sum_{u=1}^{U}FED_{iukt},k=10,\forall i,t \tag{B.53}$$

(25) Constraints of supply and demand for electricity and heat

$$\sum_{n=1}^{8}AEC_{int}\times(1-LE_t)\geq\sum_{u=1}^{U}FED_{iukt},k=11,\forall i,t \tag{B.54}$$

$$(AEC_{i2t}+AEC_{i4t})\times RHE_t+\sum_{n=9}^{11}AEC_{int}-LR_t\geq\sum_{u=1}^{U}FED_{iukt},k=12,\forall i,t \tag{B.55}$$

(26) Constraints of capacity expansion

$$AEP_{imt}\leq RCP_{imt},\forall i,m,t \tag{B.56}$$

$$CEC_{int}\leq CEC_{in1}+ECC_{int}-TY_{int},t=2,3,\ldots,6,\forall i,n \tag{B.57}$$

$$CEC_{int}\leq CEU_{int},\forall i,n,t \tag{B.58}$$

(27) Constraint of energy conversion

$$CEC_{int}\times OT_{nt}\geq AEC_{int},\forall i,n,t \tag{B.59}$$

(28) Constraint of pollutant reduction for energy generation

$$\sum_{q=1}^{3}\sum_{m=1}^{3}\sum_{t=1}^{T}AEP_{imt}\times UESP_{qmt}\times RSM_{qt}+\sum_{q=1}^{3}\sum_{n=1}^{11}\times\sum_{t=1}^{T}AEC_{int}\times UESC_{qnt}\times RSM_{qt}+\sum_{q=1}^{3}\sum_{u=1}^{U}\sum_{k=1}^{12}\times\sum_{t=1}^{T}FED_{iukt}\times CSC_{ukt}\times UPS_{it}\times RSME_{it}\leq TLP_{iqt},\forall t \tag{B.60}$$

(29) Constraints of CCS capacity

$$\sum_{m}^{M}IC_{mt}\leq\sum_{m}^{M}\left(\frac{IC_{mt}}{L_{mt}}\times\sigma_t\right)+\sum_{t}^{T}\sum_{i}^{I}\sum_{m=1}^{3}\sigma_t\times AEP_{imt}$$

$$\times UEOP_{mt} \times (1 - ROM_t) + \sum_{t}^{T} \sum_{i}^{I} \sum_{n=1}^{11} \sigma_t \times AEC_{int} \times UEOC_{nt} \times (1 - ROM_t) + \sum_{t}^{T} \sum_{k}^{K} \sum_{i}^{I} \sum_{u}^{U} \sigma_t \times FED_{iukt} \times CSC_k \times UCS_{kt} \times (1 - ROME_{ukt}), \forall t \tag{B.61}$$

$$L_{it} = \left(1 - \frac{\mu_i'}{\mu_i}\right) \times 100\% \tag{B.62}$$

$$\mu_i' = (1 - \lambda \times r_t \times \sigma_t) \times \mu_i \tag{B.63}$$

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