



1       **Process-based three-layer synergistic optimal allocation**  
2       **model for complex water resource systems considering**  
3       **reclaimed water**

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11       **Abstract**

12       The increasing water demand due to human activities has aggravated water scarcity,  
13       and conflicts among stakeholders have increased the risk of unsustainable development.

14       Ignoring the effects of trade-offs leads to misguided policy recommendations. This  
15       study highlights the concept of synergy among different aspects of water allocation  
16       process. A process-based three-layer synergistic optimal allocation (PTSOA) model is  
17       established to integrate the interests of stakeholders across subregions, decision levels  
18       and time steps while simultaneously coupling reclaimed water to establish



19 environmentally friendly solutions. A synergy degree index is constructed by applying  
20 network analysis for optimization. PTSOA is applied in Yiwu City, Southeast China,  
21 and is shown to improve the contradictions among different dimensionalities in a  
22 complex system. Overall,  $2.43 \times 10^7 \sim 3.95 \times 10^7$  m<sup>3</sup> of conventional water is saved, and  
23 notable improvements in management are achieved. The application demonstrates the  
24 efficiency and excellent performance of the PTSOA.

25 **Keywords** Three-layer optimization, water allocation, process, synergy, reclaimed  
26 water

## 27 1. Introduction

28 Water scarcity has become one of the major impediments to the sustainable  
29 development of cities (Yue et al., 2020). Emerging water scarcity concerns in cities are  
30 associated with limited available water, severe water pollution and the relentlessly  
31 growing demand for water as driven by industrial growth, population growth and higher  
32 living standards; these factors have lead to intense competition for freshwater among  
33 stakeholders of interest (Dai et al., 2018; Wu et al., 2023). However, the heterogeneous  
34 distribution of water resources at both spatial and temporal scales is common in many  
35 cities and results in water shortage risks and conflicts, which often require the  
36 optimization of water resource allocation (Friesen et al. 2017). Moreover, some  
37 satisfactory alternatives for individual stakeholders may result in negative externalities  
38 on others. Therefore, it is critical to develop a synergistic optimal allocation model to



39 alleviate conflicts and ensure the security, efficiency, equality, eco-environmental  
40 sustainability, and sustainable development of water systems simultaneously.

41 As equitable access to water resources is closely related to social stability, several  
42 qualitative and indirect methods have been developed to assess water allocation  
43 equality (D'Exelle et al. 2012). In cases with limited water resources, more water would  
44 be allocated to users with better economic conditions to achieve more economic  
45 benefits. Thus, stakeholders with poor economic status are ignored, resulting in  
46 imbalanced development. Consequently, actions are often needed by local government  
47 managers to avoid such situations. The Gini coefficient has been widely used to  
48 evaluate equality and enhance the optimization of water allocation in water use sectors  
49 (Xu et al. 2019; Hu et al. 2016; D'Exelle et al. 2012). However, it is unable to reflect  
50 the dynamic interactions among objectives, i.e., how objectives interact with each other  
51 and impact the equity of a system in cases with diverse alternative decisions. While, in  
52 the perspective of coordinated allocation, multiple goals are simultaneously considered  
53 to avoid negative effects as much as possible. Therefore, in addition to equity,  
54 coordination should be considered in water allocation systems, and these two concepts  
55 can be combined to promote systemic synergy. By identifying the dynamic interactions  
56 among objectives, the internal mechanisms of a water system can be clarified, and  
57 synergy can be achieved in cases with different potential decisions. It is also helpful to  
58 identify the hurdles and opportunities associated with sustainable development for  
59 cities and to establish specific action priorities for cities based on a comprehensive



60 understanding of the interactions among objectives. To address this knowledge gap, a  
61 correlational network approach is applied in this study, and a synergy degree index is  
62 presented to consider both the equity and coordination of water systems. Moreover,  
63 systemic analysis is used to assess the level of coordination of complex objective  
64 interactions in city water systems.

65 Network analysis, which has been widely used in studies of complex systems (Ball  
66 et al., 2000; Saavedra et al., 2011; Bond, 2017), is a holistic approach for exploring the  
67 characteristics of interactions among objectives. It provides clear visualization and  
68 conceptualization of the interactions among variables to fully characterize those  
69 interactions (Swain and Ranganathan, 2021). An array of network metrics (for example,  
70 degree centrality, betweenness centrality, eigenvector centrality, closeness centrality,  
71 and community) can be applied to quantify the importance of objectives or targets in an  
72 interaction network (Zhou and Moinuddin, 2017) and reveal the strongly connected  
73 pairs of goals or targets in the network (Allen et al., 2019). A key network metric in  
74 such analysis is connectivity, which reflects the degree of coordination among different  
75 objectives in a system; in synergy networks, high connectivity indicates that many  
76 objectives can be achieved simultaneously and that the negative effects of interactions  
77 are mild (Wu et al., 2022). Thus, to facilitate the discovery of high-quality decision  
78 alternatives, alleviate negative conflicts among multiple utilities and inform decision  
79 making, a synergy degree evaluation index is established and applied to the network  
80 analysis of this study.



81           Due to the negative externalities of individual decisions, conflicts occur not only  
82 across different users or objectives but also across hierarchical decision levels. Water  
83 use contradictions and inconsistent decision making by multiple managers inevitably  
84 results in trade-offs, including positive and negative water resource feedback in cases  
85 with limited water availability (Wang et al., 2022). In practice, district administrators  
86 allocate water to each sector in each subregion, and subregion managers then make use  
87 decisions based on the allocated amount of water resources (Safari et al., 2014). Since  
88 each decision maker places emphasis on different targets, feedback and coordination  
89 among different decision makers are of great importance. Therefore, synergistic  
90 hierarchical water allocation that achieves coordination among different decision  
91 makers is imperative to avoid conflicts, save water and maintain social stability.

92           To address these hierarchical problems, bilevel programming (BLP) has been  
93 widely used, wherein objectives at two hierarchical levels, namely, an upper level and  
94 a lower level, are co-optimized (Zhang and Vesselinov, 2016; Jin et al., 2018). The  
95 upper-level decision may be affected by the actions of the lower-level decision makers  
96 (Arora and Gupta, 2009). Yue et al. (2020) formulated a bilevel programming (BLP)  
97 framework to gain insight into the whole water allocation process with district  
98 administrators and subregional farmers. Li et al. (2022) built a two-level model with  
99 the overall interests of system managers at the top and the individual interests of water  
100 supply departments at the bottom. The multilevel programming problem (MLPP) was  
101 derived from the bilevel programming problem (BLPP) and is more applicable to real



102 world practices (Baky, 2014). However, limited studies have explored applying MLPP  
103 (more than two levels) for water resource allocation, especially in cases with  
104 unconventional water supplies.

105 To satisfy both long-term and short-term water needs and avoid unnecessary  
106 administration costs and water resource use caused by a lack of coordination among  
107 different allocation steps, temporally synergistic allocation and optimization are needed  
108 (Haguma and Leconte, 2018). In annual water resource planning, the monthly  
109 variability of hydrologic regimes and nonstationarity of the daily water demand must  
110 be considered. As an alternative example of synergistic allocation at different time steps,  
111 Vicuna et al. (2010) used a monthly nonlinear programming model and an annual  
112 sampling stochastic dynamic programming (SSDP) model to establish a monthly  
113 operating policy. Haguma et al. (2015) proposed an optimization approach with two  
114 separate time steps following the nested model approach. Haguma and Leconte (2018)  
115 constructed deterministic and stochastic optimization models with two time steps (intra-  
116 annual and interannual) and two levels of inflow variability: seasonal and interannual.  
117 The purpose of their short-time-step model was to derive aggregate performance  
118 functions associated with potential long-time-step decisions in these studies. However,  
119 short-term benefits should not be overlooked due to their appreciable impact on long-  
120 term effects. Accordingly, synergistic allocation that enhances both long-term and  
121 short-term allocations is of great importance for water resource management in cities.  
122 However, optimizing the structure of a model to achieve maximized benefits and



123 balancing the trade-offs among time steps are tasks that have rarely been studied. The  
124 synergy among different time steps is addressed with a new innovative framework and  
125 a corresponding algorithm in our study.

126 Most of the abovementioned traditional models are based on a benefit-oriented  
127 mechanism, which leads to a high degree of satisfaction in high-benefit regions and  
128 large water shortages in other regions. The existence of high-benefit regions in a city  
129 during the allocation process often exacerbates regional disparities and heterogeneous  
130 development. Moreover, spatial factors influence allocation results, especially when  
131 there is spatial hierarchical heterogeneity among water resource allocation elements (Li  
132 et al., 2022). It is thus appropriate to conceptualize water allocation problems in a  
133 multistage framework that fully considers the interests of not only the regional authority  
134 but also subregional managers (Yao et al., 2019). Hence, the synergy among subregions  
135 must be considered to optimally allocate water resources. Ideally, the benefits of all  
136 subregions should be integrated equally in the model, and the weights of  
137 hyperparameters should be adjusted to best support flexible policies.

138 The optimal allocation of conventional and unconventional water resources also  
139 significantly impacts water security and aquatic ecosystems. The reuse of reclaimed  
140 water is beneficial for alleviating high water supply pressure on conventional water  
141 resources and reducing the emission of pollutants. To effectively integrate conventional  
142 and unconventional water resources, Yang et al. (2008) and Han et al. (2008) introduced  
143 unconventional water resources as critical factors in water management. Avni et al.



144 (2013) investigated the mixing of unconventional water resources with other  
145 conventional water sources to meet the magnesium requirements for drinking water and  
146 irrigation water. Yu et al. (2017) developed a cost–benefit analysis-based utilization  
147 model for externally transferred water and desalinated water. The allocation of both  
148 conventional and unconventional water has been widely studied, but there remains a  
149 lack of methods to guide the synergistic allocation of conventional and unconventional  
150 water resources and embed reclaimed water supply systems in allocation schemes. The  
151 overexploitation of conventional water resources is not conducive to the sustainable  
152 development, while the extensive use of unconventional water could ultimately result  
153 in high economic burden. To synergistically integrate conventional and unconventional  
154 water resources and guide the coordinated allocation of these two types of water  
155 resources, corresponding mechanisms must be implemented. As a result, our study aims  
156 to couple the allocation of conventional water resources and unconventional water  
157 resources to establish synergistic solutions.

158 In summary, as insufficient water supplies and increasing water demands intensify  
159 competition for water resources and lead to conflicts among different stakeholders in  
160 different dimensions, water allocation must be optimized in cities and regions to  
161 achieve synergistic decision-making at various levels and time steps considering the  
162 value of reclaimed water. Therefore, a new process-based three-layer synergistic  
163 optimal allocation (PTSOA) model is developed here to generate numerous candidates  
164 or Pareto solutions and identify several desirable decision alternatives. The synergy of





165 time and space optimization is achieved in the new model to avoid waste and promote  
166 balanced spatial development. Furthermore, in the PTSOA model, reclaimed water is  
167 used to replenish conventional water resources in water-scarce areas.

168 The remainder of this paper is organized as follows. The mathematical model is  
169 formulated in Section 2. Section 3 gives a numerical example for Yiwu city to  
170 demonstrate the effectiveness and efficiency of the proposed methods. The results are  
171 shown in Section 4; different water allocation strategies under varying inflow  
172 conditions are explored, and some policy implications are discussed. Section 5 presents  
173 conclusions.

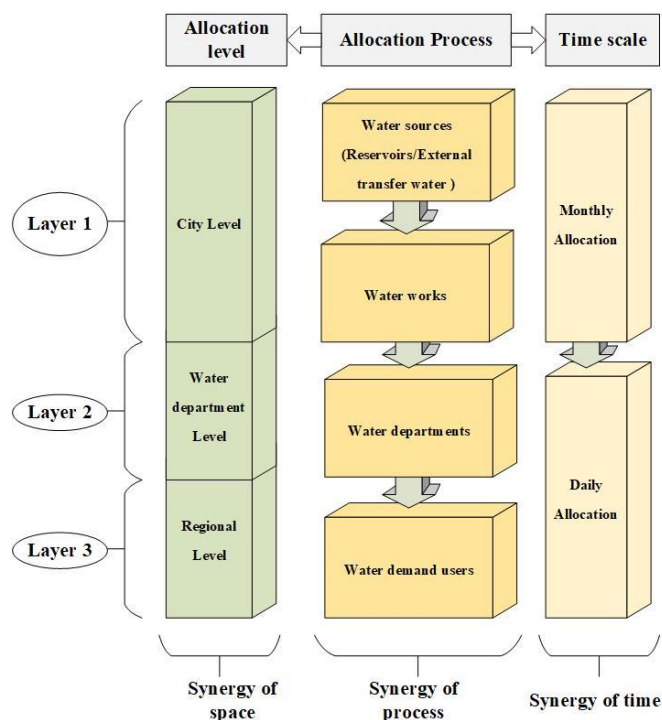
## 174 **2. Modelling**

175 With water resources becoming increasingly scarce, multidimensional synergistic  
176 optimal allocation in a hierarchical system is crucial for ensuring sustainable  
177 development in water-scarce cities. There are three dimensions of synergy in the  
178 established allocation model, as shown in Fig. 1: process synergy, decision-level  
179 synergy and time-scale synergy. The synergy of the process refers to synergistic water  
180 allocation among the three stages throughout the whole allocation process to reduce  
181 waste in bridging processes, which has rarely been considered. In the three stages, first,  
182 the original water is released from reservoirs or diverted from external water transfer  
183 projects to water works; then, the water stored in water works infrastructure is supplied  
184 to different departments that need different types of water, including both conventional



185 and reclaimed water. Finally, the water is supplied to different users. Decision-level  
186 synergy refers to synergistic water allocation considering the interests of decision  
187 makers at different levels, namely, the city, water department and regional levels, to  
188 coordinate solutions and avoid conflicts among decision makers. The city level  
189 represents the overall interests of a city from the perspective of government, the water  
190 supply department level represents the interests of water supply corporations, and the  
191 regional level focuses on the comprehensive benefits of each region in the city and  
192 mitigate development imbalance among regions. Optimal decision making at the  
193 department level is constrained by the allocation results at the city level, and so on, and  
194 the final solution should satisfy the needs of decision makers across all levels. The time  
195 scale synergy involves the coordination of the daily configuration goal with the monthly  
196 goal, the monthly goal with the yearly goal, and so on. Synergistic temporal allocation  
197 can largely alleviate time conflicts during configuration operations, ensuring that all  
198 configuration periods serve the same final configuration objectives to save water  
199 resources and improve efficiency. However, time scale synergy mainly depends on  
200 artificial operations rather than automated intelligent operations in practice. In-depth  
201 exploration has yet to be demonstrated. Consequently, the PTSOA model is constructed  
202 here to fully consider these three dimensionalities of synergy. The dimensionalities are  
203 coupled this model to achieve the efficient maximization of comprehensive benefits at  
204 all levels under the premise of saving water resources.

205



206

207

**Fig. 1. Conceptual map of the PTSOA model**

208

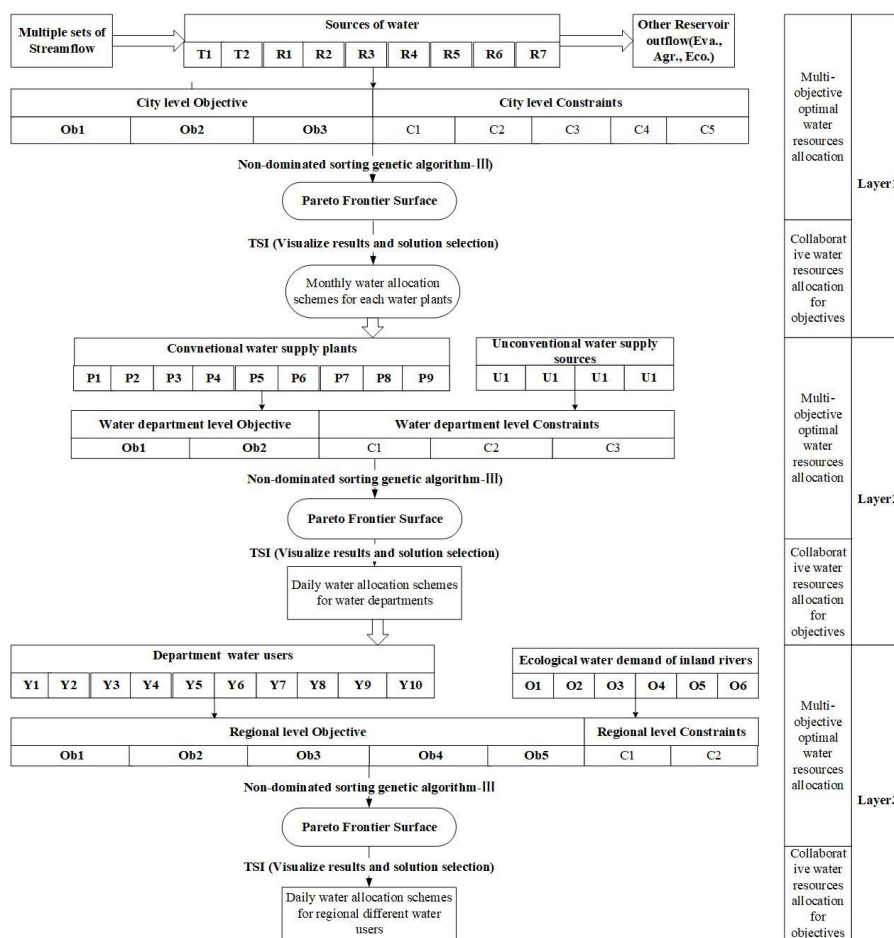
209 In water-scarce cities, using reclaimed water as an alternative water source is a  
210 proven approach to efficiently improve the environment by reducing sewage discharge.

211 The quality of inland tributaries has deteriorated in many water-scarce cities due to  
212 limited consideration of the water environment and the large-scale emission of  
213 pollutants. Transferring reclaimed water and main river water to urban inland tributaries  
214 for ecological water replenishment is a promising approach for improving the quality  
215 of urban water environments and areas with water shortages. However, there has been  
216 a lack of studies on the integration of reclaimed water reuse systems and inland water



217 distribution systems in allocation modelling. Therefore, in addition to saving water  
218 resources and improving efficiency through multidimensional synergistic allocation,  
219 the model encompasses reclaimed water reuse systems and ecological water  
220 distribution systems for inland tributaries.

221 Finally, the PTSOA model is constructed to solve the multidimensional synergistic  
222 allocation problem involving complex water resource networks that couple reclaimed  
223 water reuse systems and inland ecological water distribution systems with multiple  
224 sources, processes and regions to guarantee the sustainable development of water-  
225 scarce cities. To select the most synergistic solution of the PTSOA model, a new  
226 evaluation index named the total synergy index (TSI) is proposed to assess the synergy  
227 degree of different decision alternatives. Furthermore, the network analysis method is  
228 applied for the first time to analyse dynamic interactions in water optimal allocation.  
229 This method visually depicts the dynamic interactions and conflicts among different  
230 subareas in a city, which is helpful for system managers to realize how the water  
231 allocation scheme in one region influences that of other areas; consequently, more  
232 reasonable and flexible measures are established based on dynamic regional  
233 development targets. The detailed framework developed in this study is shown in Fig.  
234 2.



235

236

**Fig. 2. Framework of the PTSOA model**

237

## 2.1 First layer of the PTSOA decision-making process

238

Three dimensionalities of synergistic water resource allocation are coupled in the first

239

layer of the PTSOA model. The first stage of the process (original water is released

240

from reservoirs or external water transfer projects to water works) is optimized in the

241

first layer. This stage demonstrates a strong constraint effect on the later stages. To



242 satisfy the overall development goals of the city, the first-layer processes involve city-  
243 level decision-making. The city manager focuses on the overall goal of the water  
244 resource system in the city, which is the first and most important phase of the decision-  
245 making process. The established allocation scheme highly influences decision makers  
246 at other levels, and optimal allocation schemes at other levels must align with this  
247 overall goal. Additionally, since water resource planning in most Chinese cities is based  
248 on an annual planning period and monthly planning unit, the time step of the first layer  
249 is set as months. Finally, the monthly decision alternatives for the volume of water  
250 allocated from reservoirs to water works is obtained at the city decision level.

### 251 **2.1.1 Objective functions**

#### 252 **Social objective function: Minimization of total water supply shortages**

253 The social objective function is established by the city manager to minimize the total  
254 water supply shortages in a water system. The objective is established to sufficiently  
255 meet the water demands of users in a water resources system. The water deficit is  
256 considered, and this objective can reflect the ability of the water supply to meet the  
257 water demand, as shown in Eqs. (1-3):

$$258 \quad \min f_{11}(x) = D - S \quad (1)$$

$$259 \quad D = \sum_{r=1}^R \sum_{t=1}^T D_r^t \quad (2)$$

$$260 \quad S = \sum_{t=1}^T \sum_{i=1}^I \sum_{j=1}^J x_{ij}^t \alpha_{ij} + \sum_{t=1}^T \sum_{e=1}^E \sum_{j=1}^J x_{e,j}^t \beta_{ej} \quad (3)$$



261 where  $D(10^4 \text{ m}^3)$  is the total water demand of the system,  $D_r^t(10^4 \text{ m}^3)$  is the water  
 262 demand of the  $r$ th subregion at  $t$ th time step,  $r=1,2,\dots,R$ ,  $R$  is the total number of  
 263 subregions in the area,  $t=1,2,\dots,T$ ,  $T$  is the total number of months in the period,  $S(10^4$   
 264  $\text{m}^3)$  is the total water supply of the water system for all waterworks,  $x_{ij}^t(10^4 \text{ m}^3)$  is the  
 265 amount of water supplied from  $i$ th reservoir to the  $j$ th waterworks in the  $t$ th month of  
 266 the configuration period,  $i=1,2,\dots,I$ ,  $I$  refers to the total number of reservoirs,  $j=1,2,\dots,J$ ,  
 267  $J$  is the number of total water works,  $x_{ej}^t(10^4 \text{ m}^3)$  is the amount of water supplied from  
 268 the  $e$ th external transfer water source to the  $j$ th water works in the  $t$ th month of the  
 269 configuration period,  $e=1,2,\dots,E$ ,  $E$  is the total number of external transfer water  
 270 sources in the city,  $\alpha_{ij}$  is the water supply relationship coefficient between the  $i$ th  
 271 reservoir and the  $j$ th water works, where 0 indicates no supply and 1 indicates a water  
 272 supply, and  $\beta_{ej}$  is the water supply relationship coefficient between the  $e$ th external  
 273 transfer water source and the  $j$ th water works, where 0 indicates no supply and 1  
 274 indicates a water supply.

275 **Economic objective function: Maximization of the total water supply benefit**

276 A city manager operates a water allocation system to maximize the overall economic  
 277 benefit by establishing an economic objective function, as shown in Eqs. (4-7):

278 
$$\max f_{12}(x) = B - C_{rs} - C_{es} \quad (4)$$

279 
$$C_{rs} = k \times \sum_{t=1}^T \sum_{i=1}^I \sum_{j=1}^J x_{ij}^t \alpha_{ij} + \sum_{t=1}^T \sum_{i=1}^I \sum_{j=1}^J (x_{ij}^t \alpha_{ij} \times c_i) \quad (5)$$

280 
$$C_{es} = m \times \sum_{t=1}^T \sum_{j=1}^J \sum_{e=1}^E x_{ej}^t \beta_{ej} + \sum_{t=1}^T \sum_{e=1}^E \left( n_e \times \sum_{j=1}^J x_{ej}^t \beta_{ej} \right) \quad (6)$$



$$281 \quad B = \sum_{j=1}^J b_j \times \left( \sum_{t=1}^T \sum_{i=1}^I x_{ij}^t \alpha_{ij} + \sum_{t=1}^T \sum_{e=1}^E x_{ej}^t \beta_{ej} \right) \quad (7)$$

282       The overall economic benefit is the difference between the total benefit and total  
283 cost at the city level. In the equations,  $B$  (Chinese yuan, shortened to yuan in the  
284 following text) is the total direct water supply benefit (mainly considering the income  
285 from water charges for the city). The total water supply cost consists of the reservoir  
286 water supply cost  $C_{rs}$  and the external water supply cost  $C_{es}$ ;  $k$  (yuan/m<sup>3</sup>) denotes  
287 the water resources fees paid to the government;  $c_i$  (yuan/m<sup>3</sup>) denotes the water fees  
288 paid to the  $i$ th reservoir authority;  $m$  (yuan/m<sup>3</sup>) is the charge to an external  
289 administrative district per unit of externally transferred water;  $n_e$  (yuan/m<sup>3</sup>) is the  
290 charge associated with the  $e$ th external water source per unit of transferred water; and  
291  $b_j$  (yuan/m<sup>3</sup>) is the unit price of water supply revenue for the  $j$ th user.

292 **Sustainable development objective function: Maximization of the total amount of**  
293 **reserved water in reservoirs**

294 In water-scarce cities, the problem of water scarcity is a serious challenge that prevents  
295 sustainable allocation of water resources. A prominent feature of most water-scarce  
296 cities is that water inflows are limited, and the fluctuations in water availability are  
297 large. Therefore, to reduce the risk that the inflows in the next configuration period are  
298 too short to meet the basic demand of the city, such that a sustainable development  
299 objective function is developed. The sustainable development objective function seeks  
300 to maximize the amount of water remaining in the reservoir at the end of a configuration





301 period to hedge against drought risk and guarantee water use in the next period, as  
 302 shown in Eqs. (8-10):

$$303 \quad f_{13}(x) = \max \sum_{i=1}^N (V_i^{\max} - V_i) \times p(V_i^{\max} - V_i) \quad (8)$$

$$304 \quad p(V_i^{\max} - V_i) = \begin{cases} 2 \times V_i / V_i^{\max} & 0 < V_i < V_i^{\max} / 2 \\ -2 \times V_i / V_i^{\max} + 2 & V_i \geq V_i^{\max} / 2 \end{cases} \quad (9)$$

$$305 \quad V_i = \sum_{t=1}^T (R_{i,initial} + I_t^i + P_t^i - A_t^i - E_t^i - EP_t^i) - \sum_{t=1}^T \sum_{j=1}^J x_{ij}^t \alpha_{ij} \quad (10)$$

306 where  $V_i^{\max}$  ( $10^4 \text{ m}^3$ ) is the maximum allowable storage capacity of the  $i$ th water source,  
 307 which is expressed based on the limited storage capacity of a reservoir in the flood  
 308 season, and  $V_i$  ( $10^4 \text{ m}^3$ ) is the water storage capacity of the  $i$ th water source at the end  
 309 of the scheduling period. As much water as possible but less than  $V_i^{\max}$  is reserved.  
 310 However, a reserved water volume in the reservoir that is too high at the end of the  
 311 scheduling period may lead to considerable pressure on reservoirs to urgently release  
 312 water if a flood event is forecasted. The reserved water volume should be neither too  
 313 large nor too small. Thus, the benefits of reservoir retainment must be thoroughly  
 314 evaluated. Based on the characteristic of the benefit of residual water, we propose a  
 315 boundary benefit function  $p(V_i^{\max} - V_i)$  for different reserved water volumes in a  
 316 reservoir. The benefit function is a piecewise function, and when  $V_i$  is less than  
 317  $V_i^{\max} / 2$ ,  $p$  increases as  $V_i$  increases. When  $V_i$  is equal to or greater than  $V_i^{\max} / 2$ ,  
 318  $p$  decreases as  $V_i$  increases. When  $V_i = V_i^{\max}$ ,  $p$  decreases to 0.  $R_{i,initial}$  ( $10^4 \text{ m}^3$ ) is  
 319 the initial storage of the  $i$ th water source,  $I_t^i$  ( $10^4 \text{ m}^3$ ) is the inflow of the  $i$ th water source



320 at the  $t$ th time step,  $P_i^t$  ( $10^4$  m<sup>3</sup>) is the precipitation associated with the  $i$ th water source  
 321 at the  $t$ th time step,  $A_i^t$  ( $10^4$  m<sup>3</sup>) and  $E_i^t$  ( $10^4$  m<sup>3</sup>) are the agricultural and ecological  
 322 water supplies associated with the  $i$ th water source at the  $t$ th time step, respectively, and  
 323  $EP_i^t$  ( $10^4$  m<sup>3</sup>) is the evaporation from the  $i$ th water source at the  $t$ th time step.

### 324 2.1.2 Constraints

325 The layer includes six main constraints: the reservoir water supply constraint, water  
 326 demand constraint, reservoir storage constraint, water balance constraint, external water  
 327 transfer constraint, and nonnegative constraint.

#### 328 Reservoir water supply constraint

329 The maximum water available to supply from an individual reservoir is determined by  
 330 the difference between the total input and total reservoir output. The inputs include  
 331 inflow and precipitation, and the outputs mainly involve agricultural and environmental  
 332 water supplies, evaporation, water supplied for waterworks and reservoir leakage loss.

333 All these factors directly affect the decision-making process and are incorporated into  
 334 the model building process as shown in Eqs. (11-15):

$$335 \quad V_i^t \leq V_{i,\max}^t \quad (11)$$

$$336 \quad V_i^t = \sum_{j=1}^J x_{ij}^t \alpha_{ij} \quad (12)$$

$$337 \quad V_{i,\max}^t = \sum_{t=1}^{t-1} \left( R_{i,\text{initial}} + I_i^t + P_i^t - A_i^t - E_i^t - EP_i^t - \sum_{j=1}^J x_{ij}^t \alpha_{ij} - L_i^t \right) - V_{i,d} \quad (13)$$

$$338 \quad EP_i^t = ep_i^t \times s_i^t / 1000 \quad (14)$$



339 
$$V_i^t = \xi_i^t \times (R_i^{t-1} + R_i^t) \quad (15)$$

340 where  $V_i^t$  ( $10^4 \text{ m}^3$ ) denotes the total water supply from the  $i$ th reservoir at the  $t$ th time  
 341 step;  $V_{i,\max}^t$  ( $10^4 \text{ m}^3$ ) is the maximum water available to be supplied from the  $i$ th  
 342 reservoir at the  $t$ th time step;  $ep_i^t$  (mm) is the water surface evaporation from the  $i$ th  
 343 reservoir in the  $t$ th month;  $s_i^t$  ( $\text{m}^2$ ) is the monthly average surface area of the  $i$ th  
 344 reservoir in the  $t$ th month;  $V_{i,d}$  ( $10^4 \text{ m}^3$ ) is the dead storage of the  $i$ th reservoir;  $L_i^t$   
 345 ( $10^4 \text{ m}^3$ ) is the reservoir leakage loss from the  $i$ th reservoir at the  $t$ th time step;  $R_i^{t-1}$   
 346 ( $10^4 \text{ m}^3$ ) is the storage of the  $i$ th reservoir at the  $t-1$ th time step;  $R_i^t$  ( $10^4 \text{ m}^3$ ) is the  
 347 storage of the  $i$ th reservoir at the  $t$ th time step; and  $\xi_i^t$  is the  $t$ th monthly leakage  
 348 coefficient for the  $i$ th reservoir.

349 **Water demand constraint**

350 The high-quality water demand of each subarea in a city should be satisfied in the water  
 351 allocation process. High-quality water in this model refers to water that satisfies the  
 352 relevant primary (surface water can be used for drinking after simple purification  
 353 treatment, such as filtration and disinfection) and secondary water quality requirements  
 354 (water is slightly polluted and can be used for drinking after routine purification  
 355 treatment, such as flocculation, precipitation, filtration, disinfection, and other  
 356 processes) according to the Chinese Standard (GB5749), as shown in Eq. (16):

357  
 358 
$$0.8 \times D_r \leq \sum_{i=1}^T \sum_{i=1}^I \sum_{j=1}^{J_r} x_{ij}^t \alpha_{ij} + \sum_{i=1}^T \sum_{e=1}^E \sum_{j=1}^{J_r} x_{ej}^t \beta_{ej} \leq 1.2 \times D_r, r = 1, 2, \dots, R \quad (16)$$



359 where  $D_r$  ( $10^4 \text{ m}^3$ ) is the high-quality water demand in the  $r$ th subregion and there are  
 360 a total of  $R$  subregions in the city.  $J_r$  is the number of waterworks in the  $r$ th subregion.  
 361 To ensure that the water supply guarantee in each area is greater than 80%, the total  
 362 water supplied to every subarea is greater than 80% of its demand.

363 **Reservoir storage constraint**

364 
$$R_i^T \leq V_{i,f} \quad (17)$$

365 
$$R_i^T = \sum_{t=1}^T \left( R_{i,initial} + I_i^t + P_i^t - A_i^t - E_i^t - EP_i^{t1} - \sum_{j=1}^J x_{ij}^t \alpha_{ij} - V_i^t \right) \quad (18)$$

366 where  $R_i^T$  ( $10^4 \text{ m}^3$ ) is the storage of the  $i$ th reservoir at the end of the configuration  
 367 period and  $V_{i,f}$  ( $10^4 \text{ m}^3$ ) is the flood-limit storage capacity.

368 **Water balance constraint**

369 
$$R_i^{t+1} = R_i^t + I_i^t + P_i^t - A_i^t - EP_i^t - E_i^t - V_i^{t-1} - \sum_{j=1}^J x_{ij}^t \quad (19)$$

370 **External transfer water constraint**

371 
$$\sum_{t=1}^T \sum_{j=1}^J x_{ej}^t \beta_{ej} \leq E_{e,max} \quad (20)$$

372 where  $E_{e,max}$  refers to the maximum water supply capacity of an external water source  
 373 over the whole configuration period.

374 **Nonnegative constraint**

375 
$$x_{ij} \geq 0 \quad (21)$$



## 376 **2.2 Second layer of the PTSOA decision-making model**

377 Similarly, the second layer of the PTSOA model fuses all three dimensions of  
378 synergistic water resource allocation mentioned previously. The second stage of the  
379 process (the water stored in water works is supplied to different departments needing  
380 water volumes of different quality) is optimized in the second layer. After city-level  
381 decision-making, a conflict of interest inevitably occurs between traditional water  
382 supply departments and unconventional water supply departments. Because  
383 conventional and unconventional water supply departments compete for limited water  
384 demand market shares, the stability of the water allocation system may be jeopardized  
385 if excessive competition is not controlled. Thus, the second layer is implemented at the  
386 department level. Decision-making at the department level seeks to guide the two water  
387 supply departments to partake in benign competition and avoid conflicts to realize  
388 synergy. In this case, the decision plan of the first layer in the hierarchy is followed.  
389 Temporally, short-term allocation changes are needed as mentioned above; hence, the  
390 time scale of the second layer is daily. Thus, the daily decision alternatives for the  
391 volume of water allocated from water works to different water departments are obtained  
392 to make relevant decisions.

### 393 **2.2.1 Objective functions**

394 **Conventional water supply department objective function: Minimization of the**



395 **total amount of water retained in water works**

396 The managers of conventional water supply departments strive to operate conventional  
397 water systems efficiently and achieve the most equitable water share possible. The  
398 amount of conventional water (of high quality) retained in a water works system is a  
399 crucial factor affecting the efficiency and benefits of conventional water supply  
400 departments. Therefore, the benefit of conventional water departments is established by  
401 minimizing the total amount of water retained in water works at the end of a  
402 configuration period, as shown in Eq. (22):

403 
$$\min f_{21}(x) = W_L = \sum_{t=1}^T \sum_{i=1}^I \sum_{j=1}^J x_{ij}^t \alpha_{ij} + \sum_{t=1}^T \sum_{e=1}^E \sum_{j=1}^J x_{ej}^t \beta_{ej} - \sum_{t=1}^T \sum_{m=1}^M \sum_{j=1}^J \sum_{z=1}^Z q_{jz}^{t,m} \chi_{jz} \quad (22)$$

404 where  $W_L$  ( $10^4$  m<sup>3</sup>) is the total amount of water retained in a water works system at  
405 the end of a configuration period;  $q_{jz}^{t,m}$  ( $10^4$  m<sup>3</sup>) is the water supply from the  $j$ th water  
406 works system to the  $z$ th water user on the  $m$ th day in the  $t$ th month in the period of  
407 configuration;  $m=1,2,\dots,M$ ; and  $M$  is the total number of days in the  $t$ th month (28, 29,  
408 30 or 31). Additionally,  $z=1,2,\dots,Z$ , and  $Z$  is the total number of water users.  $\chi_{jz}$  is the  
409 water supply relationship coefficient between the  $j$ th water work and the  $z$ th water user,  
410 where 0 indicates no supply and 1 indicates a water supply.

411 **Unconventional water supply objective function: Maximization of the amount of**  
412 **unconventional water supplied**

413 The reclaimed water reuse system and ecological water distribution system for inland  
414 tributaries are incorporated into the PTSOA model which are associated with



415 unconventional water supply departments. The managers of unconventional water  
 416 supply departments seek to supply as much unconventional water as possible to  
 417 promote their interests. Thus, the objective of unconventional water departments is  
 418 established to maximize the amount of unconventional water supplied. Unconventional  
 419 water mainly includes reclaimed water and river water, which is of low quality (i.e., not  
 420 meeting the quality standard mentioned in Sect. 2.1.2) and is mainly used for industrial  
 421 production, ecological water replenishment for inland rivers and municipal road  
 422 sprinkling.

423 Unconventional water departments operate reclaimed water reuse systems and  
 424 ecological water distribution systems to supply unconventional water, and the  
 425 associated equations are as follows in Eqs. (23-26):

$$426 \quad \max f_{22}(x) = W_r + EW_r \quad (23)$$

$$427 \quad W_r = \sum_{t=1}^T \sum_{n=1}^N \sum_{j=1}^J r'_{nj} p(b_c, b_u) \theta_{nj} \quad (24)$$

$$428 \quad p(b_c, b_u) = \frac{1}{3} \times \frac{b_c}{b_u} - \frac{2}{3} \quad (25)$$

$$429 \quad EW_r = \sum_{t=1}^T \sum_{n=1}^N \sum_{z=1}^Z r_{nz} \theta_{nz} \quad (26)$$

430 where  $W_r$  ( $10^4 \text{ m}^3$ ) is the total amount of reclaimed water supplied for all water users;  
 431  $EW_r$  ( $10^4 \text{ m}^3$ ) is the total amount of river water supplied to maintain ecological flows  
 432 in inland tributaries;  $r'_{nj}$  ( $10^4 \text{ m}^3$ ) is the amount of water supplied to the  $j$ th user from  
 433 the  $n$ th reclaimed water source at the  $t$ th time step;  $n = 1, \dots, N$ ;  $N$  is the total number of



434 reclaimed water sources;  $p(b_c, b_u)$  is a function expressing the willingness of residents  
 435 to use reclaimed water,  $b_c$  (yuan/ $10^4$  m<sup>3</sup>) is the price per unit of conventional water;  
 436  $b_u$  (yuan/ $10^4$  m<sup>3</sup>) is the price per unit of unconventional water; and  $\theta_{nj}$  is the water  
 437 supply relationship between the  $n$ th reclaimed water source and the  $j$ th user. In this case,  
 438  $\theta_{nj} = 1$  indicates a water supply relationship, and  $\theta_{nj} = 0$  indicates no water supply  
 439 relationship.  $r_{nz}$  ( $10^4$  m<sup>3</sup>) is the amount of water supplied from the  $n$ th reclaimed water  
 440 source to the  $z$ th inland tributary;  $z = 1, 2, \dots, Z$ ;  $Z$  is the total number of inland tributaries  
 441 requiring ecological flow compensation; and  $\theta_{nz}$  is the water supply relationship  
 442 between the  $n$ th reclaimed water source and the  $z$ th inland tributary.

### 443 2.2.2 Constraints

#### 444 Conventional water supply constraint

445 According to conservation of mass, the total daily amount of conventional water  
 446 allocated in the second layer should be less than the total monthly amount of  
 447 conventional water allocated in the first layer, as described in Eq. (27):

$$448 \quad \sum_{t=1}^T \sum_{i=1}^I \sum_{j=1}^J x_{ij}^t \alpha_{ij} + \sum_{t=1}^T \sum_{e=1}^E \sum_{j=1}^J x_{ej}^t \beta_{ej} \geq \sum_{t=1}^T \sum_{m=1}^M \sum_{j=1}^J \sum_{z=1}^Z q_{jz}^{t,m} \chi_{jz}, t = 1, \dots, T \quad (27)$$

#### 449 Unconventional water constraints

450 The two types of unconventional water have separate constraints. For reclaimed water  
 451 supplied to water users, the amount should satisfy the relevant water recycling standard.

452 The ecological water used to replenish inland tributaries is mainly pumped from





453 reclaimed water works and main rivers. Therefore, this replenished volume is limited  
 454 by the pumping capacity. The constraints for unconventional water are shown in Eqs.  
 455 (28)-(29):

$$456 \quad \sum_{t=1}^T \sum_{n=1}^N \sum_{j=1}^J r_{nj}^t \theta_{nj} + \sum_{t=1}^T \sum_{n=1}^N \sum_{z=1}^Z r_{nz}^t \theta_{nz} = \sum_{t=1}^T \sum_{i=1}^I \sum_{j=1}^J x_{ij}^t \delta_{ij} \eta_{ij} + PU \quad (28)$$

$$457 \quad PU = \sum_{t=1}^T \sum_{m=1}^M \sum_{p=1}^P Q_{t,m}^{p,s} / 10^4 \quad (29)$$

458 where  $\delta_{ij}$  is the sewage discharge coefficient, which is the proportion of the water  
 459 supplied from sewage discharge;  $\eta_{ij}$  is the sewage water reuse rate, which is the  
 460 proportion of reused water in the total volume of sewage water;  $PU$  ( $10^4$  m<sup>3</sup>) is the  
 461 amount of water pumped from the main river; and  $Q_{t,m}^{p,s}$  (t/d) is the flow through the  
 462 sth pumping station on the  $m$ th day at time step  $t$ .

### 463 **Pumping constraints**

$$464 \quad Q_{t,s}^p \leq Q_{\max,s}^p \quad (30)$$

$$465 \quad Q_t^p = \sum_{s=1}^{Np} r_{t,s}^p \quad (31)$$

466 where  $Q_{\max,s}^p$  (t/d) denotes the upper flow boundary of the sth pumping station;  $r_t^s$  (t/d)  
 467 is the power of the  $p$ th pump installed at the sth pump station; and  $Np$  is the number of  
 468 pumps stalled at the sth pump station.

### 469 **Water quality constraint**

470 To control the impacts of various point and nonpoint sources on receiving water bodies  
 471 in cities, water authorities impose water quality standards for the management of river



472 basins. These standards seek to maintain the water quality at a desired target level by  
473 defining discharge limits for conventional, specific, or priority pollutants. To satisfy the  
474 relevant standards, the following water quality constraint is established:

$$475 \quad \sum_{t=1}^T \sum_{i=1}^N \sum_{j=1}^M \left( x_{ij}^t \delta_{ij} \psi_{ij} h_j^u - x_{ij}^t \delta_{ij} \eta_{ij} h_j^u \right) \times 10 \leq H^u \quad (32)$$

476 where  $\psi_{ij}$  is the sewage water treatment rate, which is the proportion of sewage water  
477 that is treated;  $h_j^u$  (mg/L) is the concentration of the  $u$ th contaminant per unit treated  
478 water required by the  $j$ th user; and  $H^u$  (kg) is the upper limit of the  $u$ th contaminant  
479 allowed to be discharged in the study area.

### 480 **2.3 Third layer of the PTSOA decision-making model**

481 After obtaining the results for the former two stages of the allocation process and the  
482 two levels of decision-making, the third model layer is constructed to achieve regional  
483 synergy *s*. It refers to the collaborative allocation of water resources in different  
484 subregions of a city, and it is intended to balance and maximize the interests of each  
485 subregion as much as possible. Additionally, the needs of different kinds of water users  
486 in different subregions can be met to the greatest extent possible with this approach.  
487 Therefore, the three dimensions of synergy are also fused in this layer. The third stage  
488 of the process (the water in different departments is supplied to different kinds of water  
489 users, namely, residential users, industrial users and municipal users, in different  
490 subregions) is optimized in this layer. After department-level decision-making,



491 conflicts of interest inevitably occur among various water users in different subregions  
492 of a city. Therefore, the third layer considers regional-level decision-making to to  
493 coordinate water needs and avoid conflicts of subregions in the city. Moreover, the  
494 various development priorities of subregions are emphasized by adjusting certain  
495 hyperparameters in the third layer. This layer is established based on the allocation  
496 scheme obtained in the second layer of the hierarchy, and the time scale of this layer is  
497 the same as that of the second.

498 Although water pollutants are controlled in the second layer, the detailed spatial  
499 distribution of pollutants remains unknown. If one of the subregions emits a greater  
500 pollution load than others such that the river pollution limit is exceeded, it constrains  
501 sustainable development and undermines the fairness of the allocation. To ensure the  
502 coordination of water quality among regions, the representative pollutant concentration  
503 of the main reach in each subregion after configuration should meet the relevant  
504 environmental capacity requirements. If these requirements are not met, then the  
505 objective function for this subregion will call for a punishment, and more  
506 environmentally friendly plans will be searched. After sewage with pollutants is  
507 transported from outlets to water bodies, advective transport, longitudinal dispersion  
508 and transverse mixing will occur. At the same time, physical, chemical and biological  
509 interactions will occur in the water body. To objectively describe the degradation of  
510 pollutants in water, it is necessary to use mathematical models to simulate physical  
511 dynamics. Due to the heterogeneity of pollutants entering water bodies and the



512 uncertainty of hydrological processes, it is usually of little practical significance to  
513 calculate the change in river water capacity over time. A steady-state model is therefore  
514 used to calculate the water capacity of the target water body (Cetintas et al., 2010;  
515 Zhang et al., 2019). When water quality changes are studied at the annual scale and  
516 complete mixing is assumed, the following equation can be used to describe the water  
517 quality change, as shown in Eq. (33):

$$518 \quad \frac{Vdc}{dt} = Q(Ce - C) + Sc + r(c)V \quad (33)$$

519 where  $V$  ( $\text{m}^3$ ) is the volume of water;  $Q$  ( $\text{m}^3/\text{a}$ ) is the flow in and out of the system  
520 at equilibrium;  $Ce$  ( $\text{g}/\text{m}^3$ ) is the contamination concentration in the inflow ( $\text{g}/\text{m}^3$ );  $C$   
521 is the pollutant concentration;  $Sc$  denotes other external pollution sources ( $\text{m}^3/\text{a}$ ); and  
522  $r(c)$  is the reaction rate of pollutants in water ( $\text{g}/\text{m}^3/\text{a}$ ). The above equation can be  
523 defined as the basic mass balance of a water body in a completely mixed system.  
524 Because the pollutants are evenly mixed in each small interval, the horizontal and  
525 vertical concentration gradients of pollutants can be neglected. Therefore, the model of  
526 water quality in mixed rivers under steady-state design conditions is adopted (Yue et  
527 al., 2021):

$$528 \quad W_c = 31.54 * [C_s \cdot (Q_p + Q_E + Q_S) - Q_p \cdot C_p] \quad (34)$$

529 where  $W_c$  represents the water environmental capacity ( $\text{t}/\text{a}$ );  $Q_p$  is the flow in the  
530 reach ( $\text{m}^3/\text{s}$ );  $C_p$  is the pollutant concentration in the river ( $\text{mg}/\text{L}$ );  $Q_E$  is the sewage  
531 discharge ( $\text{m}^3/\text{s}$ );  $Q_S$  is the total flow of nonpoint sources into the reach above the



532 control section ( $\text{m}^3/\text{s}$ ); and  $C_s$  is the target concentration of river pollutants ( $\text{mg/L}$ ).  
 533 The result calculated based on the total hydrological capacity standard is often  
 534 relatively large, which is generally referred to as nonconservative. To conform to real  
 535 conditions, the concept of a nonuniformity coefficient is introduced for correction:

$$536 \quad W'_c = \alpha \cdot W_c = 0.6 \cdot W_c \quad (35)$$

537 This coefficient is used to assign a punishment if the water quality exceeds the  
 538 relevant value in a given subregion. Based on the coefficient value, the objective  
 539 functions and constraints are adjusted accordingly. Finally, the daily decision  
 540 alternatives for water allocation from water departments to water users are obtained at  
 541 the regional decision level.

### 542 2.3.1 Objective function

543 **Regional objective function: Maximization of the comprehensive benefits of each**  
 544 **subregion**

$$545 \quad \max f_3(x) = \sum_{t=1}^T \sum_{i=1}^I \sum_{j=1}^{J_r} x'_{ij} b_{ij} - \sum_{j=1}^{J_r} \left( D_j - \sum_{t=1}^T \sum_{i=1}^I x'_{ij} \alpha_{ij} \right) \times \omega_j - P_r(r_{nz}) - G_r(x'_{ij}) \times q \quad (36)$$

$$546 \quad P_r(r_{nz}) = e_i \times \sum_{p=1}^{Pr} P_p^{pump} \times \nabla t_r + x'_{ij} \delta_{ij} \psi_{ij} \omega_{ij} \quad (37)$$

$$547 \quad \nabla t_r = \sum_{t=1}^T \sum_{n=1}^N \sum_{z=1}^{Z_r} \left\{ \left( l_{nz} + (r'_{nz} \theta_{nz} / CAS_{nz}) \right) / (Q_{nz}^{\max} / CAS_{nz}) \right\} / 3600 \quad (38)$$

$$548 \quad G_r(x_{ij}) = \sum_{z=1}^{Z_r} \sum_{u=1}^U (Q_{z,u,r}^{final} - Q_{z,u,r}^0) \quad (39)$$

549 where  $b_{ij}$  (yuan/ $\text{m}^3$ ) is benefit per unit of water supply for the  $j$ th user;  $\omega_j$  is the



550 penalty coefficient per unit of water deficiency;  $j=1,2,\dots,J_r$ ;  $J_r$  is the number of water  
551 users in  $r$ th subregion;  $r=1,2,\dots,R$ ;  $P_r(r_{nz})$  is the penalty function for cost in the  $r$ th  
552 subregion;  $e_i$  (yuan/kW·h) is the unit electricity fee;  $P_p^{pump}$  (kW·h) is the electrical  
553 power consumed by the  $p$ th pump at a pump house in each hour;  $p$  ranges from 1 to  $P_r$ ;  
554  $P_r$  is the total number of pumps in the  $r$ th subregion;  $\nabla t_r$  (h) is the time required for  
555 water transfer to provide support for the inland river flow in the  $r$ th subregion;  $\omega_{ij}$   
556 (yuan) denotes to the fee paid for sewage treatment;  $l_{nz}$  (m) is the length of a water  
557 diversion pipe from reclaimed water source  $n$  to the  $z$ th inland river;  $z$  ranges from 1 to  
558  $Z_r$ ;  $Z_r$  denotes the number of inland rivers in the  $r$ th subregion;  $CAS_{nz}$  ( $m^2$ ) is the  
559 cross-sectional area of a pipe from the  $n$ th reclaimed water source to the  $z$ th inland river;  
560  $Q_{nz}^{\max}$  ( $m^3$ ) is the maximum overflow capacity of the diversion pipe from the  $n$ th  
561 reclaimed water source to the  $z$ th inland river;  $G_r(x_{ij})$  is the penalty function for  
562 substandard water quality in the  $r$ th subregion;  $Q_{z,u,r}^{final}$  (mg/L) is the final concentration  
563 of the  $u$ th pollutant in the control section of the  $z$ th inland river in the  $r$ th subregion  
564 after optimal configuration;  $Q_{z,u,r}^0$  (mg/L) is the initial concentration of the  $u$ th  
565 pollutant in the  $z$ th inland river in the  $r$ th subregion; and  $q$  is the penalty coefficient  
566 for substandard water quality in the  $r$ th subregion. The number of objective functions  
567 in this layer depends on the number of subregions divided in the city, which is based on  
568 local conditions.



## 569 2.3.2 Constraints

### 570 Water quality constraints

571 Mathematical models are often developed to help satisfy the water quality standards at  
572 monitoring points (Zhang et al., 2019; Pourshahabi et al., 2020; Friesen et al., 2017).  
573 However, for some cities with very few monitoring points, such approaches may lead  
574 to good water quality in the monitored sections and poor water quality in other sections.  
575 In these circumstances, the quality of water bodies in each subregion of a city is not  
576 simultaneously maintained. To maintain the water quality in all subregions of a city at  
577 the desired target level, the water quality constraint in Eq. (40) is established:

$$578 \quad Q_{z,u,r}^{final} \leq Q_{z,u,r}^{control} \quad (40)$$

579 where  $Q_{z,u,r}^{control}$  (mg/L) denotes the control standard for the  $u$ th pollutant in the control  
580 section of the  $z$ th inland river in the  $r$ th subregion.

## 581 2.4 Model solution

### 582 2.4.1 Synergy degree evaluation

583 Enhancing the understanding of the synergy among water allocation alternatives to  
584 achieve broad coordination and equilibrium is crucial. The evaluation of the synergy of  
585 a water system is strongly related to multiple complex interactions, such as the  
586 interactions among different processes, users, and regions. However, these interactions  
587 have rarely been explicitly captured in prior evaluations of water allocation. One of the



588 key network metrics used in network analysis, connectivity, is a promising measure of  
589 the degree of coordination among different objectives in complex systems (Weitz et al.,  
590 2018). Connectivity reflects the connectedness of a given link to all possible links in  
591 the network, and the strength of each link is weighted, reflecting the number and  
592 strength of correlations (Felipe-Lucia et al., 2020). In this study, connectivity is used to  
593 embody coordination in the context of synergy, as shown in Eq. (26). Due to the limited  
594 supply of water resources, competition among different objectives is unavoidable, and  
595 the objectives cannot be fully optimized to equal extents, i.e., , an increase in one target  
596 output may decrease another output. Therefore, equilibrium is integrated as another  
597 vital part of the synergy devoted to maintaining a balance among the satisfaction of  
598 each goal in a system. The equilibrium based on the principle of information entropy  
599 (Gao et al., 2013; Zivieri, 2022) is shown in Eq. (27). Information entropy is a measure  
600 of the uncertainty associated with a random variable and is used to quantify the  
601 information contained in a message, usually in bits or bits/symbols; furthermore, it has  
602 been widely used to represent the fairness or equilibrium of a system (Chen et al., 2022;  
603 Zhao et al., 2022). When  $H$  is low, the level of equilibrium in the system is high. By  
604 combining the quantification of coordination and equilibrium, the synergy degree is  
605 appropriately determined (Eq. (29)). Notably, the total synergy index ( $TSI$ ) of a system  
606 is used for both generating candidate management alternatives in the generation phases  
607 of PTSOA and performing assessments of the associated level of synergy, as shown in  
608 Eqs. (41-44).





$$609 \quad SSI_{ob_i} = \frac{\sum_{j=1}^N c_{ij} \times (ob_i + ob_j)}{\sum_{j=1}^N (ob_i + ob_j)}, i \neq j \quad (41)$$

$$610 \quad H(S) = -\sum_{i=1}^N \frac{(1-u_{ob_i})}{N} \log \frac{(1-u_{ob_i})}{N} \quad (42)$$

$$611 \quad u_{ob_i} = \frac{ob_i - ob_{i,\min}}{ob_{i,\max} - ob_{i,\min}} \quad (43)$$

$$612 \quad TSI = \frac{\sum_{i=1}^N SSI_{ob_i}}{H(S)} \quad (44)$$

613 where  $SSI_{ob_i}$  is the connectivity of the  $i$ th object;  $c_{ij}$  is the Pearson correlation  
 614 between the  $i$ th object and  $j$ th object;  $ob_i$  and  $ob_j$  are the values of the  $i$ th and  $j$ th  
 615 objective functions, respectively;  $TSI$  is the synergy index of the system;  $H(S)$  is  
 616 the overall equilibrium of all objects based on the principle of information entropy;  
 617  $u_{ob_i}$  is the standardized value of the  $i$ th object;  $N$  is the total number of objects in the  
 618 system;  $ob_{i,\min}$  and  $ob_{i,\max}$  are the minimum and maximum critical thresholds of the  
 619 parameter  $ob_i$ , respectively.

## 620 2.4.2 Hierarchical optimal algorithm design for the PTSAO model

621 Based on the algorithm design with a hierarchical objective function proposed by Li et  
 622 al. (2022), a new level is added to the original two levels of the algorithm, and the  
 623 alternative generation phase is improved for better synergy. In this algorithm, the  
 624 objective functions in the upper decision level is first satisfied, and then the lower-level  
 625 objective function provides an optimal result based on the results of optimal allocation



626 in the upper level. To provide as comprehensive solutions as possible, the decision  
627 alternatives need to be classified into different sets for further selection. In addition, the  
628 synergy degree of the result of each layer is calculated to select optimal decisions  
629 among all Pareto front solutions. The detailed steps of the hierarchical optimal  
630 algorithm are as follows:

- 631 I. In the first level, calculate the objective function (city level) values for the social,  
632 economic and sustainable development components, and sort the results with  
633 NSGA-III (Pourshahabi et al., 2020; Chen et al., 2017) to obtain each Pareto  
634 front  $F_1, F_2, \dots, F_i$ .
- 635 II. Classify the Pareto fronts into  $K$  ( $K$  is determined based on the diversity of  
636 policies) elements with the K-means algorithm (Liu et al., 2022), which is used  
637 to partition a data set into  $K$  distinct and nonoverlapping clusters. To perform  
638 K-means clustering, we first specify the desired number of clusters  $K$ . Then, the  
639 K-means algorithm is used to assign each observation to exactly one of the  $K$   
640 clusters.
- 641 III. Calculate the synergy degree of each individual in the front, and select the  
642 solution that yields the greatest synergy in each cluster.  $K$  solutions are obtained  
643 in the first layer.
- 644 IV. Use the selected  $K$  solutions in the first layer to establish constraints in the  
645 second layer. Solve the objective function of the second layer with NSGA-III.
- 646 V. Calculate the synergy degree of each individual in the front and select the



647 solution that yields the greatest synergy as well as the two solutions that  
648 maximize the conventional and unconventional water supply department  
649 objective functions in all Pareto fronts with K preconditions.

650 VI. The three selected solutions in the second layer are used to establish constraints  
651 in the third layer. Solve the objective function of the third layer with NSGA-III  
652 under the three preconditions.

653 VII. The synergy degree of each individual in the front is calculated, and the solution  
654 that yields the greatest synergy in the third layer is selected. Three solutions are  
655 obtained considering the synergy in the former two layers. Finally, the  
656 synergistic configurations optimal for all stages in the whole process are  
657 identified considering the synergy among decision levels, processes and time  
658 scales.

### 659 **3. Application**

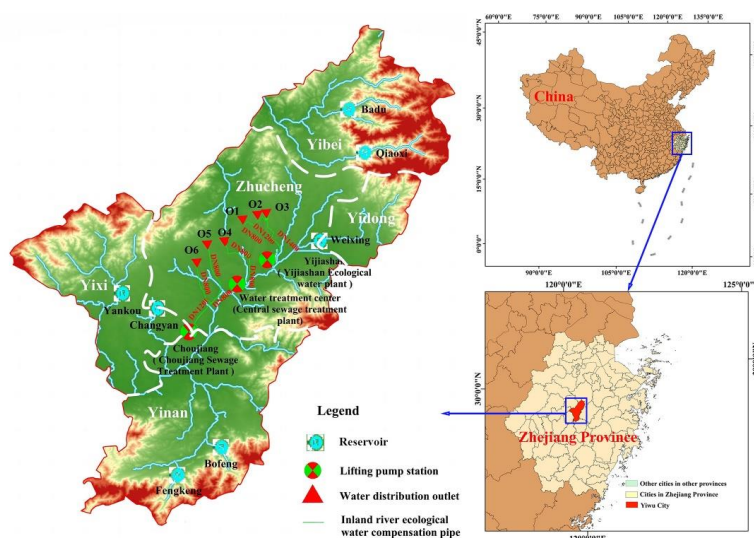
#### 660 **3.1 Study area**

661 Yiwu city is selected as a case study to validate the applicability of the PTSOA model.  
662 Yiwu city is in Southeast China, located from 119°49 'E-120 °17' E and 29°02 '13 "N-  
663 29 °33' 40" N. The city covers an area of 1105 km<sup>2</sup>. The area is characterized by a  
664 scarcity of water resources, and the conventional water supply is under severe stress.  
665 The regional water consumption depends heavily on transported water and external



666 water transfer. The per capita water resources total 622 m<sup>3</sup>, only 22.6% of the provincial  
667 average and 19.1% of the national average. Moreover, the problem of water pollution  
668 has become a bottleneck constraint for the development of Yiwu city. Therefore, it  
669 represents a typical water-scarce city with limited conventional water. Notably, water  
670 quality in Yiwu has been subjected to significant environmental stress because of the  
671 negative effects of wastewater discharge with the rapid development of industry. The  
672 current water quality is poor, with Class V water, and the main pollutant concentrations  
673 exceed the corresponding standards (Zhejiang Natural Resources and Statistical  
674 Yearbook on Environment, 2020). As shown in Fig. 3, the Yiwu River crosses the city  
675 from northeast to southeast. Additionally, there are six ecological water compensation  
676 outlets in six main tributaries in the Yiwu River.

677



678

679

Fig. 3. Map of the study area



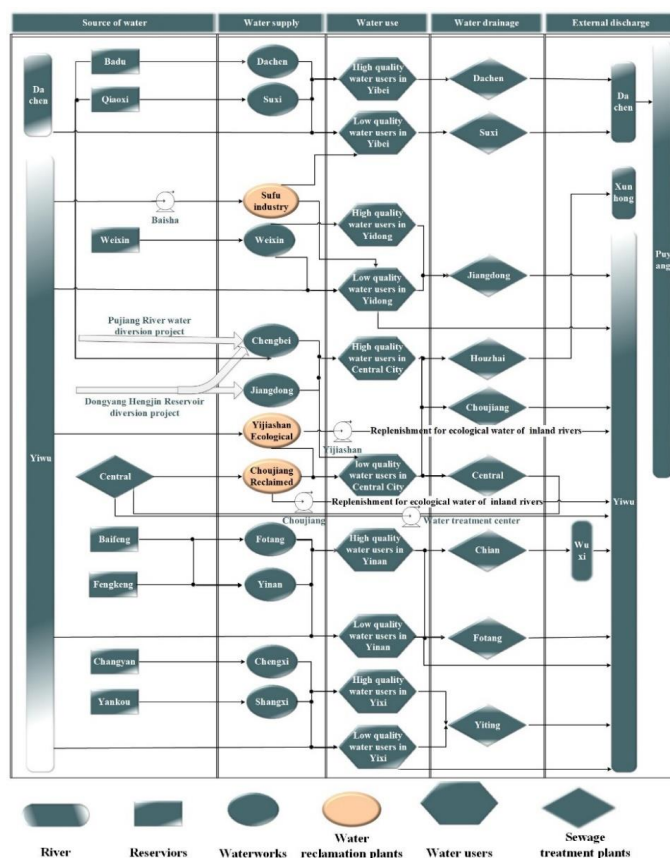
### 680 **3.2 Generalization of the water system**

681 An initial multisource, complementary and mutually regulated system has been  
682 developed for Yiwu, and this system spans the entire urban water cycle (water source-  
683 water supply-water use-drainage-drainage collection-recycling and reuse). To apply the  
684 optimal water allocation model to the complex real-world water system, all  
685 stakeholders in the water system should be schematized into a topological system, as  
686 shown in Fig. 4. The diagram comprises five modules: water sources, water supply,  
687 water use, water drainage and external discharge for all stakeholders.

688 The first module includes seven main reservoirs, two water diversion projects, the  
689 Central Sewage Treatment Plant and the Yiwu River. The seven reservoirs and two  
690 water diversion projects (as shown in Table 1) supply high-quality water. There are  
691 complex connections between the first and second modules. For example, two  
692 reservoirs supply water to one waterworks or one reservoir feeds two or three  
693 waterworks simultaneously. The reservoirs also supply some of the agricultural and  
694 ecological waters to subareas of the city. The Yiwu River, with a total length of 38.39  
695 km and 21 first-class tributaries in the city, and the Central Sewage Treatment Plant, as  
696 shown in Table 2, are low-quality water sources. Additionally, excluding water from  
697 reservoirs, most agricultural irrigation water is supplied from surface water stored in  
698 hundreds of small reservoirs and mountain ponds. Since there are no data available for  
699 agricultural irrigation water, which accounts for only a small portion of the total water



700 demand in the area, this water volume is ignored in the model. For the second module,  
701 high-quality water piped from reservoirs is transported to nine urban and rural  
702 centralized waterworks (as shown in Table 2). The Yiwu River distributes low-quality  
703 water to the Yijishan Ecological Water Plant and Sufu Industrial Water Plant through  
704 the Yijishan and Baisha Water Pump Stations, respectively. The water discharged at the  
705 Central Sewage Treatment Plant is transferred to the Choujiang Industrial Water Plant.  
706 Based on the water supply project distribution and the economic as well as social  
707 development levels, Yiwu is divided into five districts, as shown in Table 3: the Central  
708 District, Yidong District, Yibei District, Yinan District and Yixi District. The third  
709 module comprises both high-quality water users (high-quality water users consist of  
710 urban and rural domestic water users and industrial water users in the water supply  
711 network of urban and rural public water plants) and low-quality water users (low-  
712 quality water users include industrial water users, municipal water users and ecological  
713 water replenishment for inland rivers) in each district. There are nine sewage treatment  
714 plants in the fourth module (which focuses on the drainage stage), as shown in Table 2.  
715 The unused water from sewage treatment plants is discharged to the external  
716 environment. Reuse processes are also considered in the system.



717

718

Fig. 4. Schematic diagram of Yiwu city

### 719 3.3 Parameter determination

720 According to the flow duration curve of the annual natural inflow data for 51 years  
 721 (1963-2014), three years with exceedance probabilities of 50%, 75% and 90% are  
 722 selected to represent normal (1984.1–1985.1, annual mean inflow:  $1.33 \times 10^8 \text{ m}^3$ ), dry  
 723 (2008.1–2009.1, annual mean inflow:  $1.11 \times 10^8 \text{ m}^3$ ), and extremely dry (1971.1–  
 724 1972.1, annual mean inflow:  $0.63 \times 10^8 \text{ m}^3$ ) scenarios, respectively. In addition to



725 inflow, the data used in the PTSOA model mainly include the data for the parameters  
726 in each layer. Water demand values were calculated using the Yiwu City Water  
727 Resources Comprehensive Plan 2020, as shown in Table 1.

728 **Table 1** Water demands of various regions in Yiwu in 2020 ( $10^4 \text{ m}^3$ )

Subregion	Yibei	Yidong	Zhucheng	Yixi	Yinan
water demand	1695	572	11813	2198	2045

729

730 The water resources fees paid to the government total  $0.3 \text{ yuan/m}^3$ . The parameters  
731 of the reservoirs and external water division projects in Yiwu city are listed in Table 2.

732 **Table 2** Parameters of the reservoirs and external water division projects

Reservoirs & External sources	Water Fee $\text{yuan/m}^3$	Initial storage $10^4 \text{ m}^3$	Dead storage $10^4 \text{ m}^3$	Flood limit	Absolute storage capacity $10^4 \text{ m}^3$
				storage capacity $10^4 \text{ m}^3$	
Badu	0.99	1359	49	2688	2639
Qiaoxi	1.30	1505	77	2933	2856
Weixin	0.37	500	17	483	466
Baifeng	1.05	1013	15	2010	1995
Fengkeng	1.15	778	55	1501	1446
Yankou	1.49	1820	499	3140	2641
Changyan	0.70	491	41	940	899
Pujiang Project	1.00	0	0	3000	3000
Dongyang Project	1.00	0	0	5000	5000

733

734 The Tennant method is applied to calculate the ecological water demand. In this  
735 method, the relationship between the annual average discharge and habitat quality is  
736 considered, and the percentage of the annual average natural runoff is used as the  
737 recommended value of the ecological water demand for a given river channel.





738 According to the recommended values, the percentage of runoff required for the fish  
739 spawning period from April to September is 30% and the percentage runoff in the  
740 general water consumption period (October to March) is 10%.

741 Based on observations obtained with the F601 evaporator (a standard evaporation  
742 instrument widely used in China), evaporation is calculated as:

$$743 \quad EP = E \times k \quad (45)$$

744 where  $EP$  (mm) is the evaporation of a reservoir;  $E$  (mm) is the observed evaporation;  
745 and  $k$  is a reduction coefficient. According to observations, this coefficient is the same  
746 for every reservoir and varies throughout the year (Zhao, 2014). The prices of  
747 conventional water and reclaimed water are 1.7 and 2.6 yuan/m<sup>3</sup>, respectively.

748 The monthly mean monitoring data for effluent pollutant concentrations and the  
749 daily maximum processing capacities of sewage treatment plants were obtained from  
750 the monitoring systems of the sewage treatment plants. For example, the concentrations  
751 of COD, NH<sub>3</sub>-N, TN, and TP in the sewage of the Jiangdong Sewage Treatment Plant  
752 are 13.80 (mg/L), 0.22 (mg/L), 6.02 (mg/L), and 0.13 (mg/L), respectively. The daily  
753 maximum processing capacity of Jiangdong Sewage Treatment Work is 12 (10<sup>4</sup> t/d).  
754 The effluent quality of sewage treatment works satisfies the Class A Standard used in  
755 China. The maximum capacities of the Baisha pump station, Yijiashan pump station,  
756 Choujiang pump station and water treatment centre pump station are 13 t/d, 13.5 t/d, 10  
757 t/d, and 4.5 t/d, respectively.

758 Additionally, the environmental capacities of the six tributaries that are replenished



759 with ecological water are calculated according to Eqs. (33)-(35), and the results are  
760 listed in Table 3. COD, TP and TN are selected as representative pollutants in the  
761 tributaries to guarantee the water environmental quality of inland rivers. The water  
762 quality goals for the tributaries must conform to the Class III standard according to GB  
763 5749-2006 in China. The unit electricity price of pump stations in Zhejiang Province is  
764 0.41 yuan/kW·h. GB50014-2006 (2014 edition) stipulates that the comprehensive urban  
765 domestic sewage quota should be 80~90%, and the urban comprehensive domestic  
766 sewage quota should be 90% in areas with extensive drainage facilities. According to  
767 the “Yiwu Water Resources Bulletin 2020”, the urban comprehensive domestic sewage  
768 quota is set to 90%, and the sewage treatment rate is set to 100%. The benefits per unit  
769 water supply for different users in different subregions are determined from the Yiwu  
770 Water Price Adjustment Plan 2020.

771 **Table 3** Area and environmental capacity of tributaries

Name of tributary	Area (km <sup>2</sup> )	Class III		
		COD (t/a)	TN (t/a)	TP (t/a)
Chengdong	3.4	188.1	4.7	0.4
Chengzhong	8.7	432.7	31.5	3.8
Chengxi	6.3	302.5	9.5	2.3
Chenganan	7.1	318.8	0	3.6
Hongxi	12.5	778.8	138.8	7.9
Dongqingxi	38	1271.4	221.5	12.7

## 772 4. Results and discussion

773 By solving the PTSOA model for Yiwu city, synergistic optimal water allocation results  
774 for different layers (across different decision levels, water use sectors, and subregions)



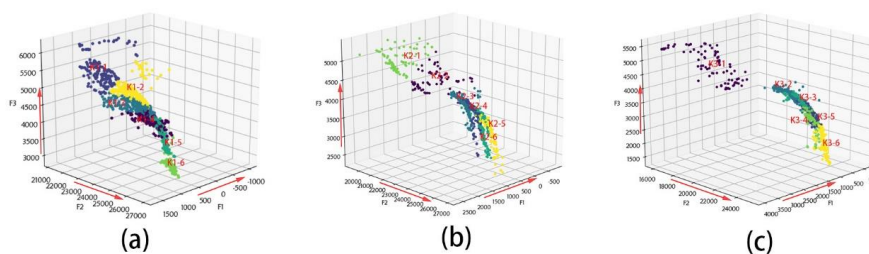
775 are obtained under normal, dry and extremely dry conditions. Pareto sets are obtained  
776 across 500 runs of the PTSOA model with the proposed hierarchical optimization  
777 algorithm.

#### 778 **4.1 Results of the first layer of the PTSOA model for synergistic** 779 **optimal water allocation**

780 To demonstrate the relationship among conflicting objectives, sets of Pareto solutions  
781 for the first layer under normal, dry and extremely dry conditions are shown in Fig. 5.  
782 The optimization using the Pareto concept allows the operator to choose an appropriate  
783 solution depending on the prevailing circumstances and analyse the trade-off among  
784 the conflicting objectives. In each of the figures, the total water supply shortage, total  
785 water supply benefit and total amount of water retained in reservoirs in Yiwu city are  
786 plotted. The colour of the markers indicates the classification of the solutions of the K-  
787 means method, as described in Sect. 2.4.2. All of the decision alternatives are classified  
788 into six groups marked in different colours for broad-scale decision-making. The names  
789 of the classes are marked in the figure in red (for example, K1-1 represents the first  
790 class of solutions in the normal scenario, and K3-2 represents the second class of  
791 solutions in the extremely dry scenario). The red arrows indicate optimization  
792 directions. The ideal solution is located at the top-right corner (low total water supply  
793 shortage, high total water supply benefit, and relatively high total amount of reserved  
794 water in reservoirs) of the plot. The geometries of the tradeoffs vary significantly across



795 the applications, as is expected given the different hydrological conditions. Generally,  
796 the total water supply shortage and the total amount of water retained in reservoirs show  
797 an inverse relationship. In contrast, the total water supply benefit shows a direct and  
798 positive influence on the total water supply shortage. The water supply reliability of the  
799 selected decision alternatives is greater than 95% under normal, dry and extremely dry  
800 conditions. The total amount of reserved water in reservoirs under normal scenarios  
801 varies in the range of  $2.91 \times 10^7 \text{ m}^3$  to  $6.14 \times 10^7 \text{ m}^3$ , which is much higher than that under  
802 the extremely dry scenario, with a value of  $1.44 \times 10^7 \text{ m}^3$  to  $2.93 \times 10^7 \text{ m}^3$ . This finding  
803 demonstrates that the optimal allocation is able to reconcile the present demand and  
804 future needs, even in extremely dry scenarios. The total water supply shortage in all  
805 scenarios is less than 5% of the water demand, which indicates that the guaranteed water  
806 supply is greater than 95%.



807 (a) (b) (c)

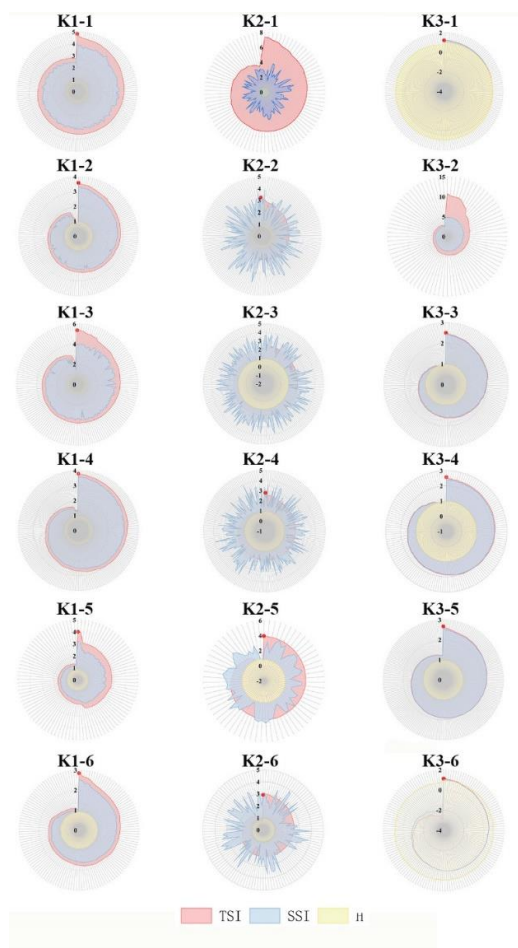
808 **Fig. 5.** Sets of Pareto solutions after 500 model simulations with the hierarchical  
809 optimal algorithm under (a) normal, (b) dry and (c) extremely dry scenarios. The red  
810 arrow indicates the direction of optimization.

811

812 We further present the TSI (total synergy index), SSI (total connectivity) and H



813 (overall equilibrium) values for different classes characterized based on the optimal  
814 PTSOA solutions under three scenarios, as shown in Fig. 6. In the PTSOA model, the  
815 Pareto solutions with the best TSI values are input to the second layer for further  
816 optimization. Thus, the red points in Fig. 6 represent the selected schemes for all classes.  
817 We observe that the variation in the TSI is consistent with that in the SSI in some, but  
818 not all cases. In some cases, difference are mainly caused by the influence of H, which  
819 influences the optimal hydrological equilibrium, especially in dry conditions. Although  
820 normal conditions are most conducive to achieving equilibrium, the better H value in  
821 extremely dry conditions than in dry conditions seems nonintuitive. However, these  
822 results suggest that when water is very limited, equally limited water is supplied to all  
823 users, thus enhancing the overall equilibrium. We note that the SSI is higher in the  
824 normal scenario than in the other two scenarios. We attribute this to relatively abundant  
825 water being useful for stakeholders to achieve synergy due to the reduced competition  
826 compared to other cases. The TSI values reach maximums of 5.36, 7.37 and 10.82 under  
827 normal, dry and extremely dry conditions, respectively. Since the TSI is used to  
828 illustrate the synergy of allocation plans under certain conditions, the three kinds of TSI  
829 values are not comparable.



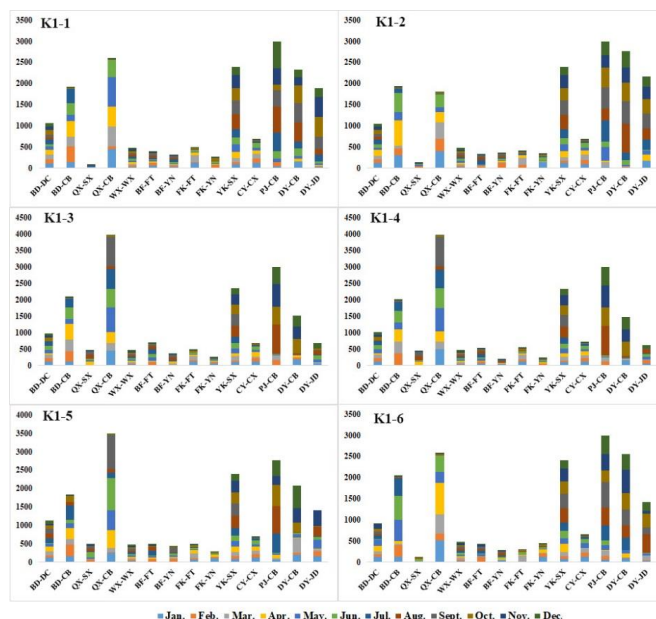
830

831 **Fig. 6.** Comparison of TSI (total synergy index), SSI (total connectivity) and H  
832 (overall equilibrium) values among various Pareto solutions in different classes for  
833 the (K1) normal, (K2) dry, and (K3) extremely dry scenarios.

834 As an example, Fig. 7 provides the specific water supply decision alternatives for  
835 the first layer that maximize synergy in each cluster under normal conditions. The water  
836 allocation plans for the seven main reservoirs and two external water diversion projects  
837 in every month of the configuration period are displayed. All reservoirs and water works



838 are represented by abbreviations based on their full names in Fig. 7. For example, QX-  
839 CB is the label for the water supplied from Qiaoxi Reservoir to Chengbei Water Works.  
840 The water volumes supplied by Qiaoxi Reservoir to Chengbei Water Works (ranging  
841 from  $1.78 \times 10^7 \text{ m}^3$  to  $3950 \times 10^4 \text{ m}^3$ ) and from the Pujiang External Water Division  
842 Project to Chengbei Water Works (ranging from  $2.57 \times 10^7 \text{ m}^3$  to  $3 \times 10^7 \text{ m}^3$ ) are relatively  
843 high in all clusters. This result is consistent with the fact that Chengbei Water Works is  
844 one of the main conventional water sources for the central city area, a region that  
845 accounts for more than 50% of the total water demand of Yiwu city. The water supplied  
846 by the two external water diversion projects from August to December is higher than  
847 that in other months. The mean monthly precipitation in these months is only 58-74%  
848 of the mean annual precipitation in Yiwu, so more external water is supplied for  
849 replenishment. Baifeng and Fengkeng Reservoirs supply similar volumes of water to  
850 their two connected waterworks.



851

852 **Fig. 7.** Water supply from each reservoir to connected water works in each month in  
 853 the normal scenario ( $10^4 \text{ m}^3$ )

854 **4.2 Results of the second layer of the PTSOA model for**  
 855 **synergistic optimal water allocation**

856 The  $6 \times 3$  decision alternatives selected in the six clusters of the optimal first-layer results  
 857 in the normal, dry and extremely dry scenarios are input into the second layer for further  
 858 optimization. As shown in Fig. 8, the total amount of water retained in water works and  
 859 the amount of unconventional water supplied show a negative correlation. In the  
 860 alternative generation phase of game bargaining between the two objectives, the greater  
 861 the total amount of water retained in water works is, the greater the amount of  
 862 unconventional water supplied will be, which indicates that more conventional water





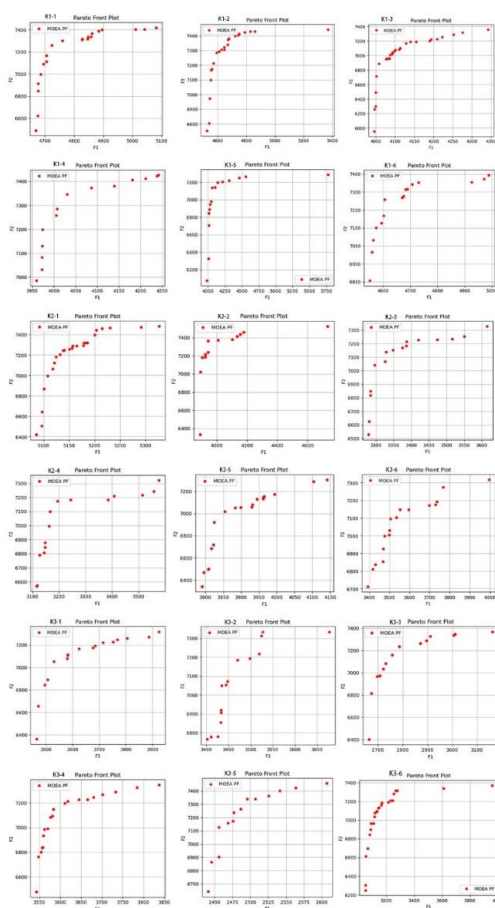
863 will be saved when more unconventional water is supplied. Conversely, the amount of  
864 unconventional water supplied is affected by the total amount of water retained in water  
865 works.

866 In the second layer, three alternatives in each scenario are selected as prior  
867 conditions for further optimization. In addition to the two individual extrema of the two  
868 objectives, the alternative that yields the best synergy is also identified, and it is similar  
869 to that in the first layer. In the normal scenario, the *TSI* values are -0.90, -1.02 and -0.88  
870 in the cases with the optimal conventional water supply, unconventional water supply  
871 and synergy, respectively. The most synergistic approach includes only  $7.08 \times 10^4$  m<sup>3</sup>  
872 more conventional water retained than that in the conventional water supply cases and  
873 only  $9.72 \times 10^4$  m<sup>3</sup> more than that in the optimal unconventional water supply case.  
874 Therefore, not only is the best *TSI* value obtained, but the requirements of both  
875 conventional and unconventional water supply departments are met. The *TSI* of the  
876 most synergistic solution is the highest under dry conditions, with a value of -0.79.

877 Overall, the total amount of water retained in the water works ranges from  $3.95 \times 10^7$   
878 m<sup>3</sup> to  $5.75 \times 10^7$  m<sup>3</sup>,  $3.12 \times 10^7$  m<sup>3</sup> to  $5.31 \times 10^7$  m<sup>3</sup>, and  $2.43 \times 10^7$  m<sup>3</sup> to  $3.96 \times 10^7$  m<sup>3</sup> for the  
879 three types of conditions. The total amount of unconventional water supplied ranges  
880 from  $5.95 \times 10^7$  m<sup>3</sup> to  $7.48 \times 10^7$  m<sup>3</sup>,  $6.34 \times 10^7$  m<sup>3</sup> to  $7.56 \times 10^7$  m<sup>3</sup>, and  $6.28 \times 10^7$  m<sup>3</sup> to  
881  $7.37 \times 10^7$  m<sup>3</sup> in the normal, dry and extremely dry scenarios, respectively. It is notable  
882 that the drier the conditions are, the lower the amount of water retained in water works  
883 and the greater the amount of unconventional water supplied. This approach is useful



884 for cities to mitigate the risk of drought. Additionally, based on the constraints regarding  
885 the contaminants allowed to be discharged, more than 1272.21 t and 48.81 t of COD  
886 and ammonia nitrogen emissions are avoided per year. In other words, the balancing of  
887 the two objectives is beneficial for managers to determine an equilibrium solution that  
888 satisfies the relevant demand and successfully avoids surplus conventional or  
889 unconventional water supply in terms of sustainable development.



890  
891 **Fig. 8.** Pareto fronts of the second layer in the PTSOA model after 500 simulations  
892 with the hierarchical optimal algorithm in the normal, dry and extremely dry



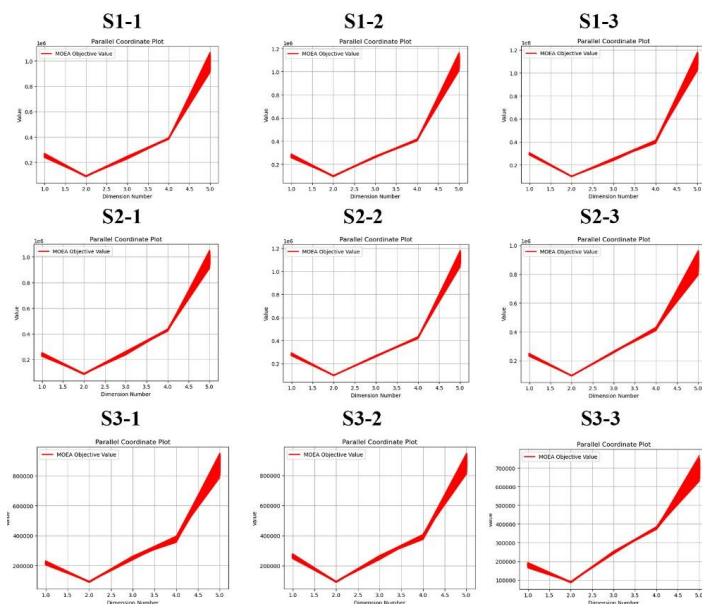
893 scenarios. F1 represents the total amount of water retained in water works ( $10^4$  m<sup>3</sup>),  
894 and F2 represents the amount of unconventional water supplied ( $10^4$  m<sup>3</sup>). The  
895 direction of optimization is from the top-right corner to the bottom-left corner.

### 896 **4.3 Results of the third layer of the PTSOA model for synergistic** 897 **optimal water allocation**

898 After selecting the three scenarios that yield the best synergy and the two best objective  
899 functions for characterizing all Pareto fronts of the second layer in each scenario, these  
900 3×3 solutions are input to the third layer for further optimization. Fig. 9 shows the  
901 tradeoffs among the five objectives in the third layer of the PTSOA model for the (S1)  
902 normal, (S2) dry, and (S3) extremely dry scenarios (these abbreviations are used to  
903 distinguish these results from those of the above two layers). The number following the  
904 ‘-’ represents the selected solution from the second layer. For example, S1-1 represents  
905 the normal scenario with the minimum total amount of water retained in water works,  
906 S1-2 represents the normal scenario with the maximum unconventional water supply  
907 and S1-3 represents the normal scenario with the maximum synergy degree in the  
908 second layer. In each of these plots, the abscissa denotes the identifier for the objective  
909 functions, which ranges from 1 to 5, and the ordinate gives the objective values in the  
910 Pareto fronts ( $10^4$  yuan). The five dimensions include the comprehensive benefits of  
911 the Yibei (1.0 dimension), Yidong (2.0 dimension), Yixi (3.0 dimension), Yinan (4.0  
912 dimension) and central city (5.0 dimension) subregions. As shown in the figure, the



913 central city achieves the most comprehensive benefit among the five cities. This is  
914 primarily attributed to the large population and intensive industry in this area. However,  
915 the benefits in the other four subregions are also high compared to recent levels and  
916 those achieved with traditional allocation methods, as shown in Table 9. Interestingly,  
917 the comprehensive benefits in the subregions are greater in the scenario with the  
918 maximum synergy degree under normal conditions than in the other two scenarios.  
919 Technically, the total comprehensive benefits in the five subregions in this scenario are  
920 approximately  $2.3 \times 10^8$ - $5.1 \times 10^8$  yuan higher than those in other cases, which indicates  
921 that the solution with the highest synergy degree in the second layer is the best choice  
922 for managers in normal years. However, the various subregions obtain the greatest  
923 benefits when maximizing the unconventional water supply in dry and extreme  
924 scenarios. This result indicates that increasing the use of unconventional water in dry  
925 and extremely dry years would significantly increase the potential benefits.



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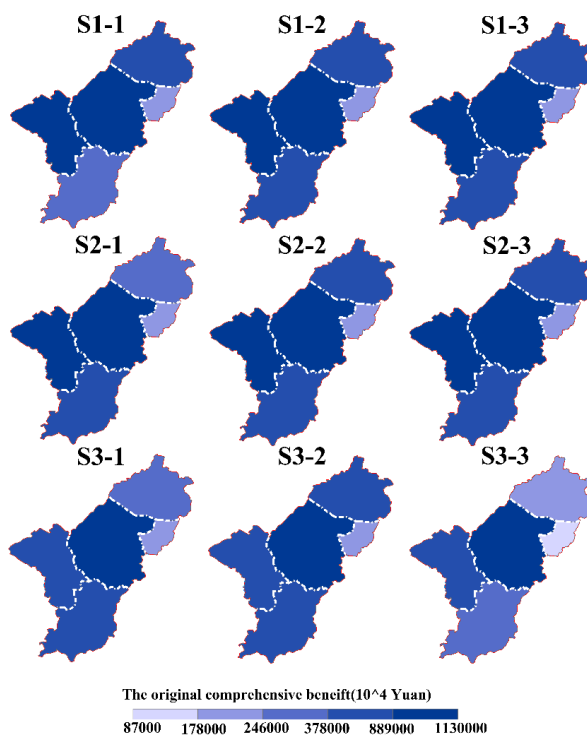
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**Fig. 9.** Illustration of parallel-reference Pareto sets from the third layer in the PTSPPOA model attained across all runs for the (S1) normal, (S2) dry, and (S3) extremely dry scenarios

Fig. 10 presents the optimal comprehensive benefit in each subregion. In all scenarios, the central city is associated with the highest comprehensive benefit, followed by Yixi and Yinan, and the comprehensive benefit in Yidong is relatively low. This result may be related to this subregion having the smallest area (72.2 km<sup>2</sup>) and the smallest population ( $7.7 \times 10^4$  people). The comprehensive benefits vary among different solutions and scenarios. Among the three normal decision alternatives, F1, F2 and F5 are highest in S1-3, with values of  $3.03 \times 10^9$  yuan,  $9.90 \times 10^8$  yuan and  $1.12 \times 10^{10}$  yuan, respectively. This indicates that considering the synergy degree could increase the



939 comprehensive benefit in most subregions in the normal scenario. Among the  
940 alternatives in the dry and extremely dry scenarios (excluding F4 and F5), other  
941 objectives are highest in S2-2, with values of  $2.84 \times 10^9$  yuan,  $9.63 \times 10^8$  yuan and  
942  $2.67 \times 10^8$  yuan, respectively. It suggests that maximizing the unconventional water  
943 supply is beneficial for the system in dry conditions. Additionally, F4 is highest, with a  
944 value of  $2.29 \times 10^9$  yuan, in S2-3 among the three solutions in the dry scenario, and F5  
945 is highest, with a value of  $9.17 \times 10^9$  yuan, in S3-1 in the extremely dry scenario.



946

947 **F10.** Comprehensive benefit in each area after the regional collaborative allocation of

948

water resources



#### 949 **4.4 Discussion**

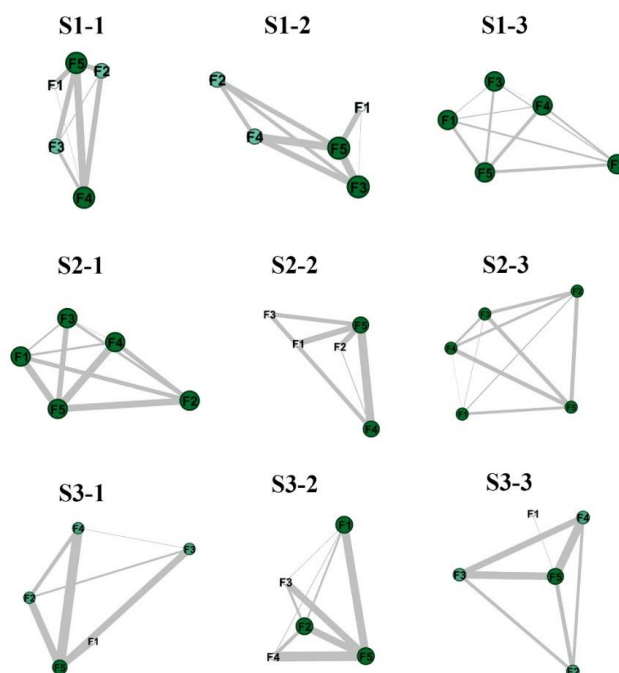
950 To assist policymakers in understanding the complex and systemic nature of water  
951 systems and reveal the dynamic interactions among objectives, network analysis and  
952 optimization was applied. By revealing the interactions among different objectives, we  
953 determine the level of synergy in complicated water systems, identify the challenges  
954 and opportunities for sustainable development of water systems in cities with various  
955 subregions, and provide valuable insights and specific action priorities for these regions.

956 In the networks shown in Fig. 11, each node represents an individual objective (F1, F2,  
957 F3, F4, and F5 represent the comprehensive benefits in Yibei, Yidong, Yixi, Yinan and  
958 the central city, respectively), and pairwise objectives that are significantly ( $P < 0.05$ )  
959 correlated are connected by a link, where the strength of each link is related to the  
960 Pearson correlation coefficient. The obtained networks with 5 nodes were weighted and  
961 undirected (directionality can be estimated only if the direction of causality is known).

962 The size of the circles in the figure indicates the connectivity of each objective. We  
963 considered trade-offs (i.e., negative correlations wherein one objective improves while  
964 the other worsens) among the objectives. In most scenarios, F5 was the relatively  
965 dominant objective, signifying that other objectives disproportionately deteriorated as  
966 progress was made towards the benefit of the central city, as shown in Fig. 11. It is  
967 evident that the trade-offs are more balanced in the scenarios with the highest degrees  
968 of synergy (S1-3, S2-3, and S3-3), which indicates that the tradeoffs and competitions



969 among the objectives are alleviated when synergy is considered. The links show that  
970 the conflicts of interest between F4 and F5 in scenarios S1-1 and S2-2 are extremely  
971 notable, suggesting that the comprehensive benefits in Yinan and the central city  
972 correspond to strong negative interactions in these cases. The connectivity of most  
973 objectives was relatively low in the tradeoff network in the extremely dry scenario, but  
974 F5 played a dominant role in terms of negative interactions among objectives, although  
975 the connectivity of F5 was lower than other connectivities in most normal and dry  
976 scenarios. Moreover, as the scenario varied from normal to extremely dry, the impact  
977 of individual regional targets on the whole system diminished.



978

979

**Fig. 11.** Network analysis of the results of layer 3





980

981       For comparison, we applied five widely used MOEAs, namely, NSGA-II, SPEA-  
982 II,  $\epsilon$ -MOEA, IBEA, and MOEA/D, to solve cases with 3+2+5 mathematical objectives  
983 (3 objectives in the first layer, 2 objectives in the second layer and 5 objectives in the  
984 third layer) with the same constraints given previously for Yiwu city under normal, dry  
985 and extremely dry conditions. The constraints and common parameters, such as the  
986 maximum number of model simulations and the simulated binary crossover (SBX) rate,  
987 are set to those used in the PTSOA model. However, it is difficult to determine feasible  
988 decision alternatives with MOEAs, even though the number of iterations is increased  
989 to 20000 (which is far beyond that considered in the previous modelling) because the  
990 complexity of the system overshadows the optimization capabilities of these traditional  
991 models. These results reconfirm the superiority, efficiency and decoupling capability of  
992 the proposed model for optimal allocation cases involving complex water systems with  
993 multiple stakeholders, multiple sources, multiple decision-makers and embodied reused  
994 systems. By embedding the targets into hierarchical layers, the excessive abandonment  
995 of some promising alternatives is avoided, and optimal allocation is progressively  
996 achieved. In general, the hierarchical structure of the PTSOA model can simulate  
997 complicated systems with multiple complex objectives and constraints.

998       In addition, the five MOEAs were used to solve the equations in the third layer of  
999 the PTSOA model, and the overall targets in the first layer were determined based on  
1000 these solutions. The necessary parameters and hyperparameters were consistent with



1001 those used in the third layer of the PTSOA model. Additionally, the benefits in the  
1002 current case with no optimization calculated based on the actual water supply are given  
1003 for comparison. The current situation was categorized as a normal scenario, and other  
1004 models were established with the same conditions to facilitate further comparison and  
1005 analysis. There were distinct decision alternatives generated by each model, and the  
1006 relevant results are listed based on their value ranges. As shown in Table 4, although  
1007 NSGA-II and  $\epsilon$ -MOEA yield slightly higher F2 values than PTSOA and F3 generated  
1008 by IBEA ( $4.8 \times 10^8$  -  $7.2 \times 10^8$  yuan) is higher than obtained with PTSOA, PTSOA  
1009 performs better than other models in most cases. The PTSOA is shown to be the best  
1010 model for obtaining comprehensive benefits for the subregions in Yiwu in the normal  
1011 scenario, demonstrating that the PTSOA model offers advantages including identifying  
1012 the best alternatives and achieving greater subregional benefits than the other models.  
1013 The proposed model yields a  $1.76 \times 10^9$  -  $15.67 \times 10^9$  yuan total comprehensive benefit  
1014 improvement and can save approximately  $3.2 \times 10^7$  -  $4.7 \times 10^7$  ( $\text{m}^3$ ) of conventional water  
1015 compared to the current values. It is also evident that the proposed model yields the  
1016 highest TSI values, reflecting the improvement achieved by considering the synergy of  
1017 the system. In terms of the targets in the first layer, except MOEA/D, other traditional  
1018 models fail to retain enough water (water requirements for living under extreme drought  
1019 conditions of the next configuration period) in the reservoirs to meet future basic needs.  
1020 For MOEA/D, although it generates a slightly higher total water supply benefit, with a  
1021 value of  $2.81 \times 10^8$  -  $3.12 \times 10^8$ , the total water supply shortage and the total amount of



1022 reserved water in the reservoirs are worse than the amounts obtained with the proposed  
1023 model. PTSOA trades some economic benefits for enhanced water supply reliability  
1024 and sustainable development, resulting in a decrease in the water supply from  
1025 conventional water plants.

1026 However, the consideration of reclaimed water in the proposed model effectively  
1027 reduces the use of traditional water and improves the quality of the water environment  
1028 by reducing sewage discharge, and other benefits are also achieved (such as meeting  
1029 the quality standards for river water and guaranteeing that the ecological water demand  
1030 of inland rivers is met). The results obtained by the PTSOA may help guide both the  
1031 government and general public. Our proposed model is superior to traditional models.  
1032 It can not only optimize water resource utilization and secure water supplies but also  
1033 enhance the synergy and environmental quality of water systems. Considering synergy  
1034 across various time scales, the proposed model ensures the synergistic allocation of  
1035 water resources at yearly, monthly and daily scales while securing both present and  
1036 future water supplies.

1037 **Table 4** Comparison of the comprehensive benefits in the five regions (F1, F2, F3, F4,  
1038 and F5) and the TSI values in the current situation and obtained using NSGA-II,  
1039 SPEA-II,  $\epsilon$ -MOEA, IBEA, MOEA/D, and PTSOA in the normal scenario

Comparison	Comprehensive benefits ( $10^9$ yuan)					TSI
	F1	F2	F3	F4	F5	
NSGA-II	2.72~2.86	0.91~1.03	2.57~2.60	3.21~3.37	7.38~9.95	-3.13~-2.82
SPEA-II	2.84~2.97	0.93~0.99	2.58~3.15	3.02~3.68	8.22~9.99	-2.39~-2.46



$\epsilon$ -MOEA	2.47~2.33	0.85~1.12	2.21~2.32	3.05~3.18	9.23~9.91	-3.41~-3.06
IBEA	2.57~2.88	0.87~0.92	3.05~3.11	3.20~3.32	5.27~8.28	-3.28~-3.11
MOEA/D	2.55~2.90	0.99~1.02	3.15~3.20	3.34~3.36	9.82~10.11	-2.37~-1.54
Current situation	2.05	0.83	2.49	3.11	9.87	-3.20
<b>PTSOA</b>	<b>2.63~3.03</b>	<b>0.95~0.99</b>	<b>2.39~2.67</b>	<b>3.84~4.11</b>	<b>10.30~11.22</b>	<b>-1.66~-0.89</b>

## 1040 5. Conclusions

1041 Applying optimal water allocation models to simultaneously enable economic benefits,  
1042 water preferences and environmental demands at different decision levels, time scales  
1043 and regions is a challenge. In this study, a new process-based three-layer synergistic  
1044 optimal allocation model (PTSOA) is developed and applied to a real and complex  
1045 water allocation system. The objective functions were divided into three layers to  
1046 coordinate conflicts of interest among decision makers at different levels and time  
1047 scales. Furthermore, the allocation of reclaimed water was embedded in the proposed  
1048 model for synergistic optimal allocation of both conventional and unconventional water.  
1049 A synergistic index based on network analysis was introduced to reduce competition  
1050 among different stakeholders and facilitate the positive effect of stakeholder  
1051 interactions. A hierarchical optimal algorithm was designed to solve the PTSOA model.

1052 The proposed model was applied to a representative city in Southeast China with  
1053 scarce water resources and a developed industry. Achieving the optimal allocation of  
1054 water resources in this kind of highly developed area offers a valuable reference for  
1055 other counties in China. Key findings can be concluded from these results, as follows.

1056 First, the results demonstrated that the PTSOA model achieved synergistic allocation



1057 among hierarchical decision-makers across various time scales and in different regions,  
1058 yielding the highest TSI (-1.66 to -0.89) among the models evaluated. Second, with a  
1059 synergistic approach, a reasonable amount of conventional water is retained for future  
1060 use in cases with potentially high risk, with volumes of  $3.95 \times 10^7$  m<sup>3</sup>,  $3.12 \times 10^7$  m<sup>3</sup>, and  
1061  $2.43 \times 10^7$  m<sup>3</sup> retained in normal, dry and extremely dry scenarios, respectively.  
1062 Moreover,  $7.35 \times 10^7$  m<sup>3</sup>,  $7.56 \times 10^7$  m<sup>3</sup>, and  $7.37 \times 10^7$  m<sup>3</sup> of conventional water is saved  
1063 in the three scenarios. Third, considering both reclaimed water and conventional water  
1064 in the optimization process efficiently improves the quality of municipal water, and  
1065 more than 1272.21 t/year and 48.81 t/year of COD and ammonia nitrogen emissions  
1066 are mitigated compared to those in the current situation. Distinct from previous models,  
1067 the proposed optimal model was implemented with the consideration of spatial  
1068 dimensions, which are important but often neglected. The results show that spatial  
1069 allocation yields an improvement of 4-95% for the comprehensive benefits in different  
1070 subregions compared to the benefits achieved with traditional models, and the total  
1071 comprehensive benefit increases by  $1.76 \times 10^9$ - $15.67 \times 10^9$  yuan compared to that in the  
1072 current situation. The synergy index established based on network analysis is used to  
1073 alleviate the competition among regions and facilitate water supply improvements.

1074 These results and conclusions provide valuable references for the evaluations of other  
1075 complicated water allocation systems. The optimal allocation scheme is determined for  
1076 a complex water system upon consideration stakeholder synergy and various  
1077 hierarchical decision levels, time scales and regions. More in-depth studies of



1078 synergistic optimal water allocation are needed in the future.

1079

1080 *Data availability.* The data used to support the findings of this study are available  
1081 from the corresponding author upon request.

1082

1083 *Author contribution.* JL and YPX designed all the experiments. JL and SWW collected  
1084 and preprocessed the data. JL and WZ conducted all the experiments and analysed the  
1085 results. JL wrote the first draft of the manuscript with contributions from SWC. YPX  
1086 supervised the study and edited the manuscript.

1087

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