

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 sub-regions, 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 [be able to](#) improve the contradictions among different dimensionalities
22 in a complex system. Overall, $2.43 \times 10^7 \sim 3.95 \times 10^7$ m³ of conventional water is saved,
23 and notable improvements in management are achieved. The application demonstrates
24 the efficiency and excellent performance of the PTSOA [model](#).

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~~[ed](#) 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. Nowadays, the water resources system become more and more complex, and

39 ~~is consisted with~~often has multiple sources and users as well as water reused
40 infrastructure. This kind of water resources system is called complex ~~water resources~~
41 ~~system in the following~~. Therefore, it is critical to develop a synergistic optimal
42 allocation model to alleviate conflicts and ensure the security, efficiency, equality, eco-
43 environmental sustainability, and sustainable development of complex water resources
44 ~~systems water systems~~ simultaneously.;

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

60 interactions among objectives, the internal mechanisms of a water system can be
61 clarified, and synergy can be achieved in cases with different potential decisions. It is
62 also helpful to identify the hurdles and opportunities associated with sustainable
63 development for cities and to establish specific action priorities for cities based on a
64 comprehensive understanding of the interactions among objectives. To address this
65 knowledge gap, a correlational network approach is applied in this study, and a synergy
66 degree index is presented to consider both ~~the~~ equity and coordination of water systems.
67 Moreover, systemic analysis is used to assess the level of coordination of complex
68 objective interactions in city water systems.

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

81 are mild (Wu et al., 2022). Thus, to facilitate the discovery of high-quality decision
82 alternatives, alleviate negative conflicts among multiple utilities and inform decision
83 making, a synergy degree evaluation index is established and applied to the network
84 analysis of this study.

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

96 To address these hierarchical problems, bi-level programming (BLP) has been
97 widely used, wherein objectives at two hierarchical levels, namely, an upper level and
98 a lower level, are co-optimized (Zhang and Vesselinov, 2016; Jin et al., 2018). The
99 upper-level decision may be affected by ~~the~~ actions of the lower-level decision makers
100 (Arora and Gupta, 2009). Yue et al. (2020) formulated a bi-level programming (BLP)
101 framework to gain insight into the whole water allocation process with district

102 administrators and sub-regional farmers. Li et al. (2022) built a two-level model with
103 the overall interests of system managers at the top and the individual interests of water
104 supply departments at the bottom. The multi-level programming problem (MLPP) was
105 derived from the bi-level programming problem (BLPP) and is more applicable to real
106 world practices (Baky, 2014). However, limited studies have explored applying MLPP
107 (more than two levels) for water resource allocation, especially in cases with
108 unconventional water supplies.

109 To satisfy both long-term and short-term water needs and avoid unnecessary
110 administration costs and water resource use caused by a lack of coordination among
111 different allocation steps, temporally synergistic allocation and optimization are needed
112 (Haguma and Leconte, 2018). In annual water resource planning, the monthly
113 variability of hydrologic regimes and non-stationarity of the daily water demand must
114 be considered. As an alternative example of synergistic allocation at different time steps,
115 Vicuna et al. (2010) used a monthly nonlinear programming model and an annual
116 sampling stochastic dynamic programming (SSDP) model to establish a monthly
117 operating policy. Haguma et al. (2015) proposed an optimization approach with two
118 separate time steps following the nested model approach. Haguma and Leconte (2018)
119 constructed deterministic and stochastic optimization models with two time steps (intra-
120 annual and inter-annual) and two levels of inflow variability: seasonal and inter-annual.
121 The purpose of their short-time-step model was to derive aggregate performance
122 functions associated with potential long-time-step decisions in these studies. However,

123 short-term benefits should not be overlooked due to their appreciable impact on long-
124 term effects. Accordingly, synergistic allocation that enhances both long-term and
125 short-term allocations is of great importance for water resource management in cities.
126 However, optimizing the structure of a model to achieve maximized benefits and
127 balancing the trade-offs among time steps are tasks that have rarely been studied. The
128 synergy among different time steps is addressed with a new innovative framework and
129 a corresponding algorithm in our study.

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

142 The optimal allocation of conventional and unconventional water resources also
143 significantly impacts water security and aquatic ecosystems. The reuse of reclaimed

144 water is beneficial for alleviating high water supply pressure on conventional water
145 resources and reducing the emission of pollutants. To effectively integrate conventional
146 and unconventional water resources, Yang et al. (2008) and Han et al. (2008) introduced
147 unconventional water resources as critical factors in water management. Avni et al.
148 (2013) investigated the mixing of unconventional water resources with other
149 conventional water sources to meet the magnesium requirements for drinking water and
150 irrigation water. Yu et al. (2017) developed a cost–benefit analysis-based utilization
151 model for externally transferred water and desalinated water. The allocation of both
152 conventional and unconventional water has been widely studied, but there remains a
153 lack of methods to guide the synergistic allocation of conventional and unconventional
154 water resources and embed reclaimed water supply systems in allocation schemes. The
155 overexploitation of conventional water resources is not conducive to ~~the~~sustainable
156 development, while ~~the~~extensive use of unconventional water could ultimately result
157 in high economic burden. To synergistically integrate conventional and unconventional
158 water resources and guide the coordinated allocation of these two types of water
159 resources, corresponding mechanisms must be implemented. As a result, our study aims
160 to couple the allocation of conventional water resources and unconventional water
161 resources to establish synergistic solutions.

162 In summary, as insufficient water supplies and increasing water demands intensify
163 competition for water resources and lead to conflicts among different stakeholders in
164 different dimensions, water allocation must be optimized in cities and regions to

165 achieve synergistic decision-making at various levels and time steps considering the
166 value of reclaimed water. Therefore, a new process-based three-layer synergistic
167 optimal allocation (PTSOA) model is developed here to generate numerous candidates
168 or Pareto solutions and identify several desirable decision alternatives. The synergy of
169 time and space optimization is achieved in the new model to avoid waste and promote
170 balanced spatial development. Furthermore, in the PTSOA model, reclaimed water is
171 used to replenish conventional water resources in water-scarce areas.

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

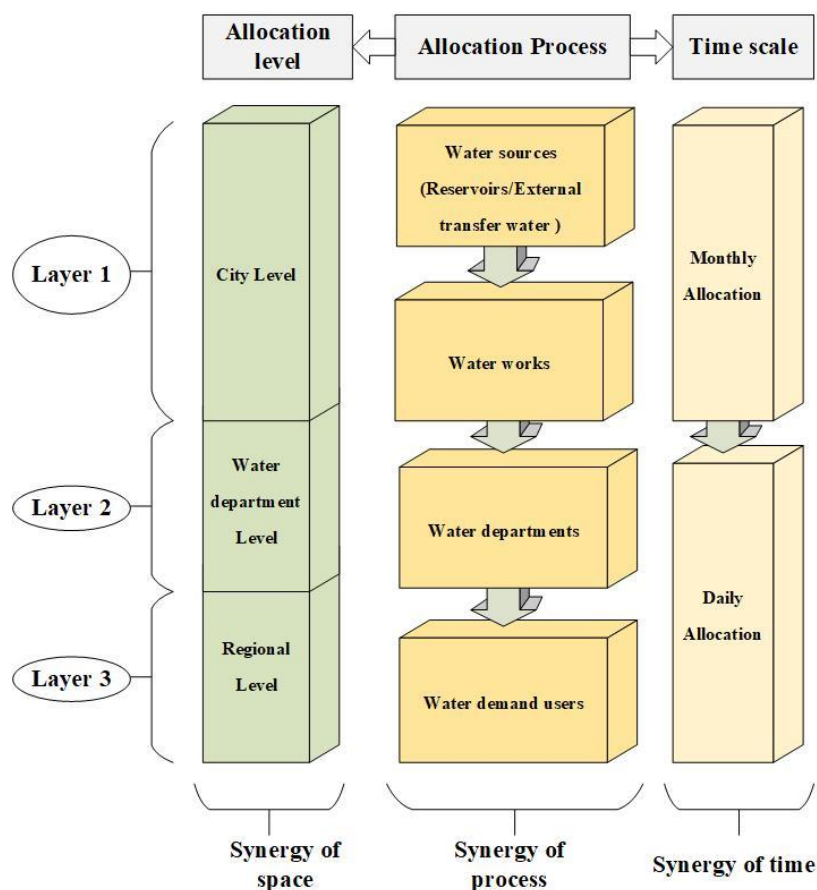
178 **2. Modelling**

179 With water resources becoming increasingly scarce, multi-dimensional synergistic
180 optimal allocation in a hierarchical system is crucial for ensuring sustainable
181 development in water-scarce cities. There are three dimensions of synergy in the
182 established allocation model, as shown in Fig. 1: process synergy, decision-level
183 synergy and time-scale synergy. The synergy of the process refers to synergistic water
184 allocation among the three stages throughout the whole allocation process to reduce

185 waste in bridging processes, which has rarely been considered. In the three stages, first,
186 the original water is released from reservoirs or diverted from external water transfer
187 projects to water works; then, the water stored in water works infrastructure is supplied
188 to different departments that need different types of water, including both conventional
189 and reclaimed water. Finally, ~~the~~ water is supplied to different users. Decision-level
190 synergy refers to synergistic water allocation considering the interests of decision
191 makers at different levels, namely, the city, water department and regional levels, to
192 coordinate solutions and avoid conflicts among decision makers. The city level
193 represents the overall interests of a city from the perspective of government, the water
194 supply department level represents the interests of water supply corporations, and the
195 regional level focuses on the comprehensive benefits of each region in the city and
196 mitigate development imbalance among regions. Optimal decision making at the
197 department level is constrained by the allocation results at the city level, and so on, and
198 the final solution should satisfy the needs of decision makers across all levels. The time
199 scale synergy involves the coordination of the daily configuration goal with the monthly
200 goal, the monthly goal with the yearly goal, and so on. Synergistic temporal allocation
201 can largely alleviate time conflicts during configuration operations, ensuring that all
202 configuration periods serve the same final configuration objectives to save water
203 resources and improve efficiency. However, time scale synergy mainly depends on
204 artificial operations rather than automated intelligent operations in practice. In-depth
205 exploration has yet to be demonstrated. Consequently, the PTSOA model is constructed

206 here to fully consider these three dimensionalities of synergy. The dimensionalities are
 207 coupled in this model to achieve the efficient maximization of comprehensive benefits
 208 at all levels under the premise of saving water resources. In Fig. 1, the grey boxes
 209 indicate the three different allocation dimensions, the green boxes indicates the three
 210 different decision levels coupled with spatial scales, the bright yellow boxes indicates
 211 every key nodes in the whole allocation process and the buff boxes indicates nested
 212 time scale.

213



214

215

Fig. 1. Conceptual map of the PTSOA model

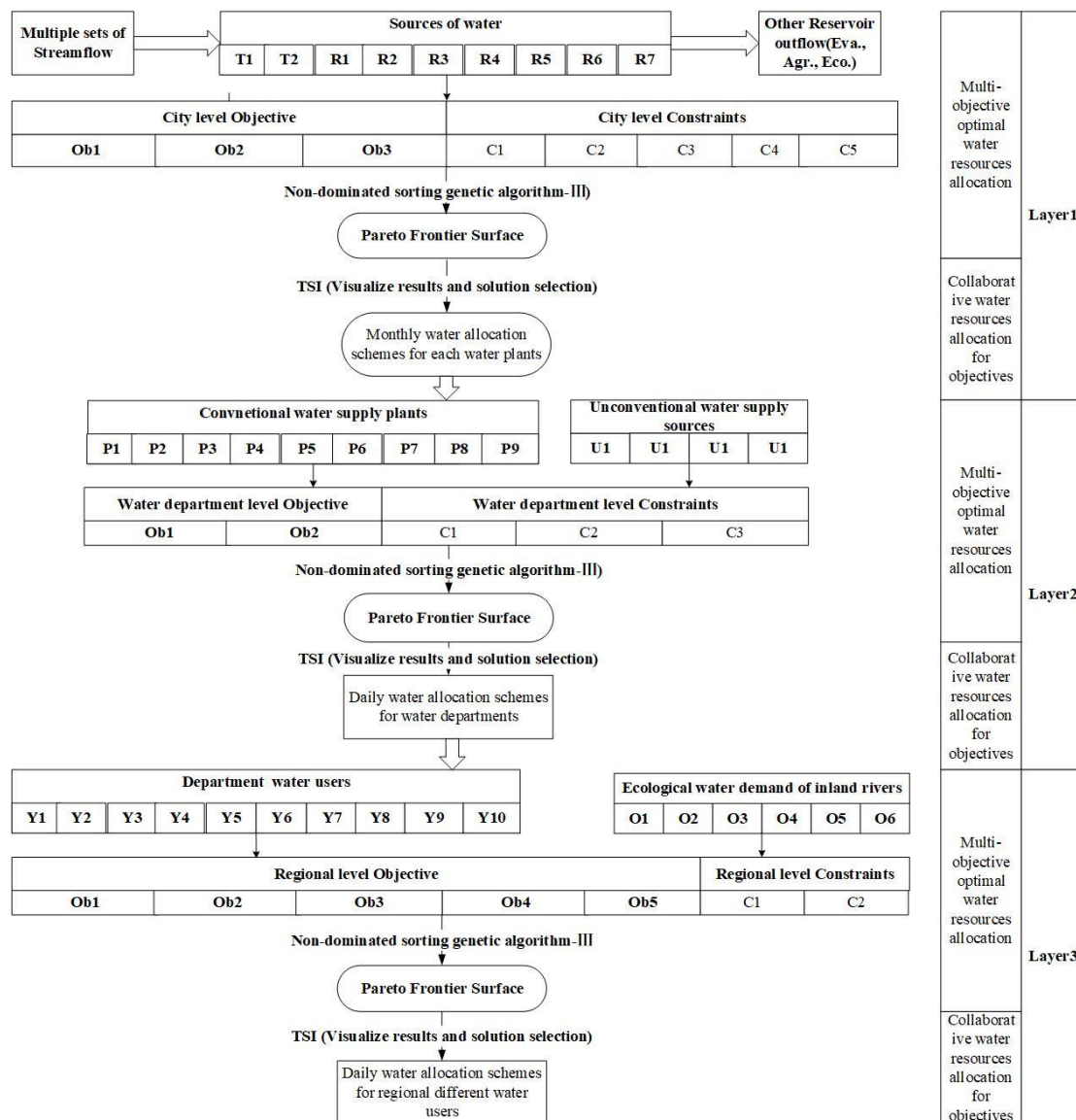
216

217 In water-scarce cities, using reclaimed water as an alternative water source is
218 proved to be useful ~~a proven approach~~ to efficiently improve the environment by
219 reducing sewage discharge. The quality of inland tributaries has deteriorated in many
220 water-scarce cities due to limited consideration of the water environment and the large-
221 scale emission of pollutants. Transferring reclaimed water and main river water to urban
222 inland tributaries for ecological water replenishment is a promising approach for
223 improving the quality of urban water environments and areas with water shortages.
224 However, there has been a lack of studies on the integration of reclaimed water reuse
225 systems and inland water distribution systems in allocation modelling. Therefore, in
226 addition to saving water resources and improving efficiency through multi-dimensional
227 synergistic allocation, the model encompasses reclaimed water reuse systems and
228 ecological water distribution systems for inland tributaries.

229 Finally, the PTSOA model is constructed to solve the multi-dimensional synergistic
230 allocation problem involving complex water resource networks that couple reclaimed
231 water reuse systems and inland ecological water distribution systems with multiple
232 sources, processes and regions to guarantee the sustainable development of water-
233 scarce cities. To select the most synergistic solution of the PTSOA model, a new
234 evaluation index named the ~~total~~-synergy index (*TSI*) is proposed to assess the synergy
235 degree of different decision alternatives. System entropy ($H(S)$) can describe the
236 evolution direction of a water resource system and was used to promote the
237 coordination of water supply departments in a water resource allocation system(Li et

238 al., 2022). So, it was is used for comparison to evaluate the validity of this proposed
239 index. Furthermore, the network analysis method is applied for the first time to analyse
240 dynamic interactions in water optimal allocation. This method visually depicts the
241 dynamic interactions and conflicts among different subareas in a city, which is helpful
242 for system managers to realize how the water allocation scheme in one region
243 influences that of other areas; consequently, more reasonable and flexible measures are
244 established based on dynamic regional development targets. The detailed framework
245 developed in this study is shown in Fig. 2. In Fig. 2 this figure, there are three layers in
246 the framework and each layer has two parts: multi-objective optimal water resources
247 allocation and collaborative water resources allocation for objectives. In the multi-
248 objective optimal water resources allocation, sub-layers contain key nodes in the
249 allocation process and relevant objectives and constraints. In the collaborative water
250 resources allocation for objectives, sub-layers contain optimization algorithm and
251 decision selection method.

252



253

254

Fig. 2. Framework of the PTSOA model

255 **2.1 First layer of the PTSOA decision-making process**

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

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

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

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

260 satisfy the overall development goals of the city, the first-layer processes involve city-
261 level decision-making. The city manager focuses on the overall goal of the complex
262 water resources system~~water resource system~~ in the city, which is the first and most
263 important phase of the decision-making process. The established allocation scheme
264 highly influences decision makers at other levels, and optimal allocation schemes at
265 other levels must align with this overall goal. Additionally, since water resource
266 planning in most Chinese cities is based on an annual planning period and monthly
267 planning unit, the time step of the first layer is set as months. Finally, the monthly
268 decision alternatives for the volume of water allocated from reservoirs to water works
269 is obtained at the city decision level.

270 **2.1.1 Objective functions of the first layer**

271 **Social objective function: Minimization~~minimization~~ of total water supply**
272 **shortages**

273 The social objective function is established by the city manager to minimize the total
274 water supply shortages in a water system. The objective is established to sufficiently
275 meet the water demands of users in a water ~~resource~~resources system. The water
276 deficit is considered, and this objective can reflect the ability of the water supply to
277 meet the water demand, as shown in Eqs. (1-3):

$$278 \quad \min f_{11}(x) = D - S \quad (1)$$

279
$$D = \sum_{r=1}^R \sum_{t=1}^T D_r^t \quad (2)$$

280
$$S = \sum_{t=1}^T \sum_{i=1}^I \sum_{j=1}^J x_{ij}^t \alpha_{ij} + \sum_{t=1}^T \sum_{e=1}^E \sum_{j=1}^J x_{ej}^t \beta_{ej} \quad (3)$$

281 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
 282 demand of the r th sub-region at t th time step, $r=1,2,\dots,R$, R is the total number of sub-
 283 regions in the area, $t=1,2,\dots,T$, T is the total number of months in the period, $S (10^4 \text{ m}^3)$
 284 is the total water supply of the water system for all waterworks, $x_{ij}^t (10^4 \text{ m}^3)$ is the
 285 amount of water supplied from i th reservoir to the j th waterworks in the t th month of
 286 the configuration period, $i=1,2,\dots,I$, I refers to the total number of reservoirs, $j=1,2,\dots,J$,
 287 J is the number of total water works, $x_{ej}^t (10^4 \text{ m}^3)$ is the amount of water supplied from
 288 the e th external transfer water source to the j th water works in the t th month of the
 289 configuration period, $e=1,2,\dots,E$, E is the total number of external transfer water
 290 sources in the city, α_{ij} is the water supply relationship coefficient between the i th
 291 reservoir and the j th water works, where 0 indicates no supply and 1 indicates a water
 292 supply, and β_{ej} is the water supply relationship coefficient between the e th external
 293 transfer water source and the j th water works, where 0 indicates no supply and 1
 294 indicates a water supply.

295 **Economic objective function: ~~Maximization~~ maximization of the total water**
 296 **supply benefit**

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

299
$$\max f_{12}(x) = B - C_{rs} - C_{es} \quad (4)$$

300
$$C_{rs} = k \times \sum_{t=1}^T \sum_{i=1}^I \sum_{j=1}^J x_{ij}^t \alpha_{ij} + \sum_{t=1}^T \sum_{i=1}^I \sum_{j=1}^J (x_{ij}^t \alpha_{ij} \times c_i) \quad (5)$$

301
$$C_{es} = m \times \sum_{t=1}^T \sum_{j=1}^J \sum_{e=1}^E x_{ej}^t \beta_{ej} + \sum_{t=1}^T \sum_{e=1}^E \left(n_e \times \sum_{j=1}^J x_{ej}^t \beta_{ej} \right) \quad (6)$$

302
$$B = \sum_{j=1}^J b_j \times \left(\sum_{t=1}^T \sum_{i=1}^I x_{ij}^t \alpha_{ij} + \sum_{t=1}^T \sum_{e=1}^E x_{ej}^t \beta_{ej} \right) \quad (7)$$

303 The overall economic benefit is the difference between the total benefit and total
 304 cost at the city level. In the equations, B (Chinese ~~yuan~~Yuan, ~~shortened to yuan in the~~
 305 ~~following text~~) is the total direct water supply benefit (mainly considering the income
 306 from water charges for the city). The total water supply cost consists of the reservoir
 307 water supply cost C_{rs} and the external water supply cost C_{es} ; k (~~yuan~~Chinese
 308 Yuan/m³) denotes the water resources fees paid to the government; c_i (~~yuan~~Chinese
 309 Yuan/m³) denotes the water fees paid to the i th reservoir authority; m (~~yuan~~Chinese
 310 Yuan/m³) is the charge to an external administrative district per unit of externally
 311 transferred water; n_e (~~yuan~~Chinese Yuan/m³) is the charge associated with the e th
 312 external water source per unit of transferred water; and b_j (~~yuan~~Chinese Yuan/m³) is
 313 the unit price of water supply revenue for the j th user.

314 **Sustainable development objective function: ~~Maximization~~ maximization of the**
 315 **total amount of reserved water in reservoirs**

316 In water-scarce cities, the problem of water scarcity is a serious challenge that prevents
 317 sustainable allocation of water resources. A prominent feature of most water-scarce

318 cities is that water inflows are limited, and the fluctuations in water availability are
319 large. Therefore, to reduce the risk that the inflows in the next configuration period are
320 too short to meet the basic demand of the city, ~~such that~~ a sustainable development
321 objective function is developed. The sustainable development objective function seeks
322 to maximize the amount of water remaining in the reservoir at the end of a configuration
323 period to hedge against drought risk and guarantee water use in the next period, as
324 shown in Eqs. (8-10):

$$325 \quad \max f_{13}(x) = \sum_{i=1}^N (V_i^{\max} - V_i) \times p(V_i^{\max} - V_i) \quad (8)$$

$$326 \quad p(V_i^{\max} - V_i) = \begin{cases} 2 \times V_i / V_i^{\max} & 0 < V_i < V_i^{\max} / 2 \\ -2 \times V_i / V_i^{\max} + 2 & V_i \geq V_i^{\max} / 2 \end{cases} \quad (9)$$

$$327 \quad V_i = \sum_{t=1}^T (R_{i,initial} + I_i^t + P_i^t - A_i^t - E_i^t - EP_i^t) - \sum_{t=1}^T \sum_{j=1}^J x_{ij}^t \alpha_{ij} \quad (10)$$

328 where V_i^{\max} (10^4 m^3) is the maximum allowable storage capacity of the i th water source,
329 which is expressed based on the limited storage capacity of a reservoir in the flood
330 season, and V_i (10^4 m^3) is the water storage capacity of the i th water source at the end
331 of the scheduling period. As much water as possible but less than V_i^{\max} is reserved.
332 However, a reserved water volume in the reservoir that is too high at the end of the
333 scheduling period may lead to considerable pressure on reservoirs to urgently release
334 water if a flood event is forecasted. The reserved water volume should be neither too
335 large nor too small. Thus, the benefits of reservoir ~~retainment-reserve stock~~ must be
336 thoroughly evaluated. Based on the characteristic of the benefit of residual water, we

337 propose a boundary benefit function $p(V_i^{\max} - V_i)$ for different reserved water
338 volumes in a reservoir. The benefit function is a piecewise function, and when V_i is
339 less than $V_i^{\max}/2$, p increases as V_i increases. When V_i is equal to or greater than
340 $V_i^{\max}/2$, p decreases as V_i increases. When $V_i = V_i^{\max}$, p decreases to 0. $R_{i,initial}$ (10^4
341 m^3) is the initial storage of the i th water source, I_i^t ($10^4 m^3$) is the inflow of the i th water
342 source at the t th time step, P_i^t ($10^4 m^3$) is the precipitation associated with the i th water
343 source at the t th time step, A_i^t ($10^4 m^3$) and E_i^t ($10^4 m^3$) are the agricultural and
344 ecological water supplies associated with the i th water source at the t th time step,
345 respectively, and EP_i^t ($10^4 m^3$) is the evaporation from the i th water source at the t th
346 time step.

347 **2.1.2 Constraints of the first layer**

348 The layer includes six main constraints: the reservoir water supply constraint, water
349 demand constraint, reservoir storage constraint, water balance constraint, external water
350 transfer constraint, and nonnegative constraint.

351 **Reservoir water supply constraint**

352 The maximum water available to supply from an individual reservoir is determined by
353 the difference between the total input and total reservoir output. The inputs include
354 inflow and precipitation, and the outputs mainly involve agricultural and environmental
355 water supplies, evaporation, water supplied for waterworks and reservoir leakage loss.
356 All these factors directly affect the decision-making process and are incorporated into

357 the model building process as shown in Eqs. (11-15):

$$358 \quad V_i^t \leq V_{i,\max}^t \quad (11)$$

$$359 \quad V_i^t = \sum_{j=1}^J x_{ij}^t \alpha_{ij} \quad (12)$$

$$360 \quad V_{i,\max}^t = \sum_{t=1}^{t-1} \left(R_{i,\text{initial}} + I_i^t + P_i^t - A_i^t - E_i^t - EP_i^t - \sum_{j=1}^J x_{ij}^t \alpha_{ij} - L_i^t \right) - V_{i,d} \quad (13)$$

$$361 \quad EP_i^t = ep_i^t \times s_i^t / 1000 \quad (14)$$

$$362 \quad V_i^t = \xi_i^t \times (R_i^{t-1} + R_i^t) \quad (15)$$

363 where V_i^t (10^4 m^3) denotes the total water supply from the i th reservoir at the t th time
 364 step; $V_{i,\max}^t$ (10^4 m^3) is the maximum water available to be supplied from the i th
 365 reservoir at the t th time step; ep_i^t (mm) is the water surface evaporation from the i th
 366 reservoir in the t th month; s_i^t (m^2) is the monthly average surface area of the i th
 367 reservoir in the t th month; $V_{i,d}$ (10^4 m^3) is the dead storage of the i th reservoir; L_i^t (10^4
 368 m^3) is the reservoir leakage loss from the i th reservoir at the t th time step; R_i^{t-1} (10^4 m^3)
 369 is the storage of the i th reservoir at the $t-1$ th time step; R_i^t (10^4 m^3) is the storage of the
 370 i th reservoir at the t th time step; and ξ_i^t is the t th monthly leakage coefficient for the
 371 i th reservoir.

372 **Water demand constraint**

373 The high-quality water demand of each subarea in a city should be satisfied in the water
 374 allocation process. High-quality water in this model refers to water that satisfies the
 375 relevant primary (surface water can be used for drinking after simple purification

376 treatment, such as filtration and disinfection) and secondary water quality requirements
 377 (water is slightly polluted and can be used for drinking after routine purification
 378 treatment, such as flocculation, precipitation, filtration, disinfection, and other
 379 processes) according to the Chinese Standard (GB5749), as shown in Eq. (16):

380

$$381 \quad 0.8 \times D_r \leq \sum_{t=1}^T \sum_{i=1}^I \sum_{j=1}^{J_r} x_{ij}^t \alpha_{ij} + \sum_{t=1}^T \sum_{e=1}^E \sum_{j=1}^{J_r} x_{ej}^t \beta_{ej} \leq 1.2 \times D_r, r = 1, 2, \dots, R \quad (16)$$

382 where D_r (10^4 m^3) is the high-quality water demand in the r th sub-region and there
 383 are a total of R sub-regions in the city. J_r is the number of waterworks in the r th sub-
 384 region. To ensure that the water supply guarantee in each area is greater than 80%, the
 385 total water supplied to every subarea is greater than 80% of its demand.

386 Reservoir storage constraint

$$387 \quad R_i^T \leq V_{i,f} \quad (17)$$

$$388 \quad R_i^T = \sum_{t=1}^T \left(R_{i,initial} + I_i^t + P_i^t - A_i^t - E_i^t - EP_i^{t1} - \sum_{j=1}^J x_{ij}^t \alpha_{ij} - V_i^t \right) \quad (18)$$

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

391 Water balance constraint

$$392 \quad R_i^{t+1} = R_i^t + I_i^t + P_i^t - A_i^t - EP_i^t - E_i^t - V_i^{t-1} - \sum_{j=1}^J x_{ij}^t \quad (19)$$

393 External transfer water constraint

$$394 \quad \sum_{t=1}^T \sum_{j=1}^J x_{ej}^t \beta_{ej} \leq E_{e,max} \quad (20)$$

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

397 **Nonnegative constraint**

398
$$x_{ij} \geq 0 \tag{21}$$

399 **2.2 Second layer of the PTSOA decision-making model**

400 Similarly, the second layer of the PTSOA model fuses all three dimensions of
401 synergistic water resource allocation mentioned previously. The second stage of the
402 process (the water stored in water works is supplied to different departments needing
403 water volumes of different quality) is optimized in the second layer. After city-level
404 decision-making, a conflict of interest inevitably occurs between traditional water
405 supply departments and unconventional water supply departments. Because
406 conventional and unconventional water supply departments compete for limited water
407 demand market shares, the stability of the water allocation system may be jeopardized
408 if excessive competition is not controlled. Thus, the second layer is implemented at the
409 department level. Decision-making at the department level seeks to guide the two water
410 supply departments to partake in benign competition and avoid conflicts to realize
411 synergy. In this case, the decision plan of the first layer in the hierarchy is followed.
412 Temporally, short-term allocation changes are needed as mentioned above; hence, the
413 time scale of the second layer is daily. Thus, the daily decision alternatives for the
414 volume of water allocated from water works to different water departments are obtained

415 to make relevant decisions.

416 **2.2.1 Objective functions of the second layer**

417 **Conventional water supply department objective function: Minimization**
418 **minimization of the total amount of water retained in water works**

419 The managers of conventional water supply departments strive to operate conventional
420 water systems efficiently and achieve the most equitable water share possible. The
421 amount of conventional water (of high quality) retained in a water works system is a
422 crucial factor affecting the efficiency and benefits of conventional water supply
423 departments. Therefore, the benefit of conventional water departments is established by
424 minimizing the total amount of water retained in water works at the end of a
425 configuration period, as shown in Eq. (22):

$$426 \quad \min f_{21}(x) = W_L = \sum_{t=1}^T \sum_{i=1}^I \sum_{j=1}^J x_{ij}^t \alpha_{ij} + \sum_{t=1}^T \sum_{e=1}^E \sum_{j=1}^J x_{ej}^t \beta_{ej} - \sum_{t=1}^T \sum_{m=1}^M \sum_{j=1}^J \sum_{z=1}^Z q_{jz}^{t,m} \chi_{jz} \quad (22)$$

427 where W_L (10^4 m³) is the total amount of water retained in a water works system at
428 the end of a configuration period; $q_{jz}^{t,m}$ (10^4 m³) is the water supply from the j th water
429 works system to the z th water user on the m th day in the t th month in the period of
430 configuration; $m=1,2,\dots,M$; and M is the total number of days in the t th month (28, 29,
431 30 or 31). Additionally, $z=1,2,\dots,Z$, and Z is the total number of water users. χ_{jz} is the
432 water supply relationship coefficient between the j th water work and the z th water user,
433 where 0 indicates no supply and 1 indicates a water supply.

434 **Unconventional water supply objective function: ~~Maximization~~ maximization of**
 435 **the amount of unconventional water supplied**

436 The reclaimed water reuse system and ecological water distribution system for inland
 437 tributaries are incorporated into the PTSOA model which are associated with
 438 unconventional water supply departments. The managers of unconventional water
 439 supply departments seek to supply as much unconventional water as possible to
 440 promote their interests. Thus, the objective of unconventional water departments is
 441 established to maximize the amount of unconventional water supplied. Unconventional
 442 water mainly includes reclaimed water and river water, which is of low quality (i.e., not
 443 meeting the quality standard mentioned in Section 2.1.2) and is mainly used for
 444 industrial production, ecological water replenishment for inland rivers and municipal
 445 road sprinkling.

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

449
$$\max f_{22}(x) = W_r + EW_r \quad (23)$$

450
$$W_r = \sum_{t=1}^T \sum_{n=1}^N \sum_{j=1}^J r_{nj}^t p(b_c, b_u) \theta_{nj} \quad (24)$$

451
$$p(b_c, b_u) = \frac{1}{3} \times \frac{b_c}{b_u} - \frac{2}{3} \quad (25)$$

452
$$EW_r = \sum_{t=1}^T \sum_{n=1}^N \sum_{z=1}^Z r_{nz} \theta_{nz} \quad (26)$$

453 where W_r (10^4 m^3) is the total amount of reclaimed water supplied for all water users;
 454 EW_r (10^4 m^3) is the total amount of river water supplied to maintain ecological flows
 455 in inland tributaries; r_{nj}^t (10^4 m^3) is the amount of water supplied to the j th user from
 456 the n th reclaimed water source at the t th time step; $n = 1, \dots, N$; N is the total number of
 457 reclaimed water sources; $p(b_c, b_u)$ is a function expressing the willingness of residents
 458 to use reclaimed water, b_c (yuanChinese Yuan/ 10^4 m^3) is the price per unit of
 459 conventional water; b_u (yuanChinese Yuan/ 10^4 m^3) is the price per unit of
 460 unconventional water; and θ_{nj} is the water supply relationship between the n th
 461 reclaimed water source and the j th user. In this case, $\theta_{nj} = 1$ indicates a water supply
 462 relationship, and $\theta_{nj} = 0$ indicates no water supply relationship. r_{nz} (10^4 m^3) is the
 463 amount of water supplied from the n th reclaimed water source to the z th inland tributary;
 464 $z = 1, 2, \dots, Z$; Z is the total number of inland tributaries requiring ecological flow
 465 compensation; and θ_{nz} is the water supply relationship between the n th reclaimed
 466 water source and the z th inland tributary.

467 **2.2.2 Constraints of the second layer**

468 **Conventional water supply constraint**

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

472
$$\sum_{t=1}^T \sum_{i=1}^I \sum_{j=1}^J x_{ij}^t \alpha_{ij} + \sum_{t=1}^T \sum_{e=1}^E \sum_{j=1}^J x_{ej}^t \beta_{ej} \geq \sum_{t=1}^T \sum_{m=1}^M \sum_{j=1}^J \sum_{z=1}^Z q_{jz}^{t,m} \chi_{jz}, t = 1, \dots, T \quad (27)$$

473 **Unconventional water constraints**

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

476 The ecological water used to replenish inland tributaries is mainly pumped from
 477 reclaimed water works and main rivers. Therefore, this replenished volume is limited
 478 by the pumping capacity. The constraints for unconventional water are shown in Eqs.

479 (28)-(29):

480
$$\sum_{t=1}^T \sum_{n=1}^N \sum_{j=1}^J r_{nj}^t \theta_{nj} + \sum_{t=1}^T \sum_{n=1}^N \sum_{z=1}^Z r_{nz} \theta_{nz} = \sum_{t=1}^T \sum_{i=1}^I \sum_{j=1}^J x_{ij}^t \delta_{ij} \eta_{ij} + PU \quad (28)$$

481
$$PU = \sum_{t=1}^T \sum_{m=1}^M \sum_{p=1}^P Q_{t,m}^{p,s} / 10^4 \quad (29)$$

482 where δ_{ij} is the sewage discharge coefficient, which is the proportion of the water
 483 supplied from sewage discharge; η_{ij} is the sewage water reuse rate, which is the
 484 proportion of reused water in the total volume of sewage water; PU (10^4 m³) is the
 485 amount of water pumped from the main river; and $Q_{t,m}^{p,s}$ (t/d) is the flow through the
 486 s th pumping station on the m th day at time step t .

487 **Pumping constraints**

488
$$Q_{t,s}^p \leq Q_{\max,s}^p \quad (30)$$

489
$$Q_t^p = \sum_{s=1}^{Np} r_{t,s}^p \quad (31)$$

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

493 **Water quality constraint**

494 To control the impacts of various point and nonpoint sources on receiving water bodies
 495 in cities, water authorities impose water quality standards for the management of river
 496 basins. These standards seek to maintain the water quality at a desired target level by
 497 defining discharge limits for conventional, specific, or priority pollutants. To satisfy the
 498 relevant standards, the following water quality constraint is established:

$$499 \quad \sum_{t=1}^T \sum_{i=1}^N \sum_{j=1}^M \left(x_{ij}^t \delta_{ij} \psi_{ij} h_j^u - x_{ij}^t \delta_{ij} \eta_{ij} h_j^u \right) \times 10 \leq H^u \quad (32)$$

500 where ψ_{ij} is the sewage water treatment rate, which is the proportion of sewage water
 501 that is treated; h_j^u (mg/L) is the concentration of the u th contaminant per unit treated
 502 water required by the j th user; and H^u (kg) is the upper limit of the u th contaminant
 503 allowed to be discharged in the study area.

504 **2.3 Third layer of the PTSOA decision-making model**

505 After obtaining the results for the former two stages of the allocation process and the
 506 two levels of decision-making, the third model layer is constructed to achieve regional
 507 [synergy](#). It refers to the collaborative allocation of water resources in different
 508 sub-regions of a city, and it is intended to balance and maximize the interests of each

509 sub-region as much as possible. Additionally, the needs of different kinds of water users
510 in different sub-regions can be met to the greatest extent possible with this approach.
511 Therefore, the three dimensions of synergy are also fused in this layer. The third stage
512 of the process (the water in different departments is supplied to different kinds of water
513 users, namely, residential users, industrial users and municipal users, in different sub-
514 regions) is optimized in this layer. After department-level decision-making, conflicts of
515 interest inevitably occur among various water users in different sub-regions of a city.
516 Therefore, the third layer considers regional-level decision-making to ~~to~~ coordinate
517 water needs and avoid conflicts of sub-regions in the city. Moreover, the various
518 development priorities of sub-regions are emphasized by adjusting certain hyper-
519 parameters in the third layer. This layer is established based on the allocation scheme
520 obtained in the second layer of the hierarchy, and the time scale of this layer is the same
521 as that of the second.

522 Although water pollutants are controlled in the second layer, the detailed spatial
523 distribution of pollutants remains unknown. If one of the sub-regions emits a greater
524 pollution load than others such that the river pollution limit is exceeded, it constrains
525 sustainable development and undermines the fairness of the allocation. To ensure the
526 coordination of water quality among regions, the representative pollutant concentration
527 of the main reach in each sub-region after configuration should meet the relevant
528 environmental capacity requirements. If these requirements are not met, ~~then~~ the
529 objective function for this sub-region will call for a punishment, and more

530 environmentally friendly plans will be searched. After sewage with pollutants is
 531 transported from outlets to water bodies, advective transport, longitudinal dispersion
 532 and transverse mixing will occur. At the same time, physical, chemical and biological
 533 interactions will occur in the water body. To objectively describe the degradation of
 534 pollutants in water, it is necessary to use mathematical models to simulate physical
 535 dynamics. Due to the heterogeneity of pollutants entering water bodies and the
 536 uncertainty of hydrological processes, it is usually of little practical significance to
 537 calculate the change in river water capacity over time. A steady-state model is therefore
 538 used to calculate the water capacity of the target water body (Cetintas et al., 2010;
 539 Zhang et al., 2019). When water quality changes are studied at the annual scale and
 540 complete mixing is assumed, the following equation can be used to describe the water
 541 quality change, as shown in Eq. (33):

$$542 \quad \frac{Vdc}{dt} = Q(Ce - C) + Sc + r(c)V \quad (33)$$

543 where V (m^3) is the volume of water; Q (m^3/a) is the flow in and out of the system
 544 at equilibrium; Ce (g/m^3) is the contamination concentration in the inflow (g/m^3); C
 545 is the pollutant concentration; Sc -denotes other external pollution sources (m^3/a); and
 546 $r(c)$ is the reaction rate of pollutants in water ($g/m^3/a$). The above equation can be
 547 defined as the basic mass balance of a water body in a completely mixed system.
 548 Because the pollutants are evenly mixed in each small interval, the horizontal and
 549 vertical concentration gradients of pollutants can be neglected. Therefore, the model of

550 water quality in mixed rivers under steady-state design conditions is adopted (Yue et
551 al., 2021):

$$552 \quad W_c = 31.54 * [C_s \cdot (Q_p + Q_E + Q_S) - Q_p \cdot C_P] \quad (34)$$

553 where W_c represents the water environmental capacity (t/a); Q_p is the flow in the
554 reach (m^3/s); C_p is the pollutant concentration in the river (mg/L); Q_E is the sewage
555 discharge (m^3/s); Q_S is the total flow of nonpoint sources into the reach above the
556 control section (m^3/s); and C_s is the target concentration of river pollutants (mg/L).

557 The result calculated based on the total hydrological capacity standard is often
558 relatively large, which is generally referred to as nonconservative. To conform to real
559 conditions, the concept of a nonuniformity coefficient is introduced for correction:

$$560 \quad W_c' = \alpha \cdot W_c = 0.6 \cdot W_c \quad (35)$$

561 This coefficient is used to assign a punishment if the water quality exceeds the
562 relevant value in a given sub-region. Based on the coefficient value, the objective
563 functions and constraints are adjusted accordingly. Finally, the daily decision
564 alternatives for water allocation from water departments to water users are obtained at
565 the regional decision level.

566 **2.3.1 Objective function of the third layer**

567 **Regional objective function: Maximization-maximization of the comprehensive**
568 **benefits of each sub-region**

569
$$\max f_3(x) = \sum_{t=1}^T \sum_{i=1}^I \sum_{j=1}^{J_r} x_{ij}^t b_{ij} - \sum_{j=1}^{J_r} \left(D_j - \sum_{t=1}^T \sum_{i=1}^I x_{ij}^t \alpha_{ij} \right) \times \omega_j - P_r(r_{nz}) - G_r(x_{ij}^t) \times q \quad (36)$$

570
$$P_r(r_{nz}) = e_i \times \sum_{p=1}^{Pr} P_p^{pump} \times \nabla t_r + x_{ij}^t \delta_{ij} \psi_{ij} \omega_{ij} \quad (37)$$

571
$$\nabla t_r = \sum_{t=1}^T \sum_{n=1}^N \sum_{z=1}^{Z_r} \left\{ \left(l_{nz} + \left(r_{nz}^t \theta_{nz} / CAS_{nz} \right) \right) / \left(Q_{nz}^{\max} / CAS_{nz} \right) \right\} / 3600 \quad (38)$$

572
$$G_r(x_{ij}) = \sum_{z=1}^{Z_r} \sum_{u=1}^U \left(Q_{z,u,r}^{final} - Q_{z,u,r}^0 \right) \quad (39)$$

573 where b_{ij} (yuanChinese Yuan/m³) is benefit per unit of water supply for the j th user;

574 ω_j is the penalty coefficient per unit of water deficiency; $j=1,2,\dots,J_r$; J_r is the number

575 of water users in r th sub-region; $r=1,2,\dots,R$; $P_r(r_{nz})$ is the penalty function for cost in

576 the r th sub-region; e_i (yuanChinese Yuan/kW·h) is the unit electricity fee; P_p^{pump}

577 (kW·h) is the electrical power consumed by the p th pump at a pump house in each hour;

578 p ranges from 1 to Pr ; Pr is the total number of pumps in the r th sub-region; ∇t_r (h)

579 is the time required for water transfer to provide support for the inland river flow in the

580 r th sub-region; ω_{ij} (yuanChinese Yuan) denotes to the fee paid for sewage treatment;

581 l_{nz} (m) is the length of a water diversion pipe from reclaimed water source n to the z th

582 inland river; z ranges from 1 to Z_r ; Z_r denotes the number of inland rivers in the r th

583 sub-region; CAS_{nz} (m²) is the cross-sectional area of a pipe from the n th reclaimed

584 water source to the z th inland river; Q_{nz}^{\max} (m³) is the maximum overflow capacity of

585 the diversion pipe from the n th reclaimed water source to the z th inland river; $G_r(x_{ij})$

586 is the penalty function for substandard water quality in the r th sub-region; $Q_{z,u,r}^{final}$ (mg/L)

587 is the final concentration of the u th pollutant in the control section of the z th inland river

588 in the r th subregion after optimal configuration; $Q_{z,u,r}^0$ (mg/L) is the initial
589 concentration of the u th pollutant in the z th inland river in the r th sub-region; and q is
590 the penalty coefficient for substandard water quality in the r th sub-region. The number
591 of objective functions in this layer depends on the number of sub-regions divided in the
592 city, which is based on local conditions.

593 **2.3.2 Constraints of the third layer**

594 **Water quality constraints**

595 Mathematical models are often developed to help satisfy the water quality standards at
596 monitoring points (Zhang et al., 2019; Pourshahabi et al., 2020; Friesen et al., 2017).
597 However, for some cities with very few monitoring points, such approaches may lead
598 to good water quality in the monitored sections and poor water quality in other sections.
599 In these circumstances, the quality of water bodies in each sub-region of a city is not
600 simultaneously maintained. To maintain the water quality in all sub-regions of a city at
601 the desired target level, the water quality constraint in Eq. (40) is established:

$$602 \quad Q_{z,u,r}^{final} \leq Q_{z,u,r}^{control} \quad (40)$$

603 where $Q_{z,u,r}^{control}$ (mg/L) denotes the control standard for the u th pollutant in the control
604 section of the z th inland river in the r th sub-region.

605 **2.4 Model solution**

606 **2.4.1 Synergy degree evaluation**

607 Enhancing the understanding of the synergy among water allocation alternatives to
608 achieve broad coordination and equilibrium is crucial. The evaluation of the synergy of
609 a complex water resources system~~water system~~ is strongly related to multiple complex
610 interactions, such as the interactions among different processes, users, and regions.
611 However, these interactions have rarely been explicitly captured in prior evaluations of
612 water allocation. One of the key network metrics used in network analysis, connectivity,
613 is a promising measure of the degree of coordination among different objectives in
614 complex systems (Weitz et al., 2018). Connectivity reflects the connectedness of a
615 given link to all possible links in the network, and the strength of each link is weighted,
616 reflecting the number and strength of correlations (Felipe-Lucia et al., 2020). In this
617 study, connectivity is used to embody coordination in the context of synergy, as shown
618 in Eq. (26). Due to the limited supply of water resources, competition among different
619 objectives is unavoidable, and the objectives cannot be fully optimized to equal extents,
620 i.e.,—, an increase in one target output may decrease another output. Therefore,
621 equilibrium is integrated as another vital part of the synergy devoted to maintaining a
622 balance among the satisfaction of each goal in a system. The equilibrium based on the
623 principle of information entropy (Gao et al., 2013; Zivieri, 2022) is shown in Eq. (27).
624 Information entropy—is a measure of the uncertainty associated with a random variable

625 and is used to quantify the information contained in a message, usually in bits or
626 bits/symbols; furthermore, it has been widely used to represent the fairness or
627 equilibrium of a system (Chen et al., 2022; Zhao et al., 2022). When H is low, the level
628 of equilibrium in the system is high. This factor is also used to be compared with the
629 proposed index. By combining the quantification of coordination and equilibrium, the
630 synergy degree is appropriately determined (Eq. (29)). Notably, the total synergy index
631 (TSI) of a system is used for both generating candidate management alternatives in the
632 generation phases of PTSOA and performing assessments of the associated level of
633 synergy, as shown in Eqs. (41-44).

$$634 \quad SSI_{ob_i} = \frac{\sum_{j=1}^N c_{ij} \times (ob_i + ob_j)}{\sum_{j=1}^N (ob_i + ob_j)}, i \neq j \quad (41)$$

$$635 \quad H(S) = -\sum_{i=1}^N \frac{(1-u_{ob_i})}{N} \log \frac{(1-u_{ob_i})}{N} \quad (42)$$

$$636 \quad u_{ob_i} = \frac{ob_i - ob_{i,\min}}{ob_{i,\max} - ob_{i,\min}} \quad (43)$$

$$637 \quad TSI = \frac{\sum_{i=1}^N SSI_{ob_i}}{H(S)} \quad (44)$$

638 where SSI_{ob_i} is the connectivity of the i th object; c_{ij} is the Pearson correlation
639 between the i th object and j th object; ob_i and ob_j are the values of the i th and j th
640 objective functions, respectively; ~~TSI is the synergy index of the system;~~ $H(S)$ is
641 the overall equilibrium of all objects based on the principle of information entropy, and

642 it is abbreviated as H in the following; u_{ob_i} is the standardized value of the i th object;
643 N is the total number of objects in the system; $ob_{i,\min}$ and $ob_{i,\max}$ are the minimum
644 and maximum critical thresholds of the parameter ob_i , respectively. SSI is ranged from
645 $0 \sim N$, and higher SSI indicates higher connectivity of the objects in the system which
646 means they are easier to promote each other, and lower SSI indicates lower connectivity
647 which means the promotion is hard to realize and obstacles to each other may occur. H
648 is ranged from $0 \sim N * \log(1/N)$,— and lower H indicates better overall equilibrium and
649 higher H indicates worse overall equilibrium from objective perspective. TSI is greater
650 than 0. When a water resource system's TSI value is higher, the degree of synergy is
651 higher; conversely, when a water resource system's degree of synergy is lower, the TSI
652 value is lower. In our application, based on actual evaluation, we define when $TSI > 5$,
653 the degree of synergy is considered satisfactory. $5 > TSI \geq 3$ is defined as moderate and
654 $3 > TSI$ is defined as low. In our application, based on actual evaluation, the criteria as
655 divided. When $TSI \geq 5$, the degree of synergy is considered satisfactory. Additionally,
656 $5 > TSI \geq 3$ is moderate synergy degree and $3 > TSI$ is low degree.

657 **2.4.2 Hierarchical optimal algorithm design for the PTSAO-PTSOA**

658 **model**

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

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

- 669 I. In the first level, calculate the objective function (city level) values for the social,
670 economic and sustainable development components, and sort the results with
671 NSGA-III (Pourshahabi et al., 2020; Chen et al., 2017) to obtain each Pareto
672 front F_1, F_2, \dots, F_i .
- 673 II. Classify the Pareto fronts into K (K is determined based on the diversity of
674 policies) elements with the K-means algorithm (Liu et al., 2022), which is used
675 to partition a data set into K distinct and non-overlapping clusters. To perform
676 K-means clustering, we first specify the desired number of clusters K . Then, the
677 K-means algorithm is used to assign each observation to exactly one of the K
678 clusters.
- 679 III. Calculate the synergy degree of each individual in the front, and select the
680 solution that yields the greatest synergy in each cluster. K solutions are obtained
681 in the first layer.
- 682 IV. Use the selected K solutions in the first layer to establish constraints in the
683 second layer. Solve the objective function of the second layer with NSGA-III.
- 684 V. Calculate the synergy degree of each individual in the front and select the

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

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

691 VII. The synergy degree of each individual in the front is calculated, and the solution
692 that yields the greatest synergy in the third layer is selected. Three solutions are
693 obtained considering the synergy in the former two layers. Finally, the
694 synergistic configurations optimal for all stages in the whole process are
695 identified considering the synergy among decision levels, processes and time
696 scales.

697 **3. Application**

698 **3.1 Study area**

699 Yiwu city is selected as a case study to validate the applicability of the PTSOA model.

700 ~~Yiwu~~ This city is in Southeast China, located from $119^{\circ}49' E$ - $120^{\circ}17' E$ and $29^{\circ}02' 13$

701 $"N-29^{\circ}33' 40" N$ ~~and. The city~~ covers an area of 1105 km^2 . The area is characterized

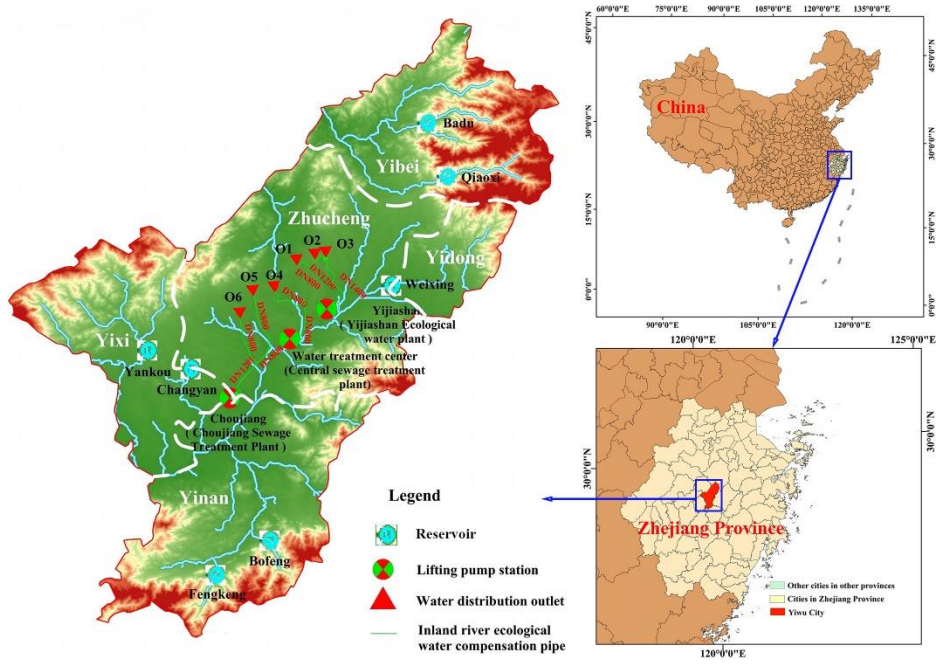
702 by a scarcity of water resources, and the conventional water supply is under severe

703 stress. The regional water consumption depends heavily on transported water and

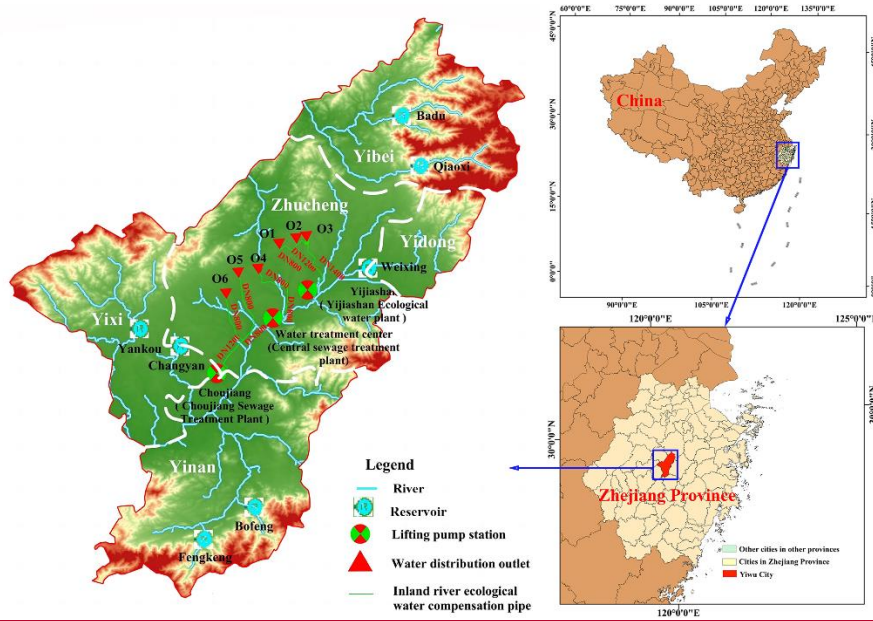
704 external water transfer. The per capita water resources is in total 622 m³, which is only
705 22.6% of the provincial average and 19.1% of the national average. Moreover, the
706 problem of water pollution has become a bottleneck constraint for the development of
707 Yiwu city. Therefore, it represents a typical water-scarce city with limited conventional
708 water. Notably, water quality in Yiwu has been subjected to significant environmental
709 stress because of the negative effects of wastewater discharge with the rapid
710 development of industry. The current water quality is poor, with Class *V*-~~water~~, and the
711 main pollutant concentrations exceed the corresponding standards (Zhejiang Natural
712 Resources and Statistical Yearbook on Environment, 2020). As shown in Fig. 3, the
713 Yiwu River crosses the city from northeast to southeast. Additionally, there are six
714 ecological water compensation outlets in six main tributaries in the Yiwu River. In Fig.
715 3, the white labels indicate five sub-regions in the city, the black labels near the
716 reservoirs are their names, the black labels named O1~O6 indicates the name of the
717 water distribution outlets and the labels near the lifting pump station are their names.

718

719



720



721

Fig. 3. Map of the study area

722

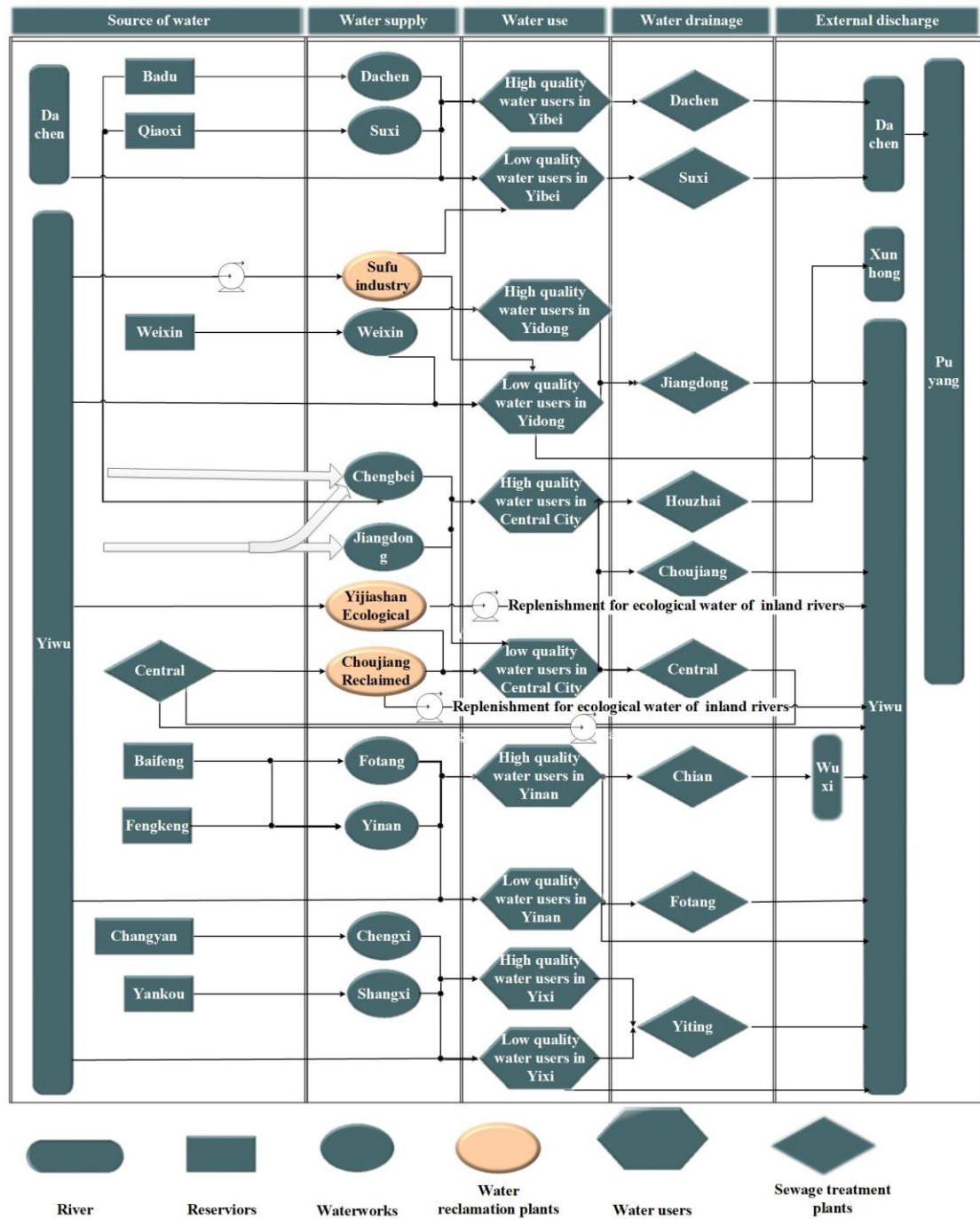
723 3.2 Generalization of the complex water resources system~~water-~~ 724 ~~system~~

725 An initial multi-source, complementary and mutually regulated system has been
726 developed for Yiwu, and this system spans the entire urban water cycle (water source-
727 water supply-water use-drainage-drainage collection-recycling and reuse). To apply the
728 optimal water allocation model to the complex real-world water system, all
729 stakeholders in the complex water resources system~~water-system~~ should be
730 schematized into a topological system, as shown in Fig. 4. The diagram comprises five
731 modules: water sources, water supply, water use, water drainage and external discharge
732 for all stakeholders.

733 The first module includes seven main reservoirs, two water diversion projects, the
734 Central Sewage Treatment Plant and the Yiwu River. The seven reservoirs and two
735 water diversion projects (as shown in Table 1) supply high-quality water. There are
736 complex connections between the first and second modules. For example, two
737 reservoirs supply water to one waterworks or one reservoir feeds two or three
738 waterworks simultaneously. The reservoirs also supply some of the agricultural and
739 ecological waters to subareas of the city. The Yiwu River, with a total length of 38.39
740 km and 21 first-class tributaries in the city, and the Central Sewage Treatment Plant, as
741 shown in Table 2, are low-quality water sources. ~~Additionally, excluding water from~~
742 ~~reservoirs, most agricultural irrigation water is supplied from surface water stored in~~

743 ~~hundreds of small reservoirs and mountain ponds. Since~~ There are no data available
744 for agricultural irrigation water, ~~which accounts for only a small portion of the total~~
745 ~~water demand in the area, and most agricultural irrigation water is supplied from surface~~
746 ~~water stored in hundreds of small reservoirs and mountain ponds (2020–Yiwu~~
747 ~~Ecological Environment Status Bulletin, 2020). So,~~ this water volume is ignored in the
748 model.

749 For the second module, high-quality water piped from reservoirs is transported to
750 nine urban and rural centralized waterworks (as shown in Table 2). The Yiwu River
751 distributes low-quality water to the Yijishan Ecological Water Plant and Sufu Industrial
752 Water Plant through the Yijishan and Baisha Water Pump Stations, respectively. The
753 water discharged at the Central Sewage Treatment Plant is transferred to the Choujiang
754 Industrial Water Plant. Based on the water supply project distribution and the economic
755 as well as social development levels⁵², Yiwu is divided into five districts, as shown in
756 Table 3: the Central District, Yidong District, Yibei District, Yinan District and Yixi
757 District. The third module comprises both high-quality water users (high-quality water
758 users consist of urban and rural domestic water users and some industrial water users
759 in the water supply network of urban and rural public water plants) and low-quality
760 water users (low-quality water users include other industrial water users, municipal
761 water users and ecological water replenishment for inland rivers) in each district. There
762 are nine sewage treatment plants in the fourth module (which focuses on the drainage
763 stage), as shown in Table 2. The unused water from sewage treatment plants is



767

768

Fig. 4. Schematic diagram of Yiwu city

769 **3.3 Parameter determination**

770 According to the flow duration curve of the annual natural inflow data for 51 years

771 (1963-2014), three years with exceedance probabilities of 50%, 75% and 90% are
 772 selected to represent normal (1984.1–1985.1, annual mean inflow: $1.33 \times 10^8 \text{ m}^3$), dry
 773 (2008.1–2009.1, annual mean inflow: $1.11 \times 10^8 \text{ m}^3$), and extremely dry (1971.1–
 774 1972.1, annual mean inflow: $0.63 \times 10^8 \text{ m}^3$) scenarios, respectively. In addition to
 775 inflow, the data used in the PTSOA model mainly include the data for the parameters
 776 in each layer. Water demand values were calculated using the Yiwu City Water
 777 Resources Comprehensive Plan 2020, as shown in Table 1.

778 **Table 1** Water demands of various regions in Yiwu in 2020 (10^4 m^3)

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

779

780 The water resources fees paid to the government are in total 0.3 ~~yuan~~Chinese
 781 Yuan/m³. The parameters of the reservoirs and external water division projects in Yiwu
 782 city are listed in Table 2.

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

Reservoirs & External sources	Water Fee yuan <u>(Chines</u> <u>e Yuan</u> /m ³)	Initial storage (10^4 m^3)	Dead storage (10^4 m^3)	Flood limit storage capacity (10^4 m^3)	Absolute storage capacity (10^4 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
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784

785 The Tennant method is applied to calculate the ecological water demand. In this
786 method, the relationship between the annual average discharge and habitat quality is
787 considered, and the percentage of the annual average natural runoff is used as the
788 recommended value of the ecological water demand for a given river channel.
789 According to the recommended values, the percentage of runoff required for the fish
790 spawning period from April to September is 30% and the percentage runoff in the
791 general water consumption period (October to March) is 10%.

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

$$794 \quad EP = E \times k \quad (45)$$

795 where EP (mm) is the evaporation of a reservoir; E (mm) is the observed evaporation;
796 and k is a reduction coefficient. According to observations, the difference of
797 this coefficient is quite slight within a small watershed (Zhao, 2014). Thus, k is
798 simplified to the same value 0.88 is the same for every reservoir and varies throughout
799 the year according to expert experience(Zhao, 2014) (Zhao, 2014). The prices of
800 conventional water and reclaimed water are 1.7 and 2.6 yuanChinese Yuan/m³,
801 respectively. In our application of the model, this precipitation component associated
802 with the water sources were calculated by the Thiessen polygon method (Liu et al.,
803 2014) based on the measured data of seven rainfall stations (Shi Caotou, Suxi, Yiwu,

804 Fotang, Baifeng, Fengkeng, Changfu) in the basin in normal (1984.1–1985.1), dry
805 (2008.1–2009.1), and extremely dry (1971.1–1972.1) scenarios, ~~relatively~~.

806 The monthly mean monitoring data for effluent pollutant concentrations and the
807 daily maximum processing capacities of sewage treatment plants were obtained from
808 the monitoring systems of the sewage treatment plants. For example, the concentrations
809 of COD, NH₃-N, TN, and TP in the sewage of the Jiangdong Sewage Treatment Plant
810 are 13.80 (mg/L), 0.22 (mg/L), 6.02 (mg/L), and 0.13 (mg/L), respectively. The daily
811 maximum processing capacity of Jiangdong Sewage Treatment Work is 12 (10⁴ t/d).
812 The effluent quality of sewage treatment works satisfies ~~the~~ Class A Standard used in
813 China. The maximum capacities of the Baisha pump station, Yijiashan pump station,
814 Choujiang pump station and water treatment centre pump station are 13 t/d, 13.5 t/d, 10
815 t/d, and 4.5 t/d, respectively.

816 Additionally, the environmental capacities of the six tributaries that are replenished
817 with ecological water are calculated according to Eqs. (33)-(35), and the results are
818 listed in Table 3. COD, TP and TN are major pollutants in Yiwu City (Yiwu Ecological
819 Environment Status Bulletin, 2020), and they are also major controlled pollutants of all
820 the monitoring sections. So, ~~these~~ ~~they~~ were selected as representative pollutants in
821 the tributaries to guarantee the water environmental quality of inland rivers. The water
822 quality goals for the tributaries must conform to ~~the~~ Class III standard according to GB
823 5749-2006 in China. The unit electricity price of pump stations in Zhejiang Province is
824 0.41 ~~yuan~~ Chinese Yuan/kW · h. GB50014-2006 (2014 edition) stipulates that the

825 comprehensive urban domestic sewage quota should be 80~90%, and the urban
826 comprehensive domestic sewage quota should be 90% in areas with extensive drainage
827 facilities. There are plenty of many influencing factors in the model, and the most
828 important ones among them are the value of water demand, the value of available water
829 and some key hyper-parameter. According to the “Yiwu Jinhua Water Resources
830 Bulletin 2020(2020)”, the urban comprehensive domestic sewage quota is set to 90%,
831 and the sewage treatment rate is set to 100%. The benefits per unit water supply for
832 different users in different subregions are determined from the Yiwu Water Price
833 Adjustment Plan (2020)-2020.

834

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

Name of tributary	Area (km ²)	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

836 **4. Results and discussion**

837 By solving the PTSOA model for Yiwu city, synergistic optimal water allocation results
838 for different layers (across different decision levels, water use sectors, and sub_regions)
839 are obtained under normal, dry and extremely dry conditions. Pareto sets are obtained
840 across 500 runs and 1000 iterations (in most cases) of the PTSOA model with the

841 proposed hierarchical optimization algorithm. If the feasible solutions could not be
842 found in some cases, the number of iteration would be increased. It took approximately
843 mean 34 h of CPU time on a computer with 32 GB memory and intel corei7@3.4 GHz
844 of CPU. Therefore, in this study, each iteration for a single trial solution takes 0.24 s of
845 CPU time on the computer with the named specifications.

846 **4.1 Results of the The ff first layer of the PTSOA model for** 847 **synergistic optimal water allocation**

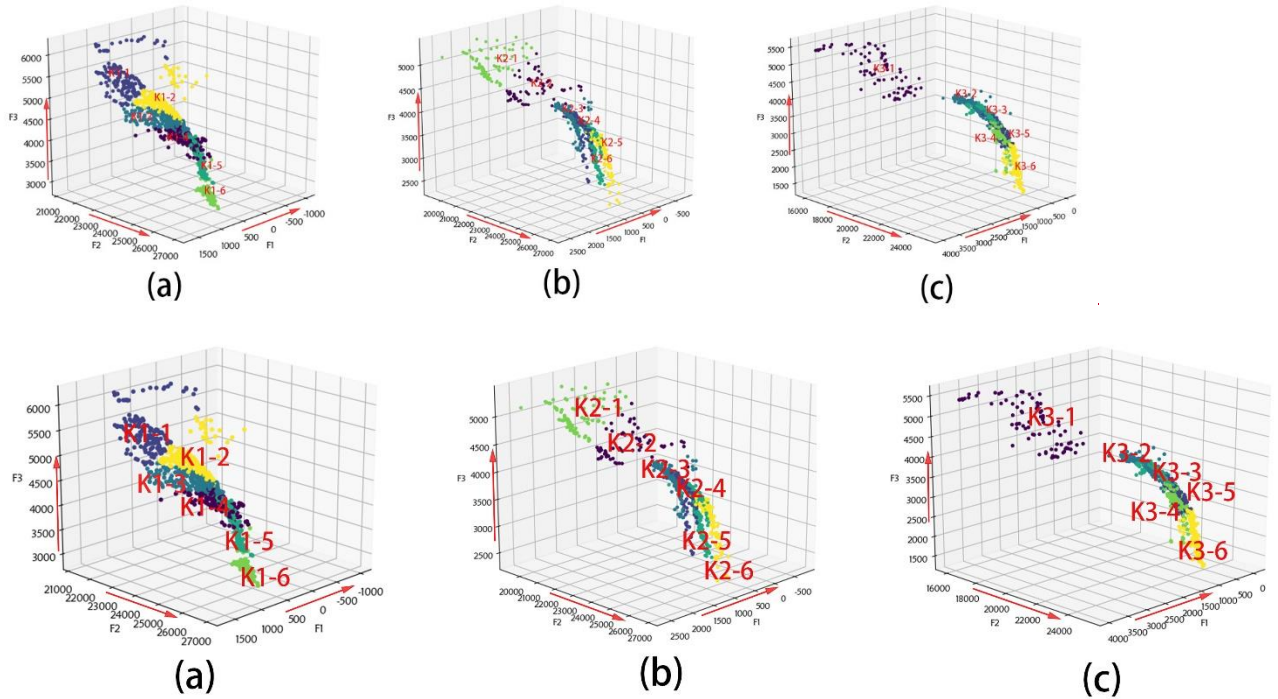
848 To demonstrate the relationship among conflicting objectives, sets of Pareto solutions
849 for the first layer under normal, dry and extremely dry conditions are shown in Fig. 5.

850 ~~The optimization using the Pareto concept allows the operator to choose an appropriate~~
851 ~~solution depending on the prevailing circumstances and analyse the trade-off among~~
852 ~~the conflicting objectives.~~ In each of the figures, the total water supply shortage, total

853 water supply benefit and total amount of water retained in reservoirs in Yiwu city are
854 plotted. The colour of the markers indicates the classification of the solutions of the K-
855 means method, as described in Section 2.4.2. All of the decision alternatives are
856 classified into six groups marked in different colours for broad-scale decision-making.

857 The names of the classes are marked in the figure in red (for example, K1-1 represents
858 the first class of solutions in the normal scenario, and K3-2 represents the second class
859 of solutions in the extremely dry scenario). The red arrows indicate optimization
860 directions. The ideal solution is located at the top-right corner (low total water supply

861 shortage, high total water supply benefit, and relatively high total amount of reserved
862 water in reservoirs) of the plot. The geometries of the trade-offs vary significantly
863 across the applications, as is expected given the different hydrological conditions.
864 Generally, the total water supply shortage and the total amount of water retained in
865 reservoirs show an inverse relationship. In contrast, the total water supply benefit shows
866 a direct and positive influence on the total water supply shortage. The water shortage
867 varies in the range of $-1.2 \times 10^6 \sim 0.8 \times 10^5$ m³, $-0.5 \times 10^5 \sim 2.0 \times 10^6$ m³, $0 \sim 3.5 \times 10^6$ m³ in
868 normal, dry and extremely dry scenarios respectively. The average water demand is
869 around 1.8×10^8 m³, and water shortage of the selected decision alternatives are all less
870 9×10^6 m³. So, The the water supply reliability of the selected decision alternatives is
871 greater than 95% under normal, dry and extremely dry conditions with the consideration
872 of water demand. The total amount of reserved water in reservoirs under normal
873 scenarios varies in the range of 2.91×10^7 m³ to 6.14×10^7 m³, which is much higher than
874 that under the extremely dry scenario, with a value of 1.44×10^7 m³ to 2.93×10^7 m³.
875 This finding demonstrates that the optimal allocation is able to reconcile the present
876 demand and future needs, even in extremely dry scenarios. The total water supply
877 shortage in all scenarios is less than 5% of the water demand, which indicates that the
878 guaranteed water supply is greater than 95%.



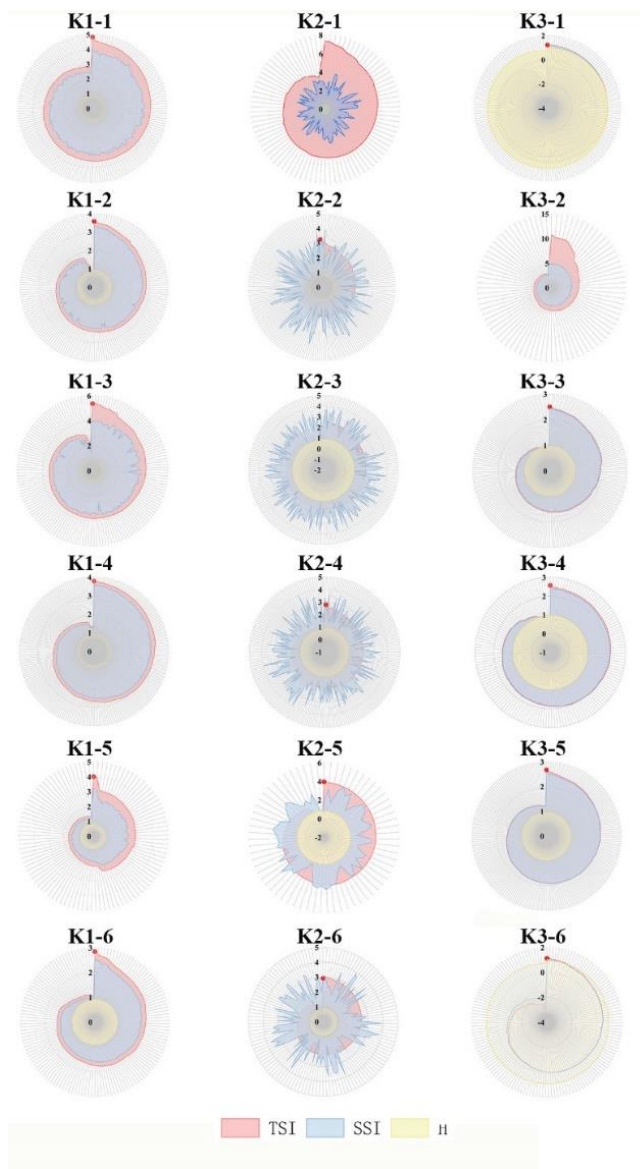
879
 880
 881 Fig. 5. Sets of Pareto solutions after 500 model simulations with the hierarchical
 882 optimal algorithm under (a) normal, (b) dry and (c) extremely dry scenarios. (F1: total
 883 water supply shortage, 10^4m^3 ; F2: total water supply benefit, 10^4 Chinese Yuan; F3:
 884 the total amount of reserved water in reservoirs, 10^4m^3 . The red arrow indicates the
 885 direction of optimization. K1-n, K2-n and K3-n represents the nth class of solutions
 886 in the normal, dry and extremely dry scenario separately, $n=1\sim 6$.)
 887 Pareto solutions after 500 model simulations with the hierarchical optimal algorithm
 888 under (a) normal, (b) dry and (c) extremely dry scenarios. The red arrow indicates the
 889 direction of optimization.

890
 891 We further present the *TSI* (total synergy index), *SSI* (total connectivity) and *H*
 892 (overall equilibrium) values for different classes characterized based on the optimal

893 PTSOA solutions under three scenarios, as shown in Fig. 6. In the PTSOA model, the
894 Pareto solutions with the best *TSI* values are input to the second layer for further
895 optimization. Thus, the red points in Fig. 6 represent the selected schemes for all classes.
896 We observe that the variation in the *TSI* is consistent with that in the *SSI* in some, but
897 not all cases. In some cases, differences are mainly caused by the influence of *H*, which
898 influences the optimal hydrological equilibrium, especially in dry conditions.
899 ~~Although normal conditions are most conducive to achieving equilibrium, the better *H*~~
900 ~~value in extremely dry conditions than in dry conditions seems nonintuitive. However,~~
901 ~~these~~ These results suggest that when water is very limited, equally limited water is
902 supplied to all users, thus enhancing the overall equilibrium. We note that the *SSI* value
903 is higher in the normal scenario than in the other two scenarios. We attribute this to
904 relatively abundant water being useful for stakeholders to achieve synergy due to the
905 reduced competition compared to other cases. The *TSI* values reach maximums of 5.36,
906 7.37 and 10.82 under normal, dry and extremely dry conditions, respectively.

907 In Fig.6, the value of *TSI* are significantly diverse among different scenarios as
908 well as different solutions. *H* is widely used to evaluate the equality of different
909 solutions (Gao et al., 2013; Li et al., 2022). As a contrast, the value of *H*, which is used
910 for comparison and construction of *TSI*, show slight differences among solutions and
911 even are the same in some classes. Therefore, it is difficult for decision makers to select
912 the best solution among all candidates if we only use *H* for evaluation and selection in
913 the decision process. Compared to *H*, *TSI* introduces *SSI* into evaluation and the

914 difference of coordination relationship between different schemes is distinguished by
 915 SSI. But H only pays attention to the equity among the stakeholders. So, TSI is more
 916 effective and validity than H in some extent. Additionally, ~~Since since~~ TSI is used
 917 to illustrate the synergy of allocation plans under certain conditions, the three kinds of
 918 TSI values are not comparable.



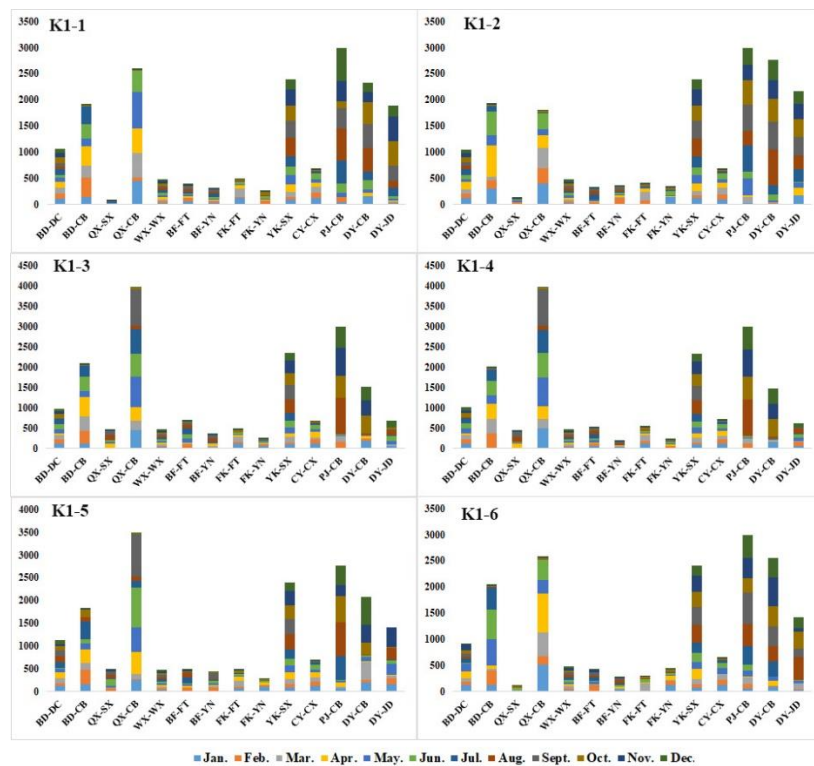
919
 920 Fig. 6. Comparison of TSI (total synergy index), SSI (total connectivity) and H
 921 (overall equilibrium) values among various Pareto solutions in different classes for

922 the (K1) normal, (K2) dry, and (K3) extremely dry scenarios. (K1-n, K2-n and K3-n
923 represents the nth class of solutions in the normal, dry and extremely dry scenario
924 separately, n=1~6.)

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

928 As an example, Fig. 7 provides the specific water supply decision alternatives for
929 the first layer that maximize synergy in each cluster under normal conditions. The water
930 allocation plans for the seven main reservoirs and two external water diversion projects
931 in every month of the configuration period are displayed. All reservoirs and water works
932 are represented by abbreviations based on their full names in Fig. 7. For example, QX-
933 CB is the label for the water supplied from Qiaoxi Reservoir to Chengbei Water Works.
934 The water volumes supplied by Qiaoxi Reservoir to Chengbei Water Works (ranging
935 from $1.78 \times 10^7 \text{ m}^3$ to $3950 \times 10^4 \text{ m}^3$) and from the Pujiang External Water Division
936 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
937 high in all clusters. This result is consistent with the fact that Chengbei Water Works is
938 one of the main conventional water sources for the central city area, a region that
939 accounts for more than 50% of the total water demand of Yiwu city. The water supplied
940 by the two external water diversion projects from August to December is higher than
941 that in other months. The mean monthly precipitation in these months is only 58-74%
942 of the mean annual precipitation in Yiwu, so more external water is supplied for

943 replenishment. Baifeng and Fengkeng Reservoirs supply similar volumes of water to
 944 their two connected waterworks.



945
 946 **Fig. 7. Water supply from each reservoir to connected water works in each month in**
 947 **the normal scenario 10^4 m^3**

948 **(K1-n represents the nth class of solutions in the normal scenario, n=1~6.)**

949 ~~Water supply from each reservoir to connected water works in each month in the~~
 950 ~~normal scenario (10^4 m^3)~~

951 **4.2 Results of the second layer of the PTSOA model for**
 952 **synergistic optimal water allocation**

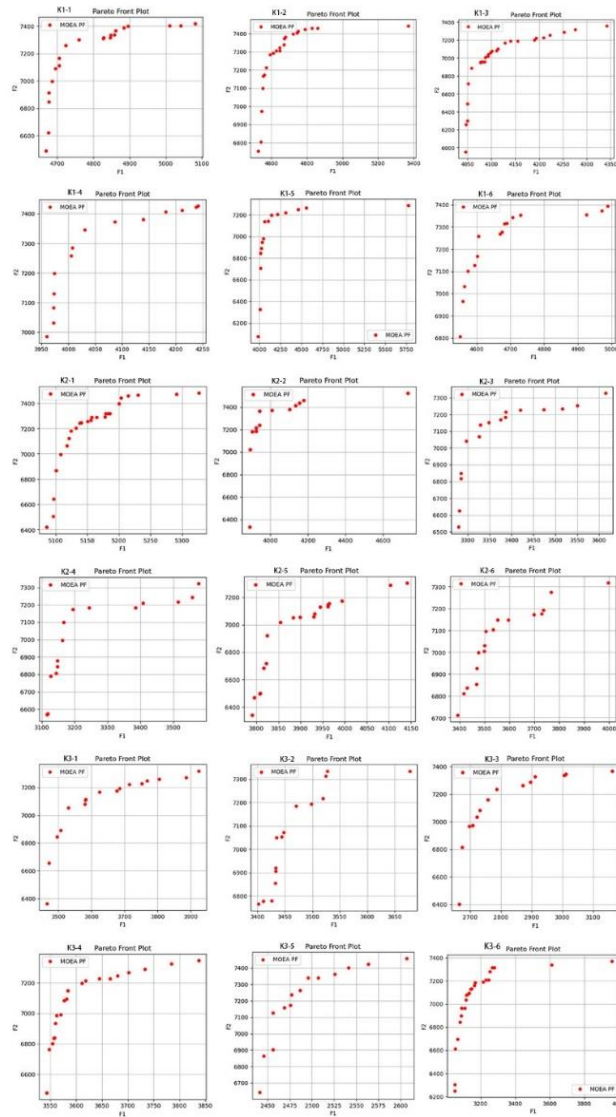
953 The 6×3 decision alternatives selected in the six clusters of the optimal first-layer results
 954 in the ~~normal, dry and extremely dry~~ scenarios are inputs into the second layer for

955 further optimization. As shown in Fig. 8, the total amount of water retained in water
956 works and the amount of unconventional water supplied show a negative correlation.
957 In the alternative generation phase of game bargaining between the two objectives, the
958 greater the total amount of water retained in water works is, the greater ~~the~~ amount of
959 unconventional water ~~supplied will be~~ will be supplied, which indicates that more
960 conventional water will be saved when more unconventional water is supplied.
961 Conversely, the amount of unconventional water supplied is affected by the total
962 amount of water retained in water works.

963 In the second layer, three alternatives in each scenario are selected as prior
964 conditions for further optimization. In addition to the two individual extrema of the two
965 objectives, the alternative that yields the best synergy is also identified, and it is similar
966 to that in the first layer. In the normal scenario, the *TSI* values are -0.90, -1.02 and -0.88
967 in the cases with the optimal conventional water supply, unconventional water supply
968 and synergy, respectively. The most synergistic approach includes ~~only~~ 7.08×10^4 m³
969 more conventional water retained than that in the conventional water supply cases and
970 ~~only~~ 9.72×10^4 m³ more than that in the optimal unconventional water supply case.
971 Therefore, not only is the best *TSI* value obtained, but the requirements of both
972 conventional and unconventional water supply departments are met. ~~The *TSI* of the~~
973 ~~most synergistic solution is the highest under dry conditions, with a value of -0.79.~~

974 Overall, the total amount of water retained in the water works ranges from 3.95×10^7
975 m³ to 5.75×10^7 m³, 3.12×10^7 m³ to 5.31×10^7 m³, and 2.43×10^7 m³ to 3.96×10^7 m³ for the

976 three types of conditions. The total amount of unconventional water supplied ranges
977 from $5.95 \times 10^7 \text{ m}^3$ to $7.48 \times 10^7 \text{ m}^3$, $6.34 \times 10^7 \text{ m}^3$ to $7.56 \times 10^7 \text{ m}^3$, and $6.28 \times 10^7 \text{ m}^3$ to
978 $7.37 \times 10^7 \text{ m}^3$ in the—_normal, dry and extremely dry scenarios, respectively. Moreover,
979 by selecting the solution with the highest TSI, $7.35 \times 10^7 \text{ m}^3$, $7.56 \times 10^7 \text{ m}^3$, and 7.37×10^7
980 m^3 of unconventional water would be supplied as an effective supplement to
981 conventional water. In the other word, conventional water would be saved by our
982 proposed model and index in the three scenarios. It is notable that the drier the
983 conditions are, the lower the amount of water retained in water works and the greater
984 the amount of unconventional water supplied. Thus, This-this approach is useful for
985 cities to mitigate the risk of drought. Additionally, based on the constraints regarding
986 the contaminants allowed to be discharged, more than 1272.21 t and 48.81 t of COD
987 and ammonia nitrogen emissions are avoided per year. ~~In other words, the balancing of~~
988 ~~the two objectives is beneficial for managers to determine an equilibrium solution that~~
989 ~~satisfies the relevant demand and successfully avoids surplus conventional or~~
990 ~~unconventional water supply in terms of sustainable development.~~



991
 992 Fig. 8. Pareto fronts of the second layer in the PTSOA model after 500 simulations
 993 with the hierarchical optimal algorithm in the normal, dry and extremely dry
 994 scenarios. (F1 represents the total amount of water retained in water works ,10⁴m³; F2
 995 represents the amount of unconventional water supplied,10⁴ m³. The direction of
 996 optimization is from the top-right corner to the bottom-left corner. K1-n, K2-n and
 997 K3-n represents the nth class of solutions in the normal, dry and extremely dry
 998 scenario separately respectively, n=1~6.)

999 Fig. 8. Pareto fronts of the second layer in the PTSOA model after 500 simulations

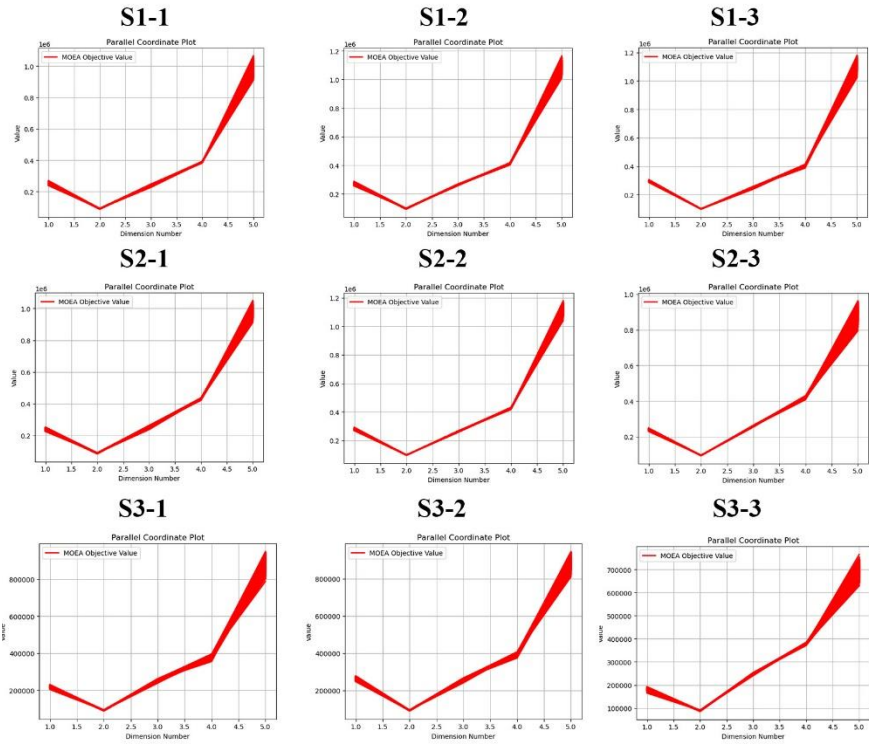
1000 with the hierarchical optimal algorithm in the normal, dry and extremely dry
1001 scenarios. F1 represents the total amount of water retained in water works ($10^4 \cdot \text{m}^3$),
1002 and F2 represents the amount of unconventional water supplied ($10^4 \cdot \text{m}^3$). The
1003 direction of optimization is from the top-right corner to the bottom-left corner.

1004 **4.3 Results of the Third layer of the PTSOA model for** 1005 **synergistic optimal water allocation**

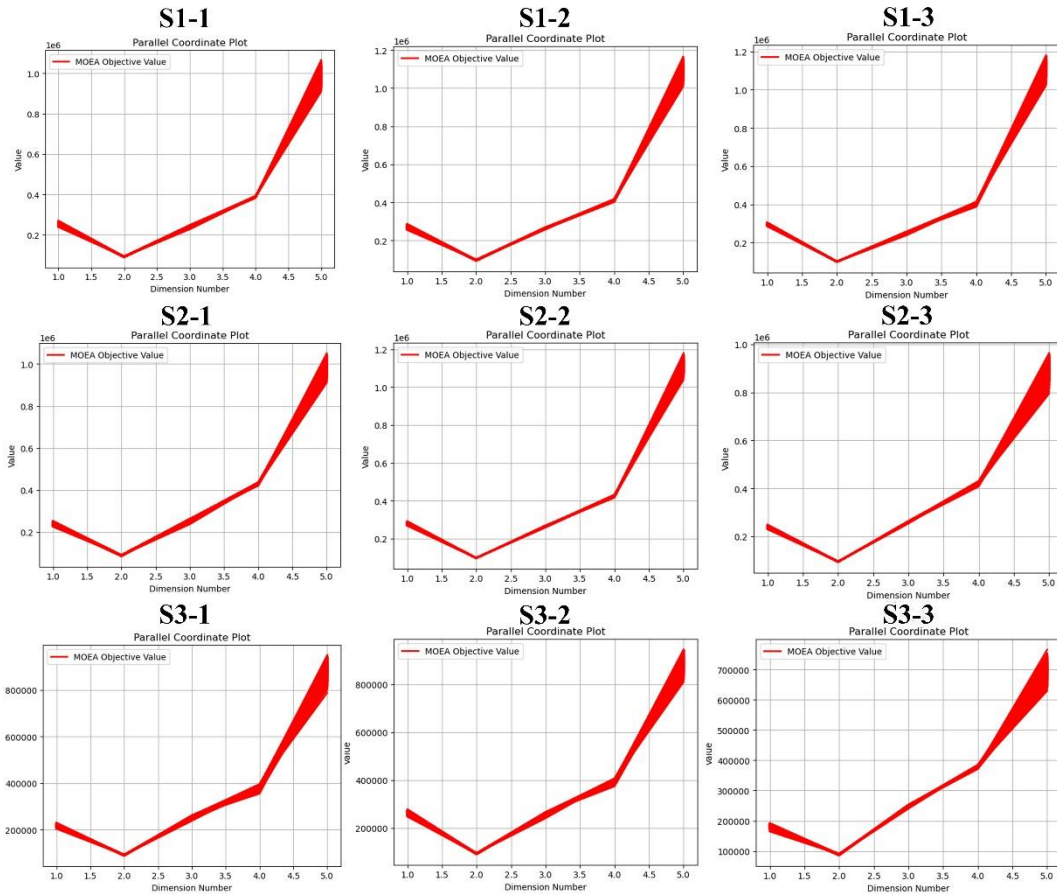
1006 After selecting the three scenarios that yield the best synergy and the two best objective
1007 functions for characterizing all Pareto fronts of the second layer in each scenario, these
1008 3×3 solutions are input to the third layer for further optimization. Fig. 9 shows the trade-
1009 offs among the five objectives in the third layer of the PTSOA model for the (S1) normal,
1010 (S2) dry, and (S3) extremely dry scenarios (these abbreviations are used to distinguish
1011 these results from those of the above two layers). The number following the ‘-’
1012 ‘ represents the selected solution from the second layer. For example, S1-1 represents
1013 the normal scenario with the minimum total amount of water retained in water works,
1014 S1-2 represents the normal scenario with the maximum unconventional water supply
1015 and S1-3 represents the normal scenario with the maximum synergy degree in the
1016 second layer. In each of these plots, the abscissa denotes the identifier for the objective
1017 functions, which ranges from 1 to 5, and the ordinate gives the objective values in the
1018 Pareto fronts (10^4 ~~yuan~~ Chinese Yuan). The five dimensions include the comprehensive
1019 benefits of the Yibei (1.0 dimension), Yidong (2.0 dimension), Yixi (3.0 dimension),

1020 Yinan (4.0 dimension) and central city (5.0 dimension) sub₂regions. As shown in the
1021 figure, the central city achieves the most comprehensive benefit among the five
1022 ~~cities~~sub₂regions. This is primarily attributed to the large population and intensive
1023 industry in this area. However, the benefits in the other four sub₂regions are also high
1024 compared to recent levels and those achieved with traditional allocation methods, as
1025 shown in Table 9. Interestingly, the comprehensive benefits in the sub₂regions are
1026 greater in the scenario with the maximum synergy degree under normal conditions than
1027 in the other two scenarios. ~~Technically, t~~The total comprehensive benefits in the five
1028 sub₂regions in this scenario are approximately $2.3 \times 10^8 \sim 5.1 \times 10^8$ ~~yuan~~Chinese Yuan
1029 higher than those in other cases, which indicates that the solution with the highest
1030 synergy degree in the second layer is the best choice for managers in normal years.
1031 ~~However, the various subregions obtain the greatest benefits when maximizing the~~
1032 ~~unconventional water supply in dry and extreme scenarios. This result indicates that~~
1033 ~~increasing the use of unconventional water in dry and extremely dry years would~~
1034 ~~significantly increase the potential benefits.~~

1035



1036



1037

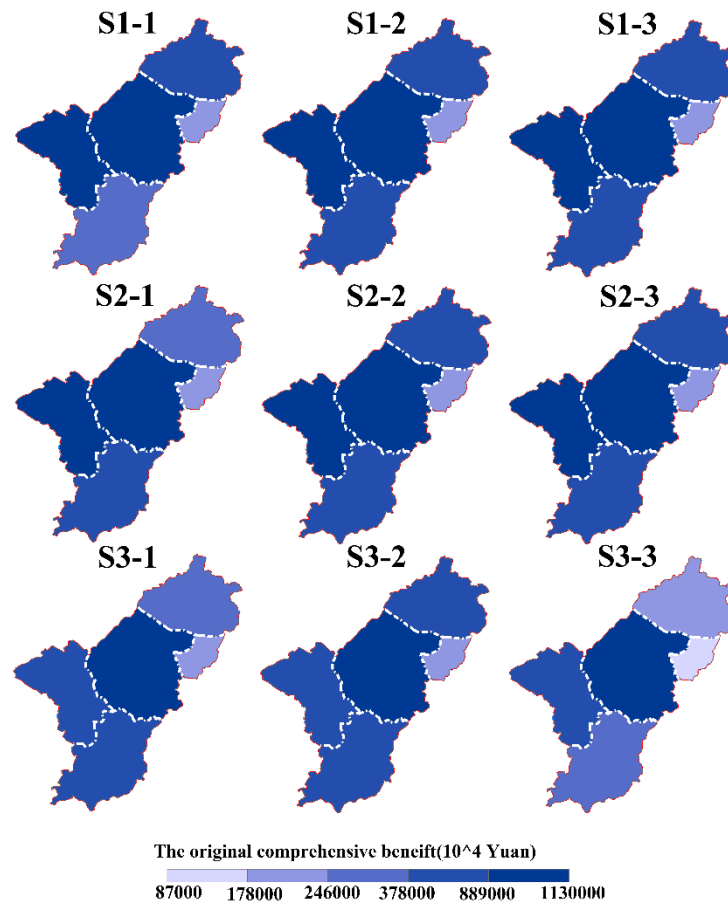
Fig. 9. Illustration of parallel-reference Pareto sets from the third layer in the

1038 PTSPOA model attained across all runs for the (S1) normal, (S2) dry, and (S3)
1039 extremely dry scenarios (S1-1 represents the normal scenario with the minimum total
1040 amount of water retained in water works, S1-2 represents the normal scenario with the
1041 maximum unconventional water supply and S1-3 represents the normal scenario with
1042 the maximum synergy degree in the second layer)

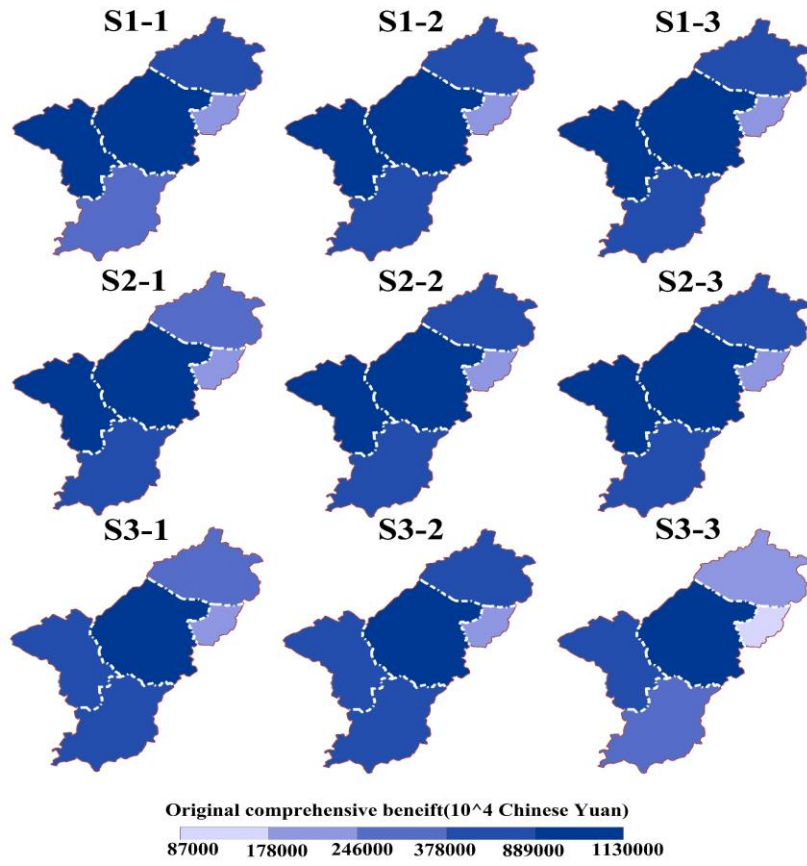
1043 ~~Fig. 9. Illustration of parallel-reference Pareto sets from the third layer in the~~
1044 ~~PTSPOA model attained across all runs for the (S1) normal, (S2) dry, and (S3)~~
1045 ~~extremely dry scenarios~~

1046
1047 Fig. 10 presents the optimal comprehensive benefit in each sub-region. In all
1048 scenarios, the central city is associated with the highest comprehensive benefit,
1049 followed by Yixi and Yinan, and the comprehensive benefit in Yidong is relatively low.
1050 This result may be related to Yidong which has this subregion having the smallest area
1051 (72.2 km²) and the smallest population (7.7×10⁴ people). ~~The comprehensive benefits~~
1052 ~~vary among different solutions and scenarios.~~ Among the three normal decision
1053 alternatives, F1, F2 and F5 are highest in S1-3, with values of 3.03×10⁹ yuanChinese
1054 Yuan, 9.90×10⁸ yuanChinese Yuan and 1.12×10¹⁰ yuanChinese Yuan, respectively. This
1055 indicates that considering the synergy degree could increase the comprehensive benefit
1056 in most sub-regions in the normal scenario. Among the alternatives in the dry and
1057 extremely dry scenarios (excluding F4 and F5), other objectives are highest in S2-2,
1058 with values of 2.84×10⁹ yuanChinese Yuan, 9.63×10⁸ yuanChinese Yuan and 2.67×10⁸

1059 yuanChinese Yuan, respectively. It suggests that maximizing the unconventional water
 1060 supply is beneficial for the system in dry conditions. Additionally, F4 is highest, with a
 1061 value of 2.29×10^9 yuanChinese Yuan, in S2-3 among the three solutions in the dry
 1062 scenario, and F5 is highest, with a value of 9.17×10^9 yuanChinese Yuan, in S3-1 in the
 1063 extremely dry scenario.



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Fig.10. Comprehensive benefit in five sub-regions after the regional collaborative allocation of water resources (S1 represents normal scenario, S2 represents dry scenario, and S3 represents extremely dry scenarios; S1-1 represents the normal scenario with the minimum total amount of water retained in water works, S1-2 represents the normal scenario with the maximum unconventional water supply and S1-3 represents the normal scenario with the maximum synergy degree in the second layer)

1074 ~~F10. Comprehensive benefit in each area after the regional-~~
1075 ~~collaborative allocation of water resources~~

1076 **4.4 Discussion**

1077 To assist policymakers in understanding the complex and systemic nature of complex
1078 water resources systems~~water systems~~ and reveal the dynamic interactions among
1079 objectives, network analysis and optimization ~~was~~were applied. Complex network
1080 analysis helps reveal the interactions among three layers with different dimensions. We
1081 determine the level of synergy in complicated water systems, identify the challenges
1082 and opportunities for sustainable development of water systems in cities with various
1083 subregions, and provide valuable insights and specific action priorities for these
1084 regions.~~By revealing the interactions among different objectives, we determine the~~
1085 ~~level of synergy in complicated water systems, identify the challenges and opportunities~~
1086 ~~for sustainable development of water systems in cities with various subregions, and~~
1087 ~~provide valuable insights and specific action priorities for these regions.~~ In the networks
1088 shown in Fig. 11, each node represents an individual objective (F1, F2, F3, F4, and F5
1089 represent the comprehensive benefits in Yibei, Yidong, Yixi, Yinan and the central city,
1090 respectively), and pairwise objectives that are significantly ($P < 0.05$) correlated are
1091 connected by a link, where the strength of each link is related to the Pearson correlation
1092 coefficient. The obtained networks with ~~5~~five nodes were weighted and undirected
1093 (directionality can be estimated only if the direction of causality is known). The size of

1094 the circles in the figure indicates the connectivity of each objective. We considered
1095 trade-offs (i.e., negative correlations wherein one objective improves while the other
1096 worsens) among the objectives. In most scenarios, F5 was the relatively dominant
1097 objective, signifying that other objectives disproportionately deteriorated as progress
1098 was made towards the benefit of the central city, as shown in Fig. 11. It is evident that
1099 the trade-offs are more balanced in the scenarios with the highest degrees of synergy
1100 (S1-3, S2-3, and S3-3), which indicates that the trade-offs and competitions among the
1101 objectives are alleviated when synergy is considered. The links show that the conflicts
1102 of interest between F4 and F5 in scenarios S1-1 and S2-2 are extremely notable,
1103 suggesting that the comprehensive benefits in Yinan and the central city correspond to
1104 strong negative interactions in these cases. The connectivity of most objectives was
1105 relatively low in the trade-off network in the extremely dry scenario, but F5 played a
1106 dominant role in terms of negative interactions among objectives, ~~although the~~
1107 ~~connectivity of F5 was lower than other connectivities in most normal and dry scenarios.~~
1108 Moreover, as the scenario varied from normal to extremely dry, the impact of individual
1109 regional targets on the whole system diminished.

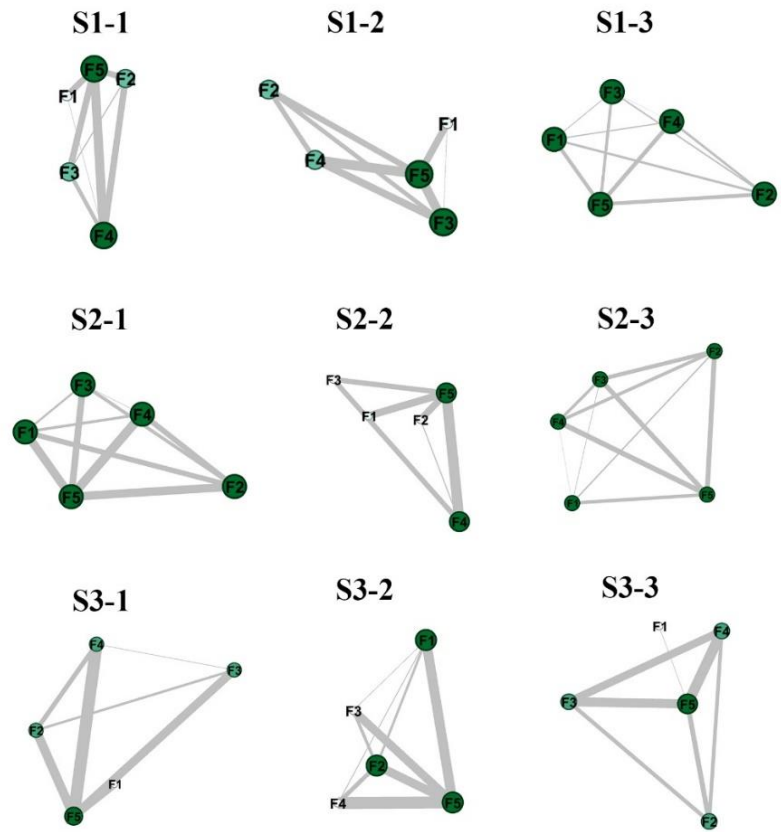


Fig. 11. Network analysis of the results of Layer 3

(The circles of F1, F2, F3, F4 and F5 represent the connectivity of each comprehensive benefit of Yibei, Yidong, Yixi, Yinan and the central city, respectively: S1 represents normal scenario, S2 represents dry scenario, and S3 represents extremely dry scenarios, S_{m-1} represents the normal scenario with the minimum total amount of water retained in water works, S_{m-2} represents the normal scenario with the maximum unconventional water supply and S_{m-3} represents the normal scenario with the maximum synergy degree in the second layer, $m=1\sim3$)

For comparison, we applied ~~five~~six widely used MOEAs, namely, NSGA-II,

1121 SPEA-II, ϵ -MOEA, IBEA, ~~and~~ MOEA/D and Borg MOEA, to solve cases with 3+2+5
1122 mathematical objectives (3 objectives in the first layer, 2 objectives in the second layer
1123 and 5 objectives in the third layer) with the same constraints given previously for Yiwu
1124 city under normal, dry and extremely dry conditions. The constraints and common
1125 parameters, such as the maximum number of model simulations and the simulated
1126 binary crossover (SBX) rate, are set to those used in the PTSOA model. However, it is
1127 difficult to determine feasible decision alternatives with MOEAs, even though the
1128 number of iterations is increased to 20000 (which is far beyond that considered in the
1129 previous modelling) because the complexity of the system overshadows the
1130 optimization capabilities of these traditional models. These results reconfirm the
1131 superiority, efficiency and decoupling capability of the proposed model for optimal
1132 allocation cases involving complex water resources systems~~complex water systems~~ with
1133 multiple stakeholders, multiple sources, multiple decision-makers and embodied reused
1134 systems. By embedding the targets into hierarchical layers, the excessive abandonment
1135 of some promising alternatives is avoided, and optimal allocation is progressively
1136 achieved. In general, the hierarchical structure of the PTSOA model can simulate
1137 complicated systems with multiple complex objectives and constraints.

1138 In addition, the ~~five~~ six MOEAs were used to solve the equations in the third layer
1139 of the PTSOA model, and the overall targets in the first layer were determined based
1140 on these solutions. The necessary parameters and hyper-parameters were consistent
1141 with those used in the third layer of the PTSOA model. Additionally, the benefits in the

1142 current case with no optimization calculated based on the actual water supply are given
1143 for comparison. The current situation was categorized as a normal scenario, and other
1144 models were established with the same conditions to facilitate further comparison and
1145 analysis. There were distinct decision alternatives generated by each model, and the
1146 relevant results are listed based on their value ranges. As shown in Table 4, although
1147 NSGA-II and ϵ -MOEA yield slightly higher F2 values than PTSOA and F3 generated
1148 by IBEA ($4.8 \times 10^8 \sim 7.2 \times 10^8$ ~~yuan~~ Chinese Yuan) is higher than obtained with PTSOA,
1149 PTSOA performs better than other models in most cases. The PTSOA model is shown
1150 to be the best model for obtaining comprehensive benefits for the sub-regions in Yiwu
1151 in the normal scenario, demonstrating that the PTSOA model offers advantages
1152 including identifying the best alternatives and achieving greater sub-regional benefits
1153 than the other models. The proposed model yields ~~a~~ $1.76 \times 10^9 \sim 15.67 \times 10^9$ ~~yuan~~ Chinese
1154 Yuan total comprehensive benefit improvement and can save approximately 3.2×10^7 -
1155 $\sim 4.7 \times 10^7$ (m^3) of conventional water compared to the current values. It is also evident
1156 that the proposed model yields the highest *TSI* values, reflecting the improvement
1157 achieved by considering the synergy of the system. In terms of the targets in the first
1158 layer, except MOEA/D, other traditional models fail to retain enough water (water
1159 requirements for living under extreme drought conditions of the next configuration
1160 period) in the reservoirs to meet future basic needs. For MOEA/D, although it generates
1161 a slightly higher total water supply benefit, with a value of $2.81 \times 10^8 \sim 3.12 \times 10^8$, the
1162 total water supply shortage and the total amount of reserved water in the reservoirs are

1163 worse than the amounts obtained with the proposed model. Borg MOEA, as an efficient
1164 and robust many-objective optimization tool, is characterized by its use of auto-
1165 adaptive multi-operator search and other adaptive features (Reed et al., 2013). The TSI
1166 value of Borg MOEA is lower than PTSOA. Therefore, in the TSI dimension, it is
1167 performance is slightly worse than the PTSOA model. However, it is noticed that the
1168 Borg MOEA algorithm could save around one-fifth of the computing time of the model
1169 (around 7h). In the future, it would be interesting to figure out how to couple the
1170 Borg MOEA algorithm with our PTSOA model in a more efficient and synergetic way.
1171 In this study, our main focus is to find the most synergetic solution through optimization
1172 in a complex system. Thus, PTSOA has accomplished superior performance level in
1173 this respect. PTSOA It trades some economic benefits for enhanced water supply
1174 reliability and sustainable development, resulting in a decrease in the water supply from
1175 conventional water plants.

1176 ~~However,~~ The consideration of reclaimed water in the proposed model effectively
1177 reduces the use of traditional water and improves the quality of the water environment
1178 by reducing sewage discharge, and other benefits are also achieved (such as meeting
1179 the quality standards for river water and guaranteeing that the ecological water demand
1180 of inland rivers is met). The results obtained by the PTSOA model may help guide both
1181 the government and general public. Our proposed model is superior to traditional
1182 models. It can not only optimize water resource utilization and secure water supplies
1183 but also enhance the synergy and environmental quality of water systems. Considering

1184 synergy across various time scales, the proposed model ensures the synergistic
 1185 allocation of water resources at yearly, monthly and daily scales while securing both
 1186 present and future water supplies.

1187 **Table 4** Comparison of the comprehensive benefits ~~in of~~ the five ~~regions-objectives~~
 1188 (F1, F2, F3, F4, and F5) and the *TSI* values in the current situation and obtained using
 1189 NSGA-II, SPEA-II, ϵ -MOEA, IBEA, MOEA/D, Borg MOEA and PTSOA in the
 1190 normal scenario

Comparison	Comprehensive benefits (10^9 yuan <u>Chinese Yuan</u>)					<i>TSI</i>
	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
ϵ -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
<u>Borg MOEA</u>	<u>2.95~3.56</u>	<u>0.80~0.98</u>	<u>1.19~2.23</u>	<u>3.11~3.82</u>	<u>12.88~13.90</u>	<u>-2.51~-1.67</u>
Current situation	2.05	0.83	2.49	3.11	9.87	-3.20
PTSOA	2.63~3.03	0.95~0.99	2.39~2.67	3.84~4.11	10.30~11.22	-1.66~-0.89

1191 5. Conclusions

1192 Applying optimal water allocation models to simultaneously enable economic benefits,
 1193 water preferences and environmental demands at different decision levels, time scales
 1194 and regions is a challenge. In this study, a new process-based three-layer synergistic
 1195 optimal allocation model (PTSOA) ~~is was~~ developed and applied to a real and complex
 1196 water allocation system ~~to figure it out~~. ~~The The objective functions model were was~~
 1197 divided into three layers to coordinate conflicts of interest among decision makers at

1198 different levels and time scales. Furthermore, the allocation of reclaimed water was
1199 embedded in the proposed model for synergistic optimal allocation of both conventional
1200 and unconventional water. A synergistic index based on network analysis was ~~put~~
1201 ~~forward introduced~~ to reduce competitions among different stakeholders and facilitate
1202 the positive effects of stakeholder interactions. A hierarchical optimal algorithm was
1203 designed to solve the ~~PTSAO-PTSOA~~ model.

1204 The proposed model was applied to a ~~representative typical~~ city in Southeast China
1205 with scarce water resources and a developed industry. Achieving the optimal allocation
1206 of water resources in this kind of ~~water-scar highly developed area city~~ offers a valuable
1207 reference for other counties in China. ~~The key findings of this study are as follows. Key~~
1208 ~~advantages of PTSOA findings can be concluded from these results, as follows.~~ First~~ly~~,
1209 the results demonstrated that the PTSOA model achieved synergistic allocation among
1210 hierarchical decision-makers across various time scales and in different regions,
1211 yielding the highest *TSI* (-1.66 to -0.89) among the ~~contrast~~ models ~~evaluated~~. Second~~ly~~,
1212 with a synergistic approach, a reasonable amount of conventional water is retained for
1213 future use in cases with potentially high risk, with volumes of 3.95×10^7 m³, 3.12×10^7
1214 m³, and 2.43×10^7 m³ retained in normal, dry and extremely dry scenarios, respectively.
1215 Moreover, 7.35×10^7 m³, 7.56×10^7 m³, and 7.37×10^7 m³ of conventional water ~~is~~ ~~can be~~
1216 saved in the three scenarios. Third~~ly~~, considering both reclaimed water and
1217 conventional water in the optimization process efficiently improves the quality of
1218 municipal water, and more than 1272.21 t/year and 48.81 t/year of COD and ammonia

1219 nitrogen emissions are mitigated compared to those in the current situation. Lastly,
1220 ~~Distinet~~ distinct from previous models, the proposed optimal model was implemented
1221 with the consideration of spatial dimensions, which are important but often neglected.
1222 The results show that spatial allocation yields an improvement of 4~95% for the
1223 comprehensive benefits in different sub-regions compared to the benefits achieved with
1224 traditional models, and the total comprehensive benefit increases by 1.76×10^9 -
1225 $\sim 15.67 \times 10^9$ ~~yuan~~ Chinese Yuan compared to that in the current situation. ~~The synergy~~
1226 ~~index established based on network analysis is used to alleviate the competition among~~
1227 ~~regions and facilitate water supply improvements.~~

1228 These results and conclusions provide valuable references for the evaluations of other
1229 complicated water allocation systems. The optimal allocation scheme ~~is~~ can be
1230 determined for a complex water resources system ~~complex water system~~ upon
1231 consideration of stakeholder synergy and various hierarchical decision levels, time
1232 scales and regions. More in-depth studies of synergistic optimal water allocation are
1233 needed in the future.

1234

1235 *Data availability.* The data used to support the findings of this study are available from
1236 the corresponding author upon request.

1237

1238 *Author contributions.* JL and YPX designed all the experiments. JL and WZ collected
1239 and preprocessed the data. JL and WZ conducted all the experiments and analysed the

1240 results. JL wrote the first draft of the manuscript with contributions from SW and SC.

1241 YPX supervised the study and edited the manuscript.

1242

1243 *Competing interests.* The authors declare that they have no conflict of interest.

1244

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1260

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