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

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Abstract

The increasing water demand due to human activities has aggravated water scarcity, and conflicts among stakeholders have increased the risk of unsustainable development. Ignoring the effects of trade-offs leads to misguided policy recommendations. This study highlights the concept of synergy among different aspects of water allocation process. A process-based three-layer synergistic optimal allocation (PTSOA) model is established to integrate the interests of stakeholders across sub-regions, decision levels 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, $2.43\times10^7\sim3.95\times10^7$ m^3 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

1. Introduction

28 Water scarcity has become one of the major impediments to sustainable development

29 of cities (Yue et al., 2020). Emerging water scarcity concerns in cities are associated

30 with limited available water, severe water pollution and relentlessly growing demand

31 for water as driven by industrial growth, population growth and higher living standards;

32 these factors have leaded to intense competition for freshwater among stakeholders of

33 interest (Dai et al., 2018; Wu et al., 2023). However, the heterogeneous distribution of

34 water resources at both spatial and temporal scales is common and results in water

35 shortage risks and conflicts, which often require the optimization of water resource

36 allocation (Friesen et al. 2017). Moreover, some satisfactory alternatives for individual

37 stakeholders may result in negative externalities on others. Nowadays, the water

38 resources system become more and more complex, and often has multiple sources and

39 users as well as water reused infrastructure. This kind of water resources system is

40 called complex system. Therefore, it is critical to develop a synergistic optimal

41 allocation model to alleviate conflicts and ensure the security, efficiency, equality, eco-

42 environmental sustainability, and sustainable development of complex water resources

43 systems simultaneously.

44 As equitable access to water resources is closely related to social stability, several

45 qualitative and indirect methods have been developed to assess water allocation

46 equality (D'Exelle et al. 2012). In cases with limited water resources, more water would

47 be allocated to users with better economic conditions to achieve more economic

48 benefits. Thus, stakeholders with poor economic status are ignored, resulting in

49 imbalanced development. Consequently, actions are often needed by local government

50 managers to avoid such situations. The Gini coefficient has been widely used to

51 evaluate equality and enhance the optimization of water allocation in water use sectors

52 (Xu et al. 2019; Hu et al. 2016; D'Exelle et al. 2012). However, it is unable to reflect

53 the dynamic interactions among objectives, i.e., how objectives interact with each other

54 and impact the equity of a system in cases with diverse alternative decisions. In the

55 perspective of coordinated allocation, multiple goals are simultaneously considered to

56 avoid negative effects as much as possible. Therefore, in addition to equity,

57 coordination should be considered in water allocation systems, and these two concepts

58 can be combined to promote systemic synergy. By identifying the dynamic interactions

59 among objectives, the internal mechanisms of a water system can be clarified, and

60 synergy can be achieved in cases with different potential decisions. It is also helpful to

61 identify the hurdles and opportunities associated with sustainable development for

62 cities and to establish specific action priorities for cities based on a comprehensive

63 understanding of the interactions among objectives. To address this knowledge gap, a

64 correlational network approach is applied in this study, and a synergy degree index is

65 presented to consider both equity and coordination of water systems. Moreover,

66 systemic analysis is used to assess the level of coordination of complex objective

67 interactions in city water systems.

68   Network analysis, which has been widely used in studies of complex systems (Ball

69 et al., 2000; Saavedra et al., 2011; Bond, 2017), is a holistic approach for exploring the

70 characteristics of interactions among objectives. It provides clear visualization and

71 conceptualization of the interactions among variables to fully characterize those

72 interactions (Swain and Ranganathan, 2021). An array of network metrics (for example,

73 degree centrality, betweenness centrality, eigenvector centrality, closeness centrality,

74 and community) can be applied to quantify the importance of objectives or targets in an

75 interaction network (Zhou and Moinuddin, 2017) and reveal the strongly connected

76 pairs of goals or targets in the network (Allen et al., 2019). A key network metric in

77 such analysis is connectivity, which reflects the degree of coordination among different

78 objectives in a system; in synergy networks, high connectivity indicates that many

79 objectives can be achieved simultaneously and that the negative effects of interactions

80 are mild (Wu et al., 2022). Thus, to facilitate the discovery of high-quality decision

81   alternatives, alleviate negative conflicts among multiple utilities and inform decision

82   making, a synergy degree evaluation index is established and applied to the network

83   analysis of this study.

84   Due to negative externalities of individual decisions, conflicts occur not only

85   across different users or objectives but also across hierarchical decision levels. Water

86   use contradictions and inconsistent decision making by multiple managers inevitably

87   results in trade-offs, including positive and negative water resource feedback in cases

88   with limited water availability (Wang et al., 2022). In practice, district administrators

89   allocate water to each sector in each sub-region, and sub-region managers then make

90   decisions based on the allocated amount of water resources (Safari et al., 2014). Since

91   each decision maker places emphasis on different targets, feedback and coordination

92   among different decision makers are of great importance. Therefore, synergistic

93   hierarchical water allocation that achieves coordination among different decision

94   makers is imperative to avoid conflicts, save water and maintain social stability.

95   To address these hierarchical problems, bi-level programming (BLP) has been

96   widely used, wherein objectives at two hierarchical levels, namely, an upper level and

97   a lower level, are co-optimized (Zhang and Vesselinov, 2016; Jin et al., 2018). The

98   upper-level decision may be affected by actions of the lower-level decision makers

99   (Arora and Gupta, 2009). Yue et al. (2020) formulated a bi-level programming (BLP)

100   framework to gain insight into the whole water allocation process with district

101   administrators and sub-regional farmers. Li et al. (2022) built a two-level model with

102 the overall interests of system managers at the top and the individual interests of water

103 supply departments at the bottom. The multi-level programming problem (MLPP) was

104 derived from the bi-level programming problem (BLPP) and is more applicable to real

105 world practices (Baky, 2014). However, limited studies have explored applying MLPP

106 (more than two levels) for water resource allocation, especially in cases with

107 unconventional water supplies.

108   To satisfy both long-term and short-term water needs and avoid unnecessary

109 administration costs and water resource use caused by lack of coordination among

110 different allocation steps, temporally synergistic allocation and optimization are needed

111 (Haguma and Leconte, 2018). In annual water resource planning, the monthly

112 variability of hydrologic regimes and non-stationarity of the daily water demand must

113 be considered. As an alternative example of synergistic allocation at different time steps,

114 Vicuna et al. (2010) used a monthly nonlinear programming model and an annual

115 sampling stochastic dynamic programming (SSDP) model to establish a monthly

116 operating policy. Haguma et al. (2015) proposed an optimization approach with two

117 separate time steps following the nested model approach. Haguma and Leconte (2018)

118 constructed deterministic and stochastic optimization models with two time steps (intra-

119 annual and inter-annual) and two levels of inflow variability: seasonal and inter-annual.

120 The purpose of their short-time-step model was to derive aggregate performance

121 functions associated with potential long-time-step decisions in these studies. However,

122 short-term benefits should not be overlooked due to their appreciable impact on long-

123   term effects. Accordingly, synergistic allocation that enhances both long-term and

124   short-term allocations is of great importance for water resource management in cities.

125   However, optimizing the structure of a model to achieve maximized benefits and

126   balancing the trade-offs among time steps are tasks that have rarely been studied. The

127   synergy among different time steps is addressed with a new innovative framework and

128   a corresponding algorithm in our study.

129   Most of the abovementioned traditional models are based on a benefit-oriented

130   mechanism, which leads to a high degree of satisfaction in high-benefit regions and

131   large water shortages in other regions. The existence of high-benefit regions in a city

132   during the allocation process often exacerbates regional disparities and heterogeneous

133   development. Moreover, spatial factors influence allocation results, especially when

134   there is spatial hierarchical heterogeneity among water resource allocation elements (Li

135   et al., 2022). It is thus appropriate to conceptualize water allocation problems in a

136   multistage framework that fully considers the interests of not only the regional authority

137   but also sub-regional managers (Yao et al., 2019). Hence, the synergy among sub-

138   regions must be considered to optimally allocate water resources. Ideally, the benefits

139   of all sub-regions should be integrated equally in the model, and the weights of hyper-

140   parameters should be adjusted to best support flexible policies.

141   The optimal allocation of conventional and unconventional water resources also

142   significantly impacts water security and aquatic ecosystems. The reuse of reclaimed

143   water is beneficial for alleviating high water supply pressure on conventional water

144 resources and reducing the emission of pollutants. To effectively integrate conventional

145 and unconventional water resources, Yang et al. (2008) and Han et al. (2008) introduced

146 unconventional water resources as critical factors in water management. Avni et al.

147 (2013) investigated the mixing of unconventional water resources with other

148 conventional water sources to meet the magnesium requirements for drinking water and

149 irrigation water. Yu et al. (2017) developed a cost–benefit analysis-based utilization

150 model for externally transferred water and desalinated water. The allocation of both

151 conventional and unconventional water has been widely studied, but there remains a

152 lack of methods to guide the synergistic allocation of conventional and unconventional

153 water resources and embed reclaimed water supply systems in allocation schemes. The

154 overexploitation of conventional water resources is not conducive to sustainable

155 development, while extensive use of unconventional water could ultimately result in

156 high economic burden. To synergistically integrate conventional and unconventional

157 water resources and guide the coordinated allocation of these two types of water

158 resources, corresponding mechanisms must be implemented. As a result, our study aims

159 to couple the allocation of conventional water resources and unconventional water

160 resources to establish synergistic solutions.

161   In summary, as insufficient water supplies and increasing water demands intensify

162 competition for water resources and lead to conflicts among different stakeholders in

163 different dimensions, water allocation must be optimized in cities and regions to

164 achieve synergistic decision-making at various levels and time steps considering the

165 value of reclaimed water. Therefore, a new process-based three-layer synergistic

166 optimal allocation (PTSOA) model is developed here to generate numerous candidates

167 or Pareto solutions and identify several desirable decision alternatives. The synergy of

168 time and space optimization is achieved in the new model to avoid waste and promote

169 balanced spatial development. Furthermore, in the PTSOA model, reclaimed water is

170 used to replenish conventional water resources in water-scarce areas.

171   The remainder of this paper is organized as follows. The mathematical model is

172 formulated in Section 2. Section 3 gives a numerical example for Yiwu city to

173 demonstrate the effectiveness and efficiency of the proposed methods. The results are

174 shown in Section 4; different water allocation strategies under varying inflow

175 conditions are explored, and policy implications are discussed. Section 5 presents

176 conclusions.

177 2. Modelling

178 With water resources becoming increasingly scarce, multi-dimensional synergistic

179 optimal allocation in a hierarchical system is crucial for ensuring sustainable

180 development in water-scarce cities. There are three dimensions of synergy in the

181 established allocation model, as shown in Fig. 1: process synergy, decision-level

182 synergy and time-scale synergy. The synergy of the process refers to synergistic water

183 allocation among the three stages throughout the whole allocation process to reduce

184 waste in bridging processes, which has rarely been considered. In the three stages, first,

185   the original water is released from reservoirs or diverted from external water transfer

186   projects to water works; then, the water stored in water works infrastructure is supplied

187   to different departments that need different types of water, including both conventional

188   and reclaimed water. Finally, water is supplied to different users. Decision-level

189   synergy refers to synergistic water allocation considering the interests of decision

190   makers at different levels, namely, the city, water department and regional levels, to

191   coordinate solutions and avoid conflicts among decision makers. The city level

192   represents the overall interests of a city from the perspective of government, the water

193   supply department level represents the interests of water supply corporations, and the

194   regional level focuses on the comprehensive benefits of each region in the city and

195   mitigate development imbalance among regions. Optimal decision making at the

196   department level is constrained by the allocation results at the city level, and so on, and

197   the final solution should satisfy the needs of decision makers across all levels. The time

198   scale synergy involves the coordination of the daily configuration goal with the monthly

199   goal, the monthly goal with the yearly goal, and so on. Synergistic temporal allocation

200   can largely alleviate time conflicts during configuration operations, ensuring that all

201   configuration periods serve the same final configuration objectives to save water

202   resources and improve efficiency. However, time scale synergy mainly depends on

203   artificial operations rather than automated intelligent operations in practice. In-depth

204   exploration has yet to be demonstrated. Consequently, the PTSOA model is constructed

205   here to fully consider these three dimensionalities of synergy. The dimensionalities are

206   coupled in this model to achieve the efficient maximization of comprehensive benefits

207   at all levels under the premise of saving water resources. In Fig. 1, the grey boxes

208   indicate the three different allocation dimensions, the green boxes indicate the three

209   different decision levels coupled with spatial scales, the bright yellow boxes indicate

210   every key nodes in the whole allocation process and the buff boxes indicate nested time

211   scale.

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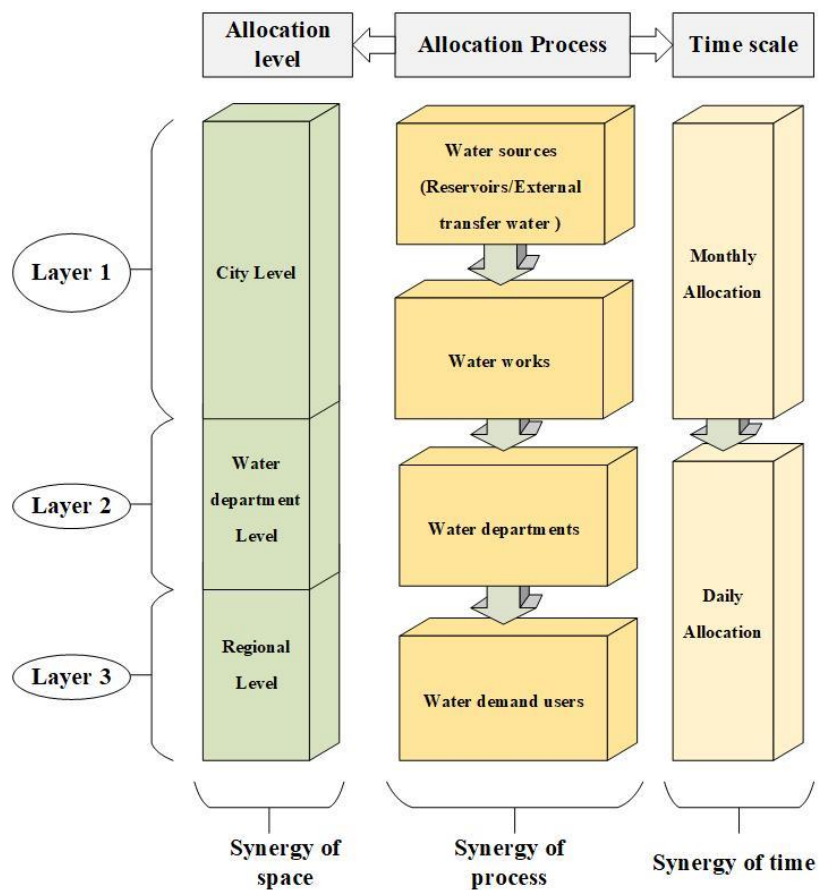
214   **Fig. 1. Conceptual map of the PTSOA model**

215

216   In water-scarce cities, using reclaimed water as an alternative water source is

217 proved to be useful to efficiently improve the environment by reducing sewage

218 discharge. The quality of inland tributaries has deteriorated in many water-scarce cities

219 due to limited consideration of the water environment and the large-scale emission of

220 pollutants. Transferring reclaimed water and main river water to urban inland tributaries

221 for ecological water replenishment is a promising approach for improving the quality

222 of urban water environments and areas with water shortages. However, there has been

223 a lack of studies on the integration of reclaimed water reuse systems and inland water

224 distribution systems in allocation modelling. Therefore, in addition to saving water

225 resources and improving efficiency through multi-dimensional synergistic allocation,

226 the model encompasses reclaimed water reuse systems and ecological water

227 distribution systems for inland tributaries.

228 Finally, the PTSOA model is constructed to solve the multi-dimensional synergistic

229 allocation problem involving complex water resource networks that couple reclaimed

230 water reuse systems and inland ecological water distribution systems with multiple

231 sources, processes and regions to guarantee the sustainable development of water-

232 scarce cities. To select the most synergistic solution of the PTSOA model, a new

233 evaluation index named the synergy index (TSI) is proposed to assess the synergy

234 degree of different decision alternatives. System entropy (H(S)) can describe the

235 evolution direction of a water resource system and was used to promote the

236 coordination of water supply departments in a water resource allocation system(Li et

237 al., 2022). So, it is used for comparison to evaluate the validity of this proposed index.

238   Furthermore, the network analysis method is applied for the first time to analyse

239   dynamic interactions in water optimal allocation. This method visually depicts the

240   dynamic interactions and conflicts among different subareas in a city, which is helpful

241   for system managers to realize how the water allocation scheme in one region

242   influences that of other areas; consequently, more reasonable and flexible measures are

243   established based on dynamic regional development targets. The detailed framework

244   developed in this study is shown in Fig. 2. In this figure, there are three layers in the

245   framework and each layer has two parts: multi-objective optimal water resources

246   allocation and collaborative water resources allocation for objectives. In the multi-

247   objective optimal water resources allocation, sub-layers contain key nodes in the

248   allocation process and relevant objectives and constraints. In the collaborative water

249   resources allocation for objectives, sub-layers contain optimization algorithm and

250   decision selection method.

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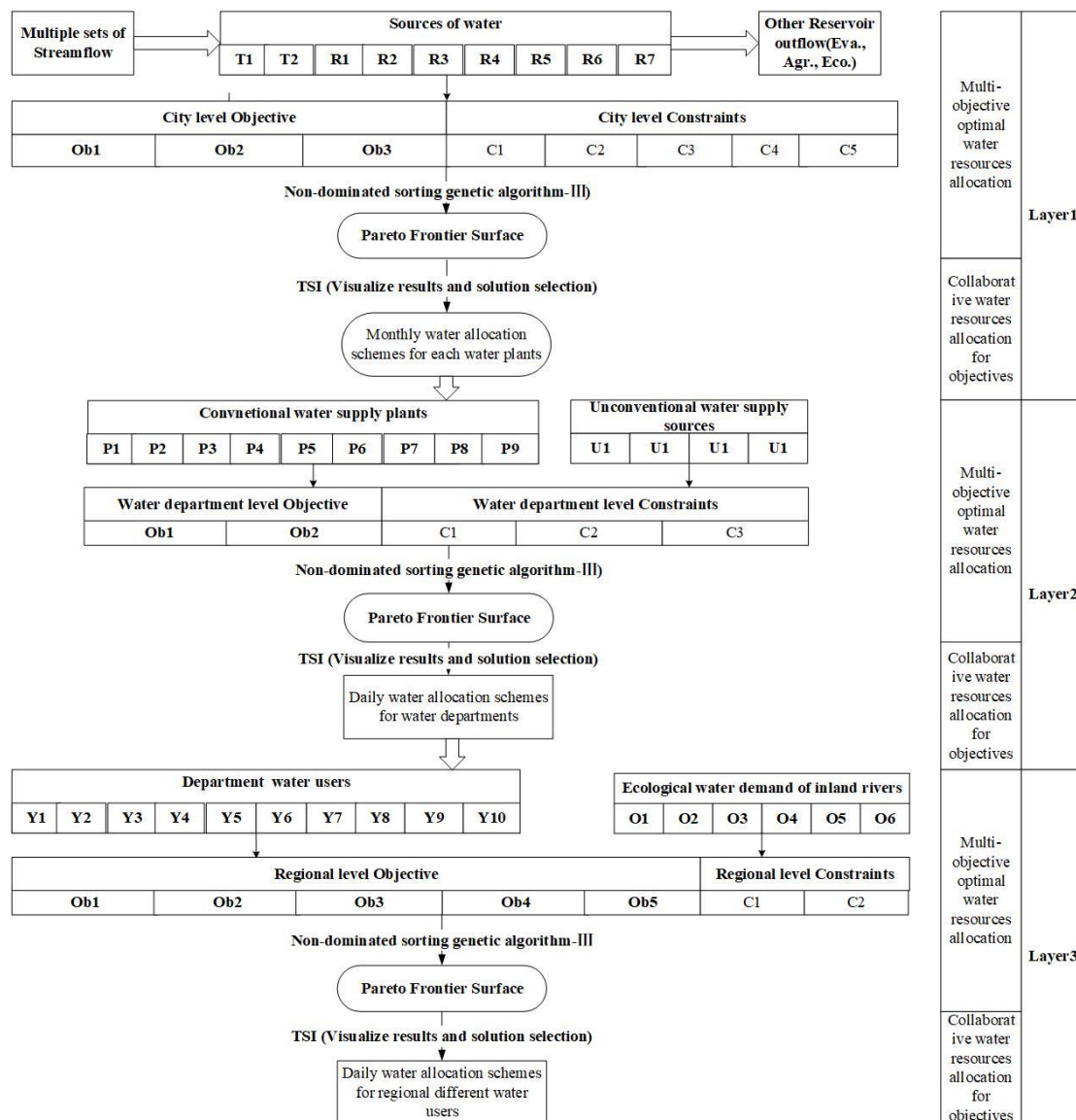
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253
Fig. 2. Framework of the PTSOA model

2.1 First layer of the PTSOA decision-making process

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

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

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

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

259 satisfy the overall development goals of the city, the first-layer processes involve city-

260 level decision-making. The city manager focuses on the overall goal of the complex

261 water resources system in the city, which is the first and most important phase of the

262 decision-making process. The established allocation scheme highly influences decision

263 makers at other levels, and optimal allocation schemes at other levels must align with

264 this overall goal. Additionally, since water resource planning in most Chinese cities is

265 based on an annual planning period and monthly planning unit, the time step of the first

266 layer is set as months. Finally, the monthly decision alternatives for the volume of water

267 allocated from reservoirs to water works is obtained at the city decision level.

2.1.1 Objective functions of the first layer

Social objective function: minimization of total water supply shortages

270 The social objective function is established by the city manager to minimize the total

271 water supply shortages in a water system. The objective is established to sufficiently

272 meet the water demands of users in a water resources system. The water deficit is

273 considered, and this objective can reflect the ability of the water supply to meet the

274 water demand, as shown in Eqs. (1-3):

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

$$D = \sum_{r=1}^{R} \sum_{t=1}^{T} D_r^t \tag{2}$$

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

278 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

279 demand of the rth sub-region at tth time step, $r=1,2,...,R$, R is the total number of sub-

280 regions in the area, $t=1,2,...,T$, T is the total number of months in the period, $S\,(10^4\,\text{m}^3)$

281 is the total water supply of the water system for all waterworks, $x_{ij}^t\,(10^4\,\text{m}^3)$ is the

282 amount of water supplied from ith reservoir to the jth waterworks in the tth month of

283 the configuration period, $i=1,2,...I$, I refers to the total number of reservoirs, $j=1,2,...J$,

284 J is the number of total water works, $x_{ej}^t\,(10^4\,\text{m}^3)$ is the amount of water supplied from

285 the eth external transfer water source to the jth water works in the tth month of the

286 configuration period, $e=1,2,...,E$, E is the total number of external transfer water

287 sources in the city, α_{ij} is the water supply relationship coefficient between the ith

288 reservoir and the jth water works, where 0 indicates no supply and 1 indicates a water

289 supply, and β_{ej} is the water supply relationship coefficient between the eth external

290 transfer water source and the jth water works, where 0 indicates no supply and 1

291 indicates a water supply.

292 **Economic objective function: maximization of the total water supply benefit**

293 A city manager operates a water allocation system to maximize the overall economic

294 benefit by establishing an economic objective function, as shown in Eqs. (4-7):

295
$$\max f_{12}(x) = B - C_{rs} - C_{es} \tag{4}$$

296
$$C_{rs} = k \times \sum_{t=1}^{T}\sum_{i=1}^{I}\sum_{j=1}^{J} x_{ij}^t \alpha_{ij} + \sum_{t=1}^{T}\sum_{i=1}^{I}\sum_{j=1}^{J}\left(x_{ij}^t \alpha_{ij} \times c_i\right) \tag{5}$$

297
$$C_{es} = m \times \sum_{t=1}^{T}\sum_{j=1}^{J}\sum_{e=1}^{E} x_{ej}^t \beta_{ej} + \sum_{t=1}^{T}\sum_{e=1}^{E}\left(n_e \times \sum_{j=1}^{J} x_{ej}^t \beta_{ej}\right) \tag{6}$$

298
$$B = \sum_{j=1}^{J} b_j \times \left(\sum_{t=1}^{T} \sum_{i=1}^{I} x_{ij}^t \alpha_{ij} + \sum_{t=1}^{T} \sum_{e=1}^{E} x_{ej}^t \beta_{ej} \right) \qquad (7)$$

299   The overall economic benefit is the difference between the total benefit and total

300 cost at the city level. In the equations, B (Chinese Yuan is the total direct water supply

301 benefit (mainly considering the income from water charges for the city). The total water

302 supply cost consists of the reservoir water supply cost C_{rs} and the external water

303 supply cost C_{es}; k (Chinese Yuan/m³) denotes the water resources fees paid to the

304 government; c_i (Chinese Yuan/m³) denotes the water fees paid to the ith reservoir

305 authority; m (Chinese Yuan/m³) is the charge to an external administrative district per

306 unit of externally transferred water; n_e (Chinese Yuan/m³) is the charge associated with

307 the eth external water source per unit of transferred water; and b_j (Chinese Yuan/m³)

308 is the unit price of water supply revenue for the jth user.

309 **Sustainable development objective function: maximization of the total amount of**

310 **reserved water in reservoirs**

311 In water-scarce cities, the problem of water scarcity is a serious challenge that prevents

312 sustainable allocation of water resources. A prominent feature of most water-scarce

313 cities is that water inflows are limited, and the fluctuations in water availability are

314 large. Therefore, to reduce the risk that the inflows in the next configuration period are

315 too short to meet the basic demand of the city, a sustainable development objective

316 function is developed. The sustainable development objective function seeks to

317 maximize the amount of water remaining in the reservoir at the end of a configuration

318 period to hedge against drought risk and guarantee water use in the next period, as

319 shown in Eqs. (8-10):

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

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

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

323 where $V_i^{\max}$ (10^4 m³) is the maximum allowable storage capacity of the ith water source,

324 which is expressed based on the limited storage capacity of a reservoir in the flood

325 season, and V_i (10^4 m³) is the water storage capacity of the ith water source at the end

326 of the scheduling period. As much water as possible but less than $V_i^{\max}$ is reserved.

327 However, a reserved water volume in the reservoir that is too high at the end of the

328 scheduling period may lead to considerable pressure on reservoirs to urgently release

329 water if a flood event is forecasted. The reserved water volume should be neither too

330 large nor too small. Thus, the benefits of reservoir reserve stock must be thoroughly

331 evaluated. Based on the characteristic of the benefit of residual water, we propose a

332 boundary benefit function $p(V_i^{\max} - V_i)$ for different reserved water volumes in a

333 reservoir. The benefit function is a piecewise function, and when V_i is less than

334 $V_i^{\max}/2$, p increases as V_i increases. When V_i is equal to or greater than $V_i^{\max}/2$, p

335 decreases as V_i increases. When $V_i = V_i^{\max}$, p decreases to 0. $R_{i,initial}$ (10^4 m³) is the

336 initial storage of the ith water source, I_i^t (10^4 m³) is the inflow of the ith water source

337   at the tth time step, P_i^t ($10^4\,\text{m}^3$) is the precipitation associated with the ith water source

338   at the tth time step, A_i^t ($10^4\,\text{m}^3$) and E_i^t ($10^4\,\text{m}^3$) are the agricultural and ecological

339   water supplies associated with the ith water source at the tth time step, respectively, and

340   EP_i^t ($10^4\,\text{m}^3$) is the evaporation from the ith water source at the tth time step.

341   2.1.2 Constraints of the first layer

342   The layer includes six main constraints: the reservoir water supply constraint, water

343   demand constraint, reservoir storage constraint, water balance constraint, external water

344   transfer constraint, and nonnegative constraint.

345   Reservoir water supply constraint

346   The maximum water available to supply from an individual reservoir is determined by

347   the difference between the total input and total reservoir output. The inputs include

348   inflow and precipitation, and the outputs mainly involve agricultural and environmental

349   water supplies, evaporation, water supplied for waterworks and reservoir leakage loss.

350   All these factors directly affect the decision-making process and are incorporated into

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

352
$$V_i^t \le V_{i,\max}^t \tag{11}$$

353
$$V_i^t = \sum_{j=1}^{J} x_{ij}^t \alpha_{ij} \tag{12}$$

354
$$V_{i,\max}^t = \sum_{t=1}^{t-1}\left(R_{i,initial} + I_i^t + P_i^t - A_i^t - E_i^t - EP_i^t - \sum_{j=1}^{J} x_{ij}^t \alpha_{ij} - L_i^t \right) - V_{i,d} \tag{13}$$

355
$$EP_i^t = ep_i^t \times s_i^t / 1000 \tag{14}$$

$$356 \qquad\qquad V_i^t = \xi_i^t \times \left(R_i^{t-1} + R_i^t \right) \qquad\qquad (15)$$

357   where V_i^t (10^4 m³) denotes the total water supply from the ith reservoir at the tth time

358   step; $V_{i,\max}^t$ (10^4 m³) is the maximum water available to be supplied from the ith

359   reservoir at the tth time step; ep_i^t (mm) is the water surface evaporation from the ith

360   reservoir in the tth month; s_i^t (m²) is the monthly average surface area of the ith

361   reservoir in the tth month; $V_{i,d}$ (10^4 m³) is the dead storage of the ith reservoir; L_i^t (10^4

362   m³) is the reservoir leakage loss from the ith reservoir at the tth time step; R_i^{t-1} (10^4 m³)

363   is the storage of the ith reservoir at the t-1th time step; R_i^t (10^4 m³) is the storage of the

364   ith reservoir at the tth time step; and ξ_i^t is the tth monthly leakage coefficient for the

365   ith reservoir.

366   **Water demand constraint**

367   The high-quality water demand of each subarea in a city should be satisfied in the water

368   allocation process. High-quality water in this model refers to water that satisfies the

369   relevant primary (surface water can be used for drinking after simple purification

370   treatment, such as filtration and disinfection) and secondary water quality requirements

371   (water is slightly polluted and can be used for drinking after routine purification

372   treatment, such as flocculation, precipitation, filtration, disinfection, and other

373   processes) according to the Chinese Standard (GB5749), as shown in Eq. (16):

374

$$375 \qquad 0.8 \times D_r \leq \sum_{t=1}^{T}\sum_{i=1}^{I}\sum_{j=1}^{Jr} x_{ij}^t \alpha_{ij} + \sum_{t=1}^{T}\sum_{e=1}^{E}\sum_{j=1}^{Jr} x_{ej}^t \beta_{ej} \leq 1.2 \times D_r, r = 1,2,...,R \qquad (16)$$

376   where D_r (10^4 m³) is the high-quality water demand in the rth sub-region and there

377   are a total of R sub-regions in the city. Jr is the number of waterworks in the rth sub-

378   region. To ensure that the water supply guarantee in each area is greater than 80%, the

379   total water supplied to every subarea is greater than 80% of its demand.

380   **Reservoir storage constraint**

381
$$R_i^T \le V_{i,f} \tag{17}$$

382
$$R_i^T = \sum_{t=1}^{T} \left(R_{i,initial} + I_i^t + P_i^t - A_i^t - E_i^t - EP_i^{t1} - \sum_{j=1}^{J} x_{ij}^t \alpha_{ij} - V_i^t \right) \tag{18}$$

383   where R_i^T (10^4 m³) is the storage of the ith reservoir at the end of the configuration

384   period and $V_{i,f}$ (10^4 m³) is the flood-limit storage capacity.

385   **Water balance constraint**

386
$$R_i^{t+1} = R_i^t + I_i^t + P_i^t - A_i^t - EP_i^t - E_i^t - V_i^{t-1} - \sum_{j=1}^{J} x_{ij}^t \tag{19}$$

387   **External transfer water constraint**

388
$$\sum_{t=1}^{T} \sum_{j=1}^{J} x_{ej}^t \beta_{ej} \le E_{e,max} \tag{20}$$

389   where $E_{e,max}$ refers to the maximum water supply capacity of an external water source

390   over the whole configuration period.

391   **Nonnegative constraint**

392
$$x_{ij} \ge 0 \tag{21}$$

2.2 Second layer of the PTSOA decision-making model

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

2.2.1 Objective functions of the second layer

Conventional water supply department objective function: minimization of the

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

413 The managers of conventional water supply departments strive to operate conventional

414 water systems efficiently and achieve the most equitable water share possible. The

415 amount of conventional water (of high quality) retained in a water works system is a

416 crucial factor affecting the efficiency and benefits of conventional water supply

417 departments. Therefore, the benefit of conventional water departments is established by

418 minimizing the total amount of water retained in water works at the end of a

419 configuration period, as shown in Eq. (22):

420
$$\min f_{21}(x) = W_L = \sum_{t=1}^{T}\sum_{i=1}^{I}\sum_{j=1}^{J} x_{ij}^{t}\alpha_{ij} + \sum_{t=1}^{T}\sum_{e=1}^{E}\sum_{j=1}^{J} x_{ej}^{t}\beta_{ej} - \sum_{t=1}^{T}\sum_{m=1}^{M}\sum_{j=1}^{J}\sum_{z=1}^{Z} q_{jz}^{t,m}\chi_{jz} \qquad (22)$$

421 where W_L (10^4 m1) is the total amount of water retained in a water works system at

422 the end of a configuration period; $q_{jz}^{t,m}$ (10^4 m³) is the water supply from the jth water

423 works system to the zth water user on the mth day in the tth month in the period of

424 configuration; $m=1,2,...,M$; and M is the total number of days in the tth month (28, 29,

425 30 or 31). Additionally, $z=1,2,...Z$, and Z is the total number of water users. χ_{jz} is the

426 water supply relationship coefficient between the jth water work and the zth water user,

427 where 0 indicates no supply and 1 indicates water supply.

428 **Unconventional water supply objective function: maximization of the amount of**

429 **unconventional water supplied**

430 The reclaimed water reuse system and ecological water distribution system for inland

431 tributaries are incorporated into the PTSOA model which are associated with

432 unconventional water supply departments. The managers of unconventional water

433 supply departments seek to supply as much unconventional water as possible to

434 promote their interests. Thus, the objective of unconventional water departments is

435 established to maximize the amount of unconventional water supplied. Unconventional

436 water mainly includes reclaimed water and river water, which is of low quality (i.e., not

437 meeting the quality standard mentioned in Section 2.1.2) and is mainly used for

438 industrial production, ecological water replenishment for inland rivers and municipal

439 road sprinkling.

440   Unconventional water departments operate reclaimed water reuse systems and

441 ecological water distribution systems to supply unconventional water, and the

442 associated equations are as follows in Eqs. (23-26):

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

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

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

$$EW_r = \sum_{t=1}^{T}\sum_{n=1}^{N}\sum_{z=1}^{Z} r_{nz}\,\theta_{nz} \tag{26}$$

447 where W_r (10^4 m³) is the total amount of reclaimed water supplied for all water users;

448 EW_r (10^4 m³) is the total amount of river water supplied to maintain ecological flows

449 in inland tributaries; r_{nj}^{t} (10^4 m³) is the amount of water supplied to the jth user from

450 the nth reclaimed water source at the tth time step; $n = 1,...,N$; N is the total number of

451 reclaimed water sources; $p(b_c, b_u)$ is a function expressing the willingness of residents

452 to use reclaimed water, b_c (Chinese Yuan/10^4 m^3) is the price per unit of conventional

453 water; b_u (Chinese Yuan/10^4 m^3) is the price per unit of unconventional water; and θ_{nj}

454 is the water supply relationship between the nth reclaimed water source and the jth user.

455 In this case, $\theta_{nj} = 1$ indicates a water supply relationship, and $\theta_{nj} = 0$ indicates no

456 water supply relationship. r_{nz} (10^4 m^3) is the amount of water supplied from the nth

457 reclaimed water source to the zth inland tributary; $z = 1, 2, ..., Z$; Z is the total number of

458 inland tributaries requiring ecological flow compensation; and θ_{nz} is the water supply

459 relationship between the nth reclaimed water source and the zth inland tributary.

460 2.2.2 Constraints of the second layer

461 **Conventional water supply constraint**

462 According to conservation of mass, the total daily amount of conventional water

463 allocated in the second layer should be less than the total monthly amount of

464 conventional water allocated in the first layer, as described in Eq. (27):

465
$$\sum_{t=1}^{T}\sum_{i=1}^{I}\sum_{j=1}^{J} x_{ij}^{t}\alpha_{ij} + \sum_{t=1}^{T}\sum_{e=1}^{E}\sum_{j=1}^{J} x_{ej}^{t}\beta_{ej} \geq \sum_{t=1}^{T}\sum_{m=1}^{M}\sum_{j=1}^{J}\sum_{z=1}^{Z} q_{jz}^{t,m}\chi_{jz}, t = 1,...,T \qquad (27)$$

466 **Unconventional water constraints**

467 The two types of unconventional water have separate constraints. For reclaimed water

468 supplied to water users, the amount should satisfy the relevant water recycling standard.

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

470   reclaimed water works and main rivers. Therefore, this replenished volume is limited

471   by the pumping capacity. The constraints for unconventional water are shown in Eqs.

472   (28)-(29):

473
$$\sum_{t=1}^{T}\sum_{n=1}^{N}\sum_{j=1}^{J} r_{nj}^{t}\theta_{nj} + \sum_{t=1}^{T}\sum_{n=1}^{N}\sum_{z=1}^{Z} r_{nz}\theta_{nz} = \sum_{t=1}^{T}\sum_{i=1}^{I}\sum_{j=1}^{J} x_{ij}^{t}\delta_{ij}\eta_{ij} + PU \tag{28}$$

474
$$PU = \sum_{t=1}^{T}\sum_{m=1}^{M}\sum_{p=1}^{P} Q_{t,m}^{p,s}/10^{4} \tag{29}$$

475   where δ_{ij} is the sewage discharge coefficient, which is the proportion of the water

476   supplied from sewage discharge; η_{ij} is the sewage water reuse rate, which is the

477   proportion of reused water in the total volume of sewage water; PU (10^{4} m^{3}) is the

478   amount of water pumped from the main river; and $Q_{t,m}^{p,s}$ (t/d) is the flow through the

479   sth pumping station on the mth day at time step t.

480   **Pumping constraints**

481
$$Q_{t,s}^{p} \leq Q_{\max,s}^{P} \tag{30}$$

482
$$Q_{t}^{P} = \sum_{s=1}^{Np} r_{t,s}^{p} \tag{31}$$

483   where $Q_{\max,s}^{P}$ (t/d) denotes the upper flow boundary of the sth pumping station; r_{t}^{s} (t/d)

484   is the power of the pth pump installed at the sth pump station; and Np is the number of

485   pumps stalled at the sth pump station.

486   **Water quality constraint**

487   To control the impacts of various point and nonpoint sources on receiving water bodies

488   in cities, water authorities impose water quality standards for the management of river

489 basins. These standards seek to maintain the water quality at a desired target level by

490 defining discharge limits for conventional, specific, or priority pollutants. To satisfy the

491 relevant standards, the following water quality constraint is established:

492
$$\sum_{t=1}^{T}\sum_{i=1}^{N}\sum_{j=1}^{M}\left(x_{ij}^{t}\delta_{ij}\psi_{ij}h_{j}^{u}-x_{ij}^{t}\delta_{ij}\eta_{ij}h_{j}^{u}\right)\times 10 \leq H^{u} \tag{32}$$

493 where ψ_{ij} is the sewage water treatment rate, which is the proportion of sewage water

494 that is treated; h_{j}^{u} (mg/L) is the concentration of the uth contaminant per unit treated

495 water required by the jth user; and H^{u} (kg) is the upper limit of the uth contaminant

496 allowed to be discharged in the study area.

2.3 Third layer of the PTSOA decision-making model

498 After obtaining the results for the former two stages of the allocation process and the

499 two levels of decision-making, the third model layer is constructed to achieve regional

500 synergy. It refers to the collaborative allocation of water resources in different sub-

501 regions of a city, and it is intended to balance and maximize the interests of each sub-

502 region as much as possible. Additionally, the needs of different kinds of water users in

503 different sub-regions can be met to the greatest extent possible with this approach.

504 Therefore, the three dimensions of synergy are also fused in this layer. The third stage

505 of the process (the water in different departments is supplied to different kinds of water

506 users, namely, residential users, industrial users and municipal users, in different sub-

507 regions) is optimized in this layer. After department-level decision-making, conflicts of

508   interest inevitably occur among various water users in different sub-regions of a city.

509   Therefore, the third layer considers regional-level decision-making to coordinate water

510   needs and avoid conflicts of sub-regions in the city. Moreover, the various development

511   priorities of sub-regions are emphasized by adjusting certain hyper-parameters in the

512   third layer. This layer is established based on the allocation scheme obtained in the

513   second layer of the hierarchy, and the time scale of this layer is the same as that of the

514   second.

515   Although water pollutants are controlled in the second layer, the detailed spatial

516   distribution of pollutants remains unknown. If one of the sub-regions emits a greater

517   pollution load than others such that the river pollution limit is exceeded, it constrains

518   sustainable development and undermines the fairness of the allocation. To ensure the

519   coordination of water quality among regions, the representative pollutant concentration

520   of the main reach in each sub-region after configuration should meet the relevant

521   environmental capacity requirements. If these requirements are not met, the objective

522   function for this sub-region will call for a punishment, and more environmentally

523   friendly plans will be searched. After sewage with pollutants is transported from outlets

524   to water bodies, advective transport, longitudinal dispersion and transverse mixing will

525   occur. At the same time, physical, chemical and biological interactions will occur in the

526   water body. To objectively describe the degradation of pollutants in water, it is

527   necessary to use mathematical models to simulate physical dynamics. Due to the

528   heterogeneity of pollutants entering water bodies and the uncertainty of hydrological

529   processes, it is usually of little practical significance to calculate the change in river

530   water capacity over time. A steady-state model is therefore used to calculate the water

531   capacity of the target water body (Cetintas et al., 2010; Zhang et al., 2019). When water

532   quality changes are studied at the annual scale and complete mixing is assumed, the

533   following equation can be used to describe the water quality change, as shown in Eq.

534   (33):

535
$$\frac{Vdc}{dt} = Q(Ce - C) + Sc + r(c)V \tag{33}$$

536   where V (m³) is the volume of water; Q (m³/a) is the flow in and out of the system

537   at equilibrium; Ce (g/m³) is the contamination concentration in the inflow (g/m³); C

538   is the pollutant concentration; Sc denotes other external pollution sources (m³/a); and

539    $r(c)$ is the reaction rate of pollutants in water (g/m³/a). The above equation can be

540   defined as the basic mass balance of a water body in a completely mixed system.

541   Because the pollutants are evenly mixed in each small interval, the horizontal and

542   vertical concentration gradients of pollutants can be neglected. Therefore, the model of

543   water quality in mixed rivers under steady-state design conditions is adopted (Yue et

544   al., 2021):

545
$$W_c = 31.54 * \left[C_s \cdot (Q_p + Q_E + Q_S) - Q_p \cdot C_P \right] \tag{34}$$

546   where W_c represents the water environmental capacity (t/a); Q_p is the flow in the

547   reach (m³/s); C_P is the pollutant concentration in the river (mg/L); Q_E is the sewage

548   discharge (m³/s); Q_S is the total flow of nonpoint sources into the reach above the

549 control section (m³/s); and C_s is the target concentration of river pollutants (mg/L).

550 The result calculated based on the total hydrological capacity standard is often

551 relatively large, which is generally referred to as nonconservative. To conform to real

552 conditions, the concept of a nonuniform coefficient is introduced for correction:

553
$$W_c' = \alpha \cdot W_c = 0.6 \cdot W_c \tag{35}$$

554 This coefficient is used to assign a punishment if the water quality exceeds the

555 relevant value in a given sub-region. Based on the coefficient value, the objective

556 functions and constraints are adjusted accordingly. Finally, the daily decision

557 alternatives for water allocation from water departments to water users are obtained at

558 the regional decision level.

559 ## 2.3.1 Objective function of the third layer

560 **Regional objective function: maximization of the comprehensive benefits of each**

561 **sub-region**

562
$$\max f_3(x) = \sum_{t=1}^{T}\sum_{i=1}^{I}\sum_{j=1}^{Jr} x_{ij}^t b_{ij} - \sum_{j=1}^{Jr}\left(D_j - \sum_{t=1}^{T}\sum_{i=1}^{I} x_{ij}^t \alpha_{ij}\right)\times\omega_j - P_r(r_{nz}) - G_r(x_{ij}^t)\times q \tag{36}$$

563
$$P_r(r_{nz}) = e_i \times \sum_{p=1}^{Pr} P_p^{pump} \times \nabla t_r + x_{ij}^t \delta_{ij}\psi_{ij}\omega_{ij} \tag{37}$$

564
$$\nabla t_r = \sum_{t=1}^{T}\sum_{n=1}^{N}\sum_{z=1}^{Zr}\left\{\left(l_{nz} + \left(r_{nz}^t \theta_{nz}/CAS_{nz}\right)\right)\Big/\left(Q_{nz}^{max}/CAS_{nz}\right)\right\}\Big/3600 \tag{38}$$

565
$$G_r(x_{ij}) = \sum_{z=1}^{Zr}\sum_{u=1}^{U}\left(Q_{z,u,r}^{final} - Q_{z,u,r}^0\right) \tag{39}$$

566 where b_{ij} (Chinese Yuan/m³) is benefit per unit of water supply for the jth user; ω_j is

567 the penalty coefficient per unit of water deficiency; $j=1,2,...,Jr$; Jr is the number of

568 water users in rth sub-region; r= 1,2,…,R; $P_r(r_{nz})$ is the penalty function for cost in

569 the rth sub-region; e_i (Chinese Yuan/kW·h) is the unit electricity fee; P_p^{pump} (kW·h)

570 is the electrical power consumed by the pth pump at a pump house in each hour; p

571 ranges from 1 to Pr; Pr is the total number of pumps in the rth sub-region; ∇t_r (h) is

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

573 rth sub-region; ω_{ij} (Chinese Yuan) denotes to the fee paid for sewage treatment; l_{nz}

574 (m) is the length of a water diversion pipe from reclaimed water source n to the zth

575 inland river; z ranges from 1 to Zr; Zr denotes the number of inland rivers in the rth

576 sub-region; CAS_{nz} (m^2) is the cross-sectional area of a pipe from the nth reclaimed

577 water source to the zth inland river; Q_{nz}^{max} (m^3) is the maximum overflow capacity of

578 the diversion pipe from the nth reclaimed water source to the zth inland river; $G_r(x_{ij})$

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

580 is the final concentration of the uth pollutant in the control section of the zth inland river

581 in the rth subregion after optimal configuration; $Q_{z,u,r}^0$ (mg/L) is the initial

582 concentration of the uth pollutant in the zth inland river in the rth sub-region; and q is

583 the penalty coefficient for substandard water quality in the rth sub-region. The number

584 of objective functions in this layer depends on the number of sub-regions divided in the

585 city, which is based on local conditions.

2.3.2 Constraints of the third layer

Water quality constraints

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

$$Q_{z,u,r}^{final} \leq Q_{z,u,r}^{control} \tag{40}$$

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

2.4 Model solution

2.4.1 Synergy degree evaluation

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

605 One of the key network metrics used in network analysis, connectivity, is a promising

606 measure of the degree of coordination among different objectives in complex systems

607 (Weitz et al., 2018). Connectivity reflects the connectedness of a given link to all

608 possible links in the network, and the strength of each link is weighted, reflecting the

609 number and strength of correlations (Felipe-Lucia et al., 2020). In this study,

610 connectivity is used to embody coordination in the context of synergy, as shown in Eq.

611 (26). Due to the limited supply of water resources, competition among different

612 objectives is unavoidable, and the objectives cannot be fully optimized to equal extents,

613 i.e.,, an increase in one target output may decrease another output. Therefore,

614 equilibrium is integrated as another vital part of the synergy devoted to maintaining a

615 balance among the satisfaction of each goal in a system. The equilibrium based on the

616 principle of information entropy (Gao et al., 2013; Zivieri, 2022) is shown in Eq. (27).

617 Information entropy is a measure of the uncertainty associated with a random variable

618 and is used to quantify the information contained in a message, usually in bits or

619 bits/symbols; furthermore, it has been widely used to represent the fairness or

620 equilibrium of a system (Chen et al., 2022; Zhao et al., 2022). When H is low, the level

621 of equilibrium in the system is high. This factor is also used to be compared with the

622 proposed index. By combining the quantification of coordination and equilibrium, the

623 synergy degree is appropriately determined (Eq. (29)). Notably, the total synergy index

624 (*TSI*) of a system is used for both generating candidate management alternatives in the

625 generation phases of PTSOA and performing assessments of the associated level of

626 synergy, as shown in Eqs. (41-44).

$$SSI_{ob_i} = \frac{\sum\limits_{j=1}^{N} c_{ij} \times \left(ob_i + ob_j\right)}{\sum\limits_{j=1}^{N} \left(ob_i + ob_j\right)}, i \neq j \tag{41}$$

627

628 $$\tag{42}$$

$$u_{ob_i} = \frac{ob_i - ob_{i,\min}}{ob_{i,\max} - ob_{i,\min}} \tag{43}$$

629

$$TSI = \frac{\sum\limits_{i=1}^{N} SSI_{ob_i}}{H(S)} \tag{44}$$

630

631 where SSI_{ob_i} is the connectivity of the ith object; c_{ij} is the Pearson correlation

632 between the ith object and jth object; ob_i and ob_j are the values of the ith and jth

633 objective functions, respectively; $H(S)$ is the overall equilibrium of all objects based

634 on the principle of information entropy, and it is abbreviated as H in the following;

635 u_{ob_i} is the standardized value of the ith object; N is the total number of objects in the

636 system; $ob_{i,\min}$ and $ob_{i,\max}$ are the minimum and maximum critical thresholds of the

637 parameter ob_i, respectively. *SSI* is ranged from 0~N, and higher *SSI* indicates higher

638 connectivity of the objects in the system which means they are easier to promote each

639 other. *H* is ranged from 0~N*log(1/N) and lower *H* indicates better overall equilibrium

640 from objective perspective. *TSI* is greater than 0. When a water resource system's *TSI*

641 value is higher, the degree of synergy is higher. In our application, based on actual

642 evaluation, we define when *TSI*≥5, the degree of synergy is considered satisfactory.

643 5>*TSI*≥3 is defined as moderate and 3>*TSI* is defined as low.

2.4.2 Hierarchical optimal algorithm design for the PTSOA model

Based on the algorithm design with a hierarchical objective function proposed by Li et al. (2022), a new level is added to the original two levels of the algorithm, and the alternative generation phase is improved for better synergy. In this algorithm, the objective functions in the upper decision level is first satisfied, and then the lower-level objective function provides an optimal result based on the results of optimal allocation in the upper level. To provide as comprehensive solutions as possible, the decision alternatives need to be classified into different sets for further selection. In addition, the synergy degree of the result of each layer is calculated to select optimal decisions among all Pareto front solutions. The detailed steps of the hierarchical optimal algorithm are as follows:

I.   In the first level, calculate the objective function (city level) values for the social, economic and sustainable development components, and sort the results with NSGA-III (Pourshahabi et al., 2020; Chen et al., 2017) to obtain each Pareto front F_1, F_2, …, F_i.

II.   Classify the Pareto fronts into K (K is determined based on the diversity of policies) elements with the K-means algorithm (Liu et al., 2022), which is used to partition a data set into K distinct and non-overlapping clusters. To perform K-means clustering, we first specify the desired number of clusters K. Then, the K-means algorithm is used to assign each observation to exactly one of the K clusters.

III. Calculate the synergy degree of each individual in the front, and select the

666 solution that yields the greatest synergy in each cluster. *K* solutions are obtained

667 in the first layer.

668 IV. Use the selected *K* solutions in the first layer to establish constraints in the

669 second layer. Solve the objective function of the second layer with NSGA-Ⅲ.

670 V. Calculate the synergy degree of each individual in the front and select the

671 solution that yields the greatest synergy as well as the two solutions that

672 maximize the conventional and unconventional water supply department

673 objective functions in all Pareto fronts with *K* preconditions.

674 VI. The three selected solutions in the second layer are used to establish constraints

675 in the third layer. Solve the objective function of the third layer with NSGA-Ⅲ

676 under the three preconditions.

677 VII. The synergy degree of each individual in the front is calculated, and the solution

678 that yields the greatest synergy in the third layer is selected. Three solutions are

679 obtained considering the synergy in the former two layers. Finally, the

680 synergistic configurations optimal for all stages in the whole process are

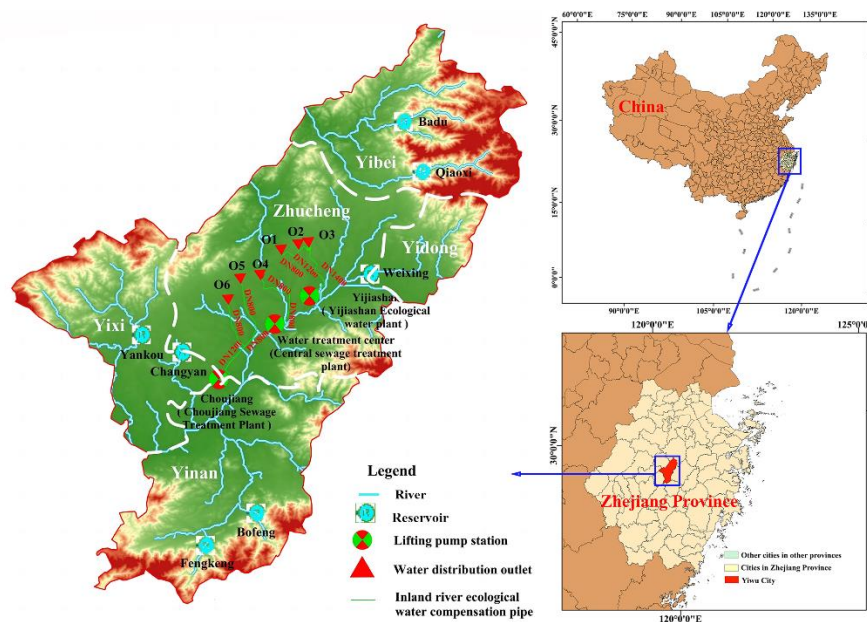
681 identified considering the synergy among decision levels, processes and time

682 scales.

3. Application

3.1 Study area

Yiwu city is selected as a case study to validate the applicability of the PTSOA model. This city is in Southeast China, located from 119°49 'E-120 °17' E and 29°02 '13 "N-29 °33' 40" N and covers an area of 1105 km^2. The area is characterized by a scarcity of water resources, and the conventional water supply is under severe stress. The regional water consumption depends heavily on transported water and external water transfer. The per capita water resource is in total 622 m^3, which is only 22.6% of the provincial average and 19.1% of the national average. Moreover, the problem of water pollution has become a bottleneck constraint for the development of Yiwu city. Therefore, it represents a typical water-scarce city with limited conventional water. Notably, water quality in Yiwu has been subjected to significant environmental stress because of the negative effects of wastewater discharge with the rapid development of industry. The current water quality is poor, with Class V, and the main pollutant concentrations exceed the corresponding standards (Zhejiang Natural Resources and Statistical Yearbook on Environment, 2020). As shown in Fig. 3, the Yiwu River crosses the city from northeast to southeast. Additionally, there are six ecological water compensation outlets in six main tributaries in the Yiwu River. In Fig. 3, the white labels indicate five sub-regions in the city, the black labels near the reservoirs are their names, the black labels named O1~O6 indicate the name of the water distribution outlets and

703 the labels near the lifting pump station are their names.

704

705 **Fig. 3. Map of the study area**

3.2 Generalization of the complex water resources system

707 An initial multi-source, complementary and mutually regulated system has been

708 developed for Yiwu, and this system spans the entire urban water cycle (water source-

709 water supply-water use-drainage-drainage collection-recycling and reuse). To apply the

710 optimal water allocation model to the complex real-world water system, all

711 stakeholders in the complex water resources system should be schematized into a

712 topological system, as shown in Fig. 4. The diagram comprises five modules: water

713 sources, water supply, water use, water drainage and external discharge for all

714 stakeholders.

715 The first module includes seven main reservoirs, two water diversion projects, the

716   Central Sewage Treatment Plant and the Yiwu River. The seven reservoirs and two

717   water diversion projects (as shown in Table 1) supply high-quality water. There are

718   complex connections between the first and second modules. For example, two

719   reservoirs supply water to one waterworks or one reservoir feeds two or three

720   waterworks simultaneously. The reservoirs also supply some of the agricultural and

721   ecological waters to subareas of the city. The Yiwu River, with a total length of 38.39

722   km and 21 first-class tributaries in the city, and the Central Sewage Treatment Plant, as

723   shown in Table 2, are low-quality water sources. There are no data available for

724   agricultural irrigation water, and most agricultural irrigation water is supplied from

725   surface water stored in hundreds of small reservoirs and mountain ponds (Yiwu

726   Ecological Environment Status Bulletin, 2020). So, this water volume is ignored in the

727   model.

728   For the second module, high-quality water piped from reservoirs is transported to

729   nine urban and rural centralized waterworks (as shown in Table 2). The Yiwu River

730   distributes low-quality water to the Yijishan Ecological Water Plant and Sufu Industrial

731   Water Plant through the Yijishan and Baisha Water Pump Stations, respectively. The

732   water discharged at the Central Sewage Treatment Plant is transferred to the Choujiang

733   Industrial Water Plant. Based on the water supply project distribution and the economic

734   as well as social development levels, Yiwu is divided into five districts, as shown in

735   Table 3: the Central District, Yidong District, Yibei District, Yinan District and Yixi

736   District. The third module comprises both high-quality water users (high-quality water

737   users consist of urban and rural domestic water users and some industrial water users

738   in the water supply network of urban and rural public water plants) and low-quality

739   water users (low-quality water users include other industrial water users, municipal

740   water users and ecological water replenishment for inland rivers) in each district. There

741   are nine sewage treatment plants in the fourth module (which focuses on the drainage

742   stage), as shown in Table 2. The unreused water from sewage treatment plants is

743   discharged to the external environment. Reuse processes are also considered in the

744   system.

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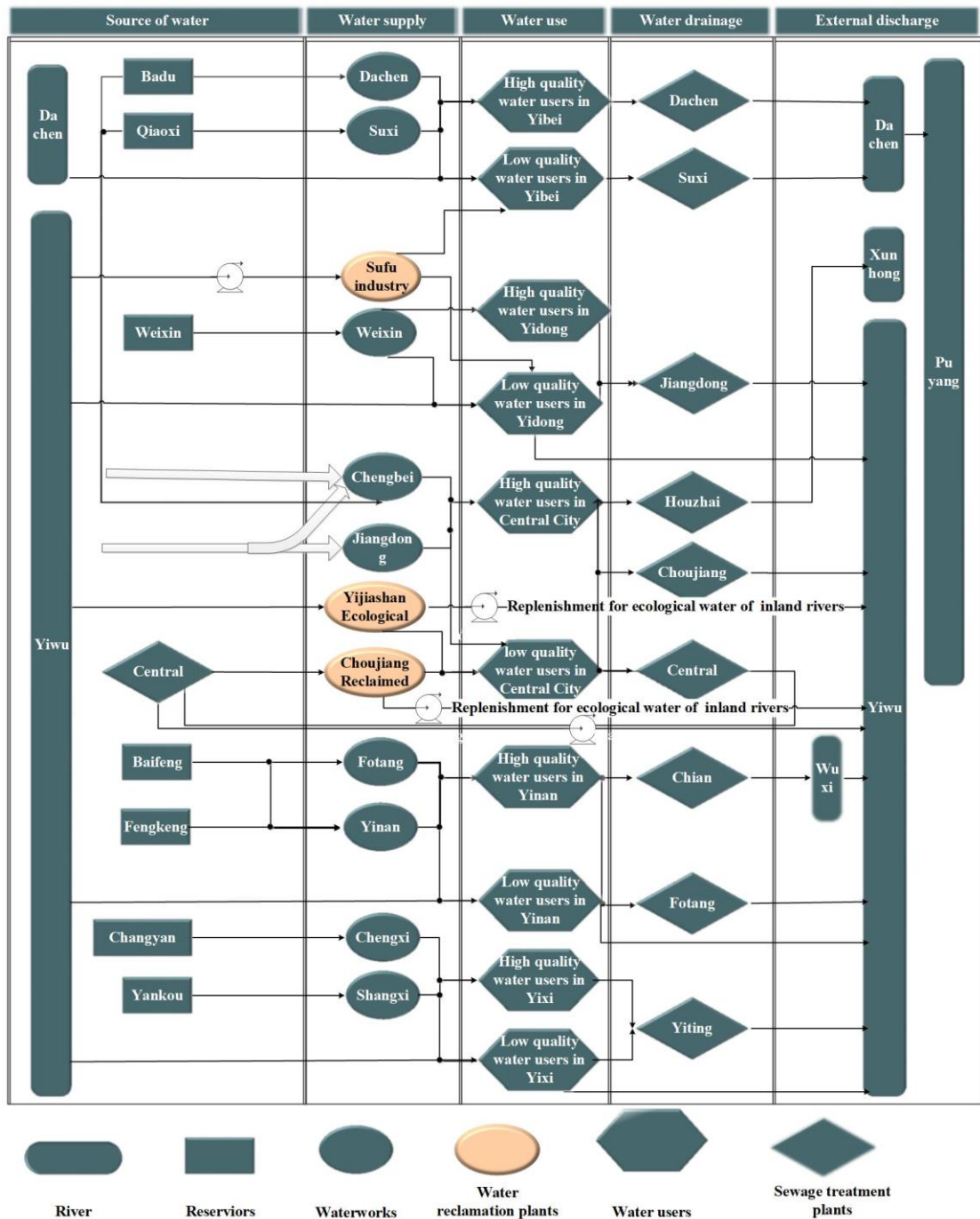


Fig. 4. Schematic diagram of Yiwu city

3.3 Parameter determination

According to the flow duration curve of the annual natural inflow data for 51 years (1963-2014), three years with exceedance probabilities of 50%, 75% and 90% are

751 selected to represent normal (1984.1–1985.1, annual mean inflow: 1.33×10^8 m³), dry

752 (2008.1–2009.1, annual mean inflow: 1.11×10^8 m³), and extremely dry (1971.1–

753 1972.1, annual mean inflow: 0.63×10^8 m³) scenarios, respectively. In addition to

754 inflow, the data used in the PTSOA model mainly include the data for the parameters

755 in each layer. Water demand values were calculated using the Yiwu City Water

756 Resources Comprehensive Plan 2020, as shown in Table 1.

757 **Table 1** Water demands of various regions in Yiwu in 2020 (10^4 m³)

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

758

759 The water resources fees paid to the government are in total 0.3 Chinese Yuan/m³.

760 The parameters of the reservoirs and external water division projects in Yiwu city are

761 listed in Table 2.

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

Reservoirs & External sources	Water Fee (Chinese Yuan/m³)	Initial storage (10^4 m³)	Dead storage (10^4 m³)	Flood limit storage capacity (10^4 m³)	Absolute storage capacity (10^4 m³)
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

763 The Tennant method is applied to calculate the ecological water demand. In this

764   method, the relationship between the annual average discharge and habitat quality is

765   considered, and the percentage of the annual average natural runoff is used as the

766   recommended value of the ecological water demand for a given river channel.

767   According to the recommended values, the percentage of runoff required for the fish

768   spawning period from April to September is 30% and the percentage runoff in the

769   general water consumption period (October to March) is 10%.

770   Based on observations obtained with the F601 evaporator (a standard evaporation

771   instrument widely used in China), evaporation is calculated as:

$$EP = E \times k \tag{45}$$

773   where EP (mm) is the evaporation of a reservoir; E (mm) is the observed evaporation;

774   and k is a reduction coefficient. According to observations, the difference of

775   this coefficient is quite slight within a small watershed (Zhao, 2014). Thus, k is

776   simplified to the same value 0.88 for every reservoir and varies throughout the year

777   according to expert experience(Zhao, 2014). The prices of conventional water and

778   reclaimed water are 1.7 and 2.6 Chinese Yuan/m³, respectively. In our application of the

779   model, this precipitation component associated with the water sources were calculated

780   by the Thiessen polygon method (Liu et al., 2014) based on the measured data of seven

781   rainfall stations (Shi Caotou, Suxi, Yiwu, Fotang, Baifeng, Fengkeng, Changfu) in the

782   basin in normal (1984.1–1985.1), dry (2008.1–2009.1), and extremely dry (1971.1–

783   1972.1) scenarios.

784   The monthly mean monitoring data for effluent pollutant concentrations and the

785   daily maximum processing capacities of sewage treatment plants were obtained from

786   the monitoring systems of the sewage treatment plants. For example, the concentrations

787   of COD, NH3-N, TN, and TP in the sewage of the Jiangdong Sewage Treatment Plant

788   are 13.80 (mg/L), 0.22 (mg/L), 6.02 (mg/L), and 0.13 (mg/L), respectively. The daily

789   maximum processing capacity of Jiangdong Sewage Treatment Work is 12 (10^4 t/d).

790   The effluent quality of sewage treatment works satisfies Class A Standard used in China.

791   The maximum capacities of the Baisha pump station, Yijiashan pump station,

792   Choujiang pump station and water treatment centre pump station are 13 t/d, 13.5 t/d, 10

793   t/d, and 4.5 t/d, respectively.

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

795   with ecological water are calculated according to Eqs. (33)-(35), and the results are

796   listed in Table 3. COD, TP and TN are major pollutants in Yiwu City (Yiwu Ecological

797   Environment Status Bulletin, 2020), and they are also major controlled pollutants of all

798   the monitoring sections. So, they were selected as representative pollutants in the

799   tributaries to guarantee the water environmental quality of inland rivers. The water

800   quality goals for the tributaries must conform to Class III standard according to GB

801   5749-2006 in China. The unit electricity price of pump stations in Zhejiang Province is

802   0.41 Chinese Yuan/kW · h. GB50014-2006 (2014 edition) stipulates that the

803   comprehensive urban domestic sewage quota should be 80~90%, and the urban

804   comprehensive domestic sewage quota should be 90% in areas with extensive drainage

805   facilities. There are many influencing factors in the model and the most important ones

806   among them are the value of water demand, the value of available water and some key

807   hyper-parameter. According to the "Jinhua Water Resources Bulletin (2020)", the urban

808   comprehensive domestic sewage quota is set to 90%, and the sewage treatment rate is

809   set to 100%. The benefits per unit water supply for different users in different

810   subregions are determined from the Yiwu Water Price Adjustment Plan (2020).

811

812   **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

4. Results and discussion

813

814   By solving the PTSOA model for Yiwu city, synergistic optimal water allocation results

815   for different layers (across different decision levels, water use sectors, and sub-regions)

816   are obtained under normal, dry and extremely dry conditions. Pareto sets are obtained

817   across 500 runs and 1000 iterations (in most cases) of the PTSOA model with the

818   proposed hierarchical optimization algorithm. If the feasible solutions could not be

819   found in some cases, the number of iteration would be increased. It took approximately

820   34 h of CPU time on a computer with 32 GB memory and intel corei7@3.4 GHz of

821   CPU. Therefore, in this study, each iteration for a single trial solution takes 0.24 s of

822   CPU time on the computer with the named specifications.

823   **4.1 First layer of the PTSOA model for synergistic optimal**

824   **water allocation**

825   To demonstrate the relationship among conflicting objectives, sets of Pareto solutions

826   for the first layer under normal, dry and extremely dry conditions are shown in Fig. 5.

827   In each of the figures, the total water supply shortage, total water supply benefit and

828   total amount of water retained in reservoirs in Yiwu city are plotted. The colour of the

829   markers indicates the classification of the solutions of the K-means method, as

830   described in Section 2.4.2. All of the decision alternatives are classified into six groups

831   marked in different colours for broad-scale decision-making. The names of the classes

832   are marked in the figure in red (for example, K1-1 represents the first class of solutions

833   in the normal scenario, and K3-2 represents the second class of solutions in the

834   extremely dry scenario). The red arrows indicate optimization directions. The ideal

835   solution is located at the top-right corner (low total water supply shortage, high total

836   water supply benefit, and relatively high total amount of reserved water in reservoirs)

837   of the plot. The geometries of the trade-offs vary significantly across the applications,

838   as is expected given different hydrological conditions. Generally, the total water supply

839   shortage and the total amount of water retained in reservoirs show an inverse

840   relationship. In contrast, the total water supply benefit shows a direct and positive

841   influence on the total water supply shortage. The water shortage varies in the range of

842     $-1.2\times10^6 \sim 0.8\times10^5$ m³, $-0.5\times10^5 \sim 2.0\times10^6$ m³, $0 \sim 3.5\times10^6$ m³ in normal, dry and

843   extremely dry scenarios respectively. The average water demand is around 1.8×10^8 m³,

844   and water shortage of the selected decision alternatives are all less 9×10^6 m³. So,the

845   water supply reliability of the selected decision alternatives is greater than 95% under

846   normal, dry and extremely dry conditions with the consideration of water demand. The

847   total amount of reserved water in reservoirs under normal scenarios varies in the range

848   of 2.91×10^7 m³ to 6.14×10^7 m³, which is much higher than that under the extremely dry

849   scenario, with a value of 1.44×10^7 m³ to 2.93×107 m³. This finding demonstrates that

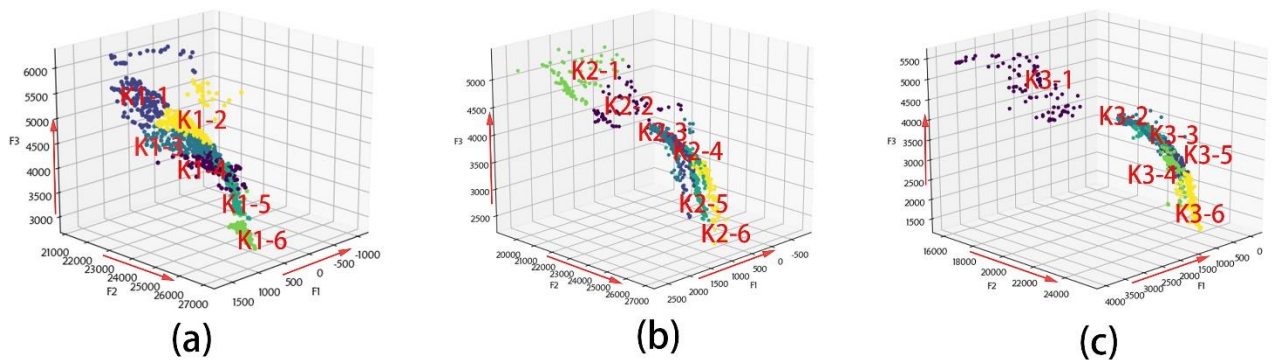
850   the optimal allocation is able to reconcile the present demand and future needs, even in

851   extremely dry scenarios. The total water supply shortage in all scenarios is less than 5%

852   of the water demand, which indicates that the guaranteed water supply is greater than

853   95%.

854

(a)   (b)   (c)

856   Fig. 5. Sets of Pareto solutions after 500 model simulations with the hierarchical

857   optimal algorithm under (a) normal, (b) dry and (c) extremely dry scenarios. (F1: total

858   water supply shortage, 10^4m³; F2: total water supply benefit, 10^4 Chinese Yuan; F3:

859   the total amount of reserved water in reservoirs, $10^4 m^3$. The red arrow indicates the

860   direction of optimization. K1-n,K2-n and K3-n represents the nth class of solutions

861   in the normal, dry and extremely dry scenario separately, n=1~6.)

862   We further present the *TSI*, *SSI* (total connectivity) and *H* (overall equilibrium)

863   values for different classes characterized based on the optimal PTSOA solutions under

864   three scenarios, as shown in Fig. 6. In the PTSOA model, the Pareto solutions with the

865   best *TSI* values are input to the second layer for further optimization. Thus, the red

866   points in Fig. 6 represent the selected schemes for all classes. We observe that the

867   variation in the *TSI* is consistent with that in the *SSI* in some, but not all cases. In some

868   cases, differences are mainly caused by the influence of H, which influences the optimal

869   hydrological equilibrium, especially in dry condition. These results suggest that when

870   water is very limited, equally limited water is supplied to all users, thus enhancing the

871   overall equilibrium. We note that the *SSI* value is higher in the normal scenario than in

872   the other two scenarios. We attribute this to relatively abundant water being useful for

873   stakeholders to achieve synergy due to the reduced competition compared to other cases.

874   The *TSI* values reach maximums of 5.36, 7.37 and 10.82 under normal, dry and

875   extremely dry conditions, respectively.

876   In Fig.6, the value of *TSI* are significantly diverse among different scenarios as

877   well as different solutions. H is widely used to evaluate the equality of different

878   solutions (Gao et al., 2013;Li et al., 2022). As a contrast, the value of *H*, which is used

879   for comparison and construction of *TSI*, show slight differences among solutions and

880 even are the same in some classes. Therefore, it is difficult for decision makers to select

881 the best solution among all candidates if we only use H for evaluation and selection in

882 the decision process. Compared to H, TSI introduces SSI into evaluation and the

883 difference of coordination relationship between different schemes is distinguished by

884 SSI. But H only pays attention to the equity among the stakeholders. So, TSI is more

885 effective and valid than H in some extent. Additionally, since TSI is used to illustrate

886 the synergy of allocation plans under certain conditions, the three kinds of TSI values

887 are not comparable.

888

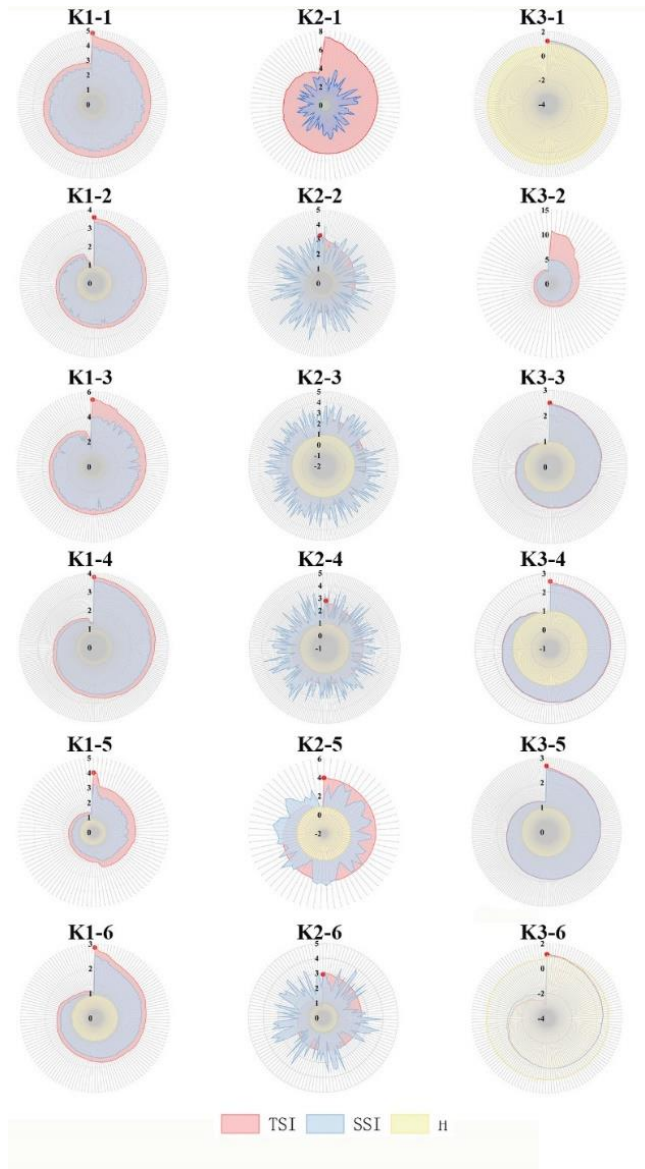



Fig. 6. Comparison of *TSI* (total synergy index), *SSI* (total connectivity) and *H*

(overall equilibrium) values among various Pareto solutions in different classes for

the (K1) normal, (K2) dry, and (K3) extremely dry scenarios. (K1-n,K2-n and K3-n

represents the nth class of solutions in the normal, dry and extremely dry scenario

separately, n=1~6.)

As an example, Fig. 7 provides the specific water supply decision alternatives for

the first layer that maximize synergy in each cluster under normal conditions. The water

896   allocation plans for the seven main reservoirs and two external water diversion projects

897   in every month of the configuration period are displayed. All reservoirs and water works

898   are represented by abbreviations based on their full names in Fig. 7. For example, QX-

899   CB is the label for the water supplied from Qiaoxi Reservoir to Chengbei Water Works.

900   The water volumes supplied by Qiaoxi Reservoir to Chengbei Water Works (ranging

901   from 1.78×10^7 m³ to 3950×10^4 m³) and from the Pujiang External Water Division

902   Project to Chengbei Water Works (ranging from 2.57×10^7 m³ to 3×10^7 m³) are relatively

903   high in all clusters. This result is consistent with the fact that Chengbei Water Works is

904   one of the main conventional water sources for the central city area, a region that

905   accounts for more than 50% of the total water demand of Yiwu city. The water supplied

906   by the two external water diversion projects from August to December is higher than

907   that in other months. The mean monthly precipitation in these months is only 58-74%

908   of the mean annual precipitation in Yiwu, so more external water is supplied for

909   replenishment. Baifeng and Fengkeng Reservoirs supply similar volumes of water to

910   their two connected waterworks.

911

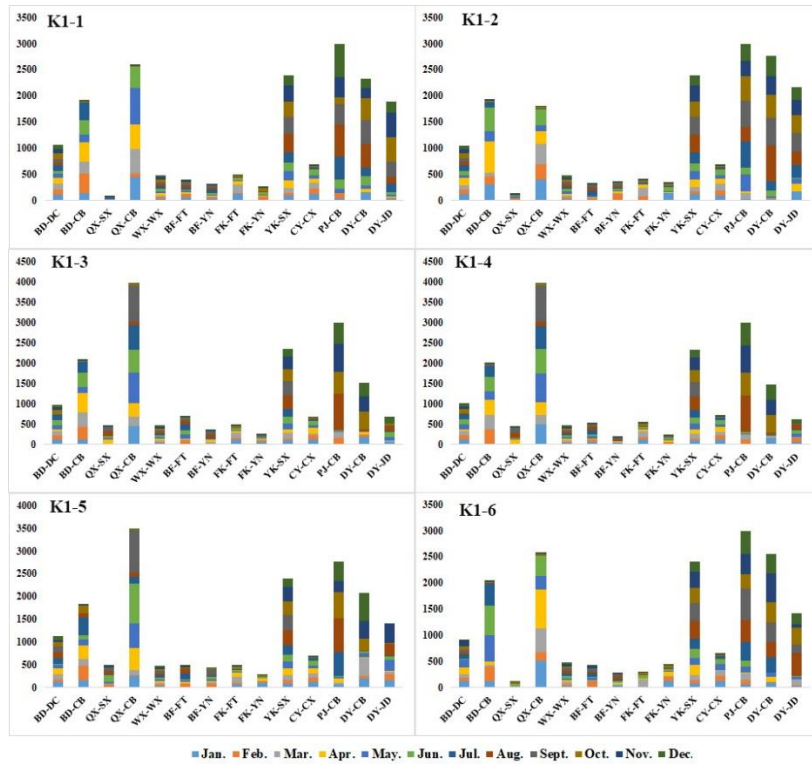



Fig. 7. Water supply from each reservoir to connected water works in each month in

the normal scenario 10^4 m^3

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

915

4.2 Second layer of the PTSOA model for synergistic optimal water allocation

The 6×3 decision alternatives selected in the six clusters of the optimal first-layer results

in the scenarios are inputs into the second layer for further optimization. As shown in

Fig. 8, the total amount of water retained in water works and the amount of

unconventional water supplied show a negative correlation. In the alternative

generation phase of game bargaining between the two objectives, the greater the total

923   amount of water retained in water works is, the greater amount of unconventional water

924   will be supplied, which indicates that more conventional water will be saved when more

925   unconventional water is supplied. Conversely, the amount of unconventional water

926   supplied is affected by the total amount of water retained in water works.

927   In the second layer, three alternatives in each scenario are selected as prior

928   conditions for further optimization. In addition to the two individual extrema of the two

929   objectives, the alternative that yields the best synergy is also identified, and it is similar

930   to that in the first layer. In the normal scenario, the *TSI* values are -0.90, -1.02 and -0.88

931   in the cases with the optimal conventional water supply, unconventional water supply

932   and synergy, respectively. The most synergistic approach includes 7.08×10^4 m³ more

933   conventional water retained than that in the conventional water supply cases and

934   9.72×10^4 m³ more than that in the optimal unconventional water supply case. Therefore,

935   not only is the best *TSI* value obtained, but the requirements of both conventional and

936   unconventional water supply departments are met.

937   Overall, the total amount of water retained in the water works ranges from 3.95×10^7

938   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

939   three types of conditions. The total amount of unconventional water supplied ranges

940   from 5.95×10^7 m³ to 7.48×10^7 m³, 6.34×10^7 m³ to 7.56×10^7 m³, and 6.28×10^7 m³ to

941   7.37×10^7 m³ in the normal, dry and extremely dry scenarios, respectively. Moreover, by

942   selecting the solution with the highest *TSI*, 7.35×10^7 m³, 7.56×10^7 m³, and 7.37×10^7 m³

943   of unconventional water would be supplied as an effective supplement to conventional

944 water. In the other word, conventional water would be saved by our proposed model

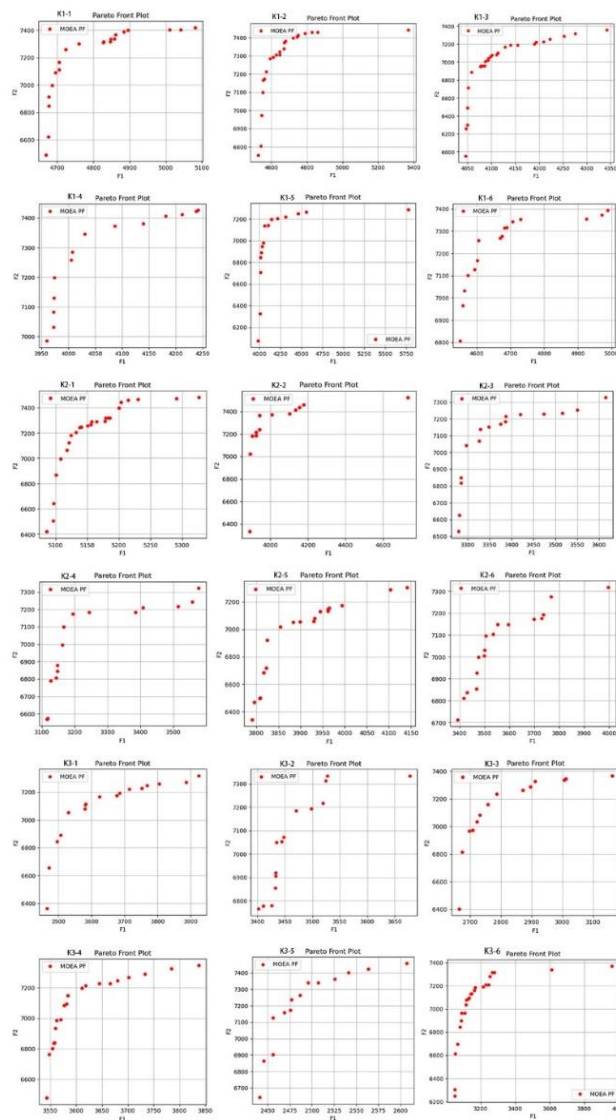
945 and index in the three scenarios. It is notable that the drier the conditions are, the lower

946 the amount of water retained in water works and the greater the amount of

947 unconventional water supplied. Thus, this approach is useful for cities to mitigate the

948 risk of drought. Additionally, based on the constraints regarding the contaminants

949 allowed to be discharged, more than 1272.21 t and 48.81 t of COD and ammonia

950 nitrogen emissions are avoided per year.

951

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

953   with the hierarchical optimal algorithm in the normal, dry and extremely dry

954   scenarios. (F1 represents the total amount of water retained in water works ,$10^4 m^3$; F2

955   represents the amount of unconventional water supplied,$10^4 \, m^3$. The direction of

956   optimization is from the top-right corner to the bottom-left corner. K1-n,K2-n and

957   K3-n represent the nth class of solutions in the normal, dry and extremely dry scenario

958   respectively, n=1~6.)

959

4.3 Third layer of the PTSOA model for synergistic optimal water allocation

962   Fig. 9 shows the trade-offs among the five objectives in the third layer of the PTSOA

963   model for the (S1) normal, (S2) dry, and (S3) extremely dry scenarios (these

964   abbreviations are used to distinguish these results from those of the above two layers).

965   The number following '-' represents the selected solution from the second layer. For

966   example, S1-1 represents the normal scenario with the minimum total amount of water

967   retained in water works, S1-2 represents the normal scenario with the maximum

968   unconventional water supply and S1-3 represents the normal scenario with the

969   maximum synergy degree in the second layer. In each of these plots, the abscissa

970   denotes the identifier for the objective functions, which ranges from 1 to 5, and the

971   ordinate gives the objective values in the Pareto fronts (10^4 Chinese Yuan). The five

972   dimensions include the comprehensive benefits of the Yibei (1.0 dimension), Yidong

973 (2.0 dimension), Yixi (3.0 dimension), Yinan (4.0 dimension) and central city (5.0

974 dimension) sub-regions. As shown in the figure, the central city achieves the most

975 comprehensive benefit among the five sub-regions. This is primarily attributed to the

976 large population and intensive industry in this area. However, the benefits in the other

977 four sub-regions are also high compared to recent levels and those achieved with

978 traditional allocation methods, as shown in Table 9. Interestingly, the comprehensive

979 benefits in the sub-regions are greater in the scenario with the maximum synergy degree

980 under normal conditions than in the other two scenarios. The total comprehensive

981 benefits in the five sub-regions in this scenario are approximately 2.3×10^8~5.1×10^8

982 Chinese Yuan higher than those in other cases, which indicates that the solution with

983 the highest synergy degree in the second layer is the best choice for managers in normal

984 years.

985

986

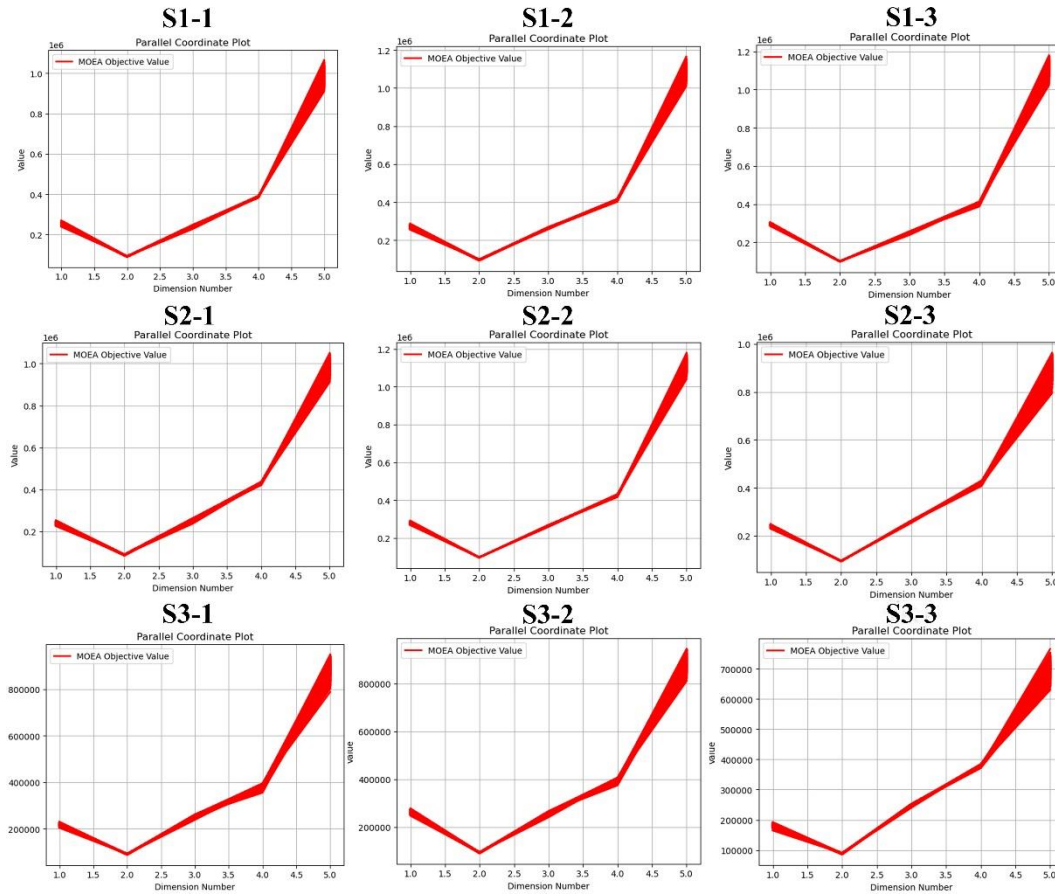



Fig. 9. Illustration of parallel-reference Pareto sets from the third layer in the

PTSPOA model attained across all runs for the (S1) normal, (S2) dry, and (S3)

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)

Fig. 10 presents the optimal comprehensive benefit in each sub-region. In all

scenarios, the central city is associated with the highest comprehensive benefit,

followed by Yixi and Yinan, and the comprehensive benefit in Yidong is relatively low.

997   This result may be related to Yidong which has the smallest area (72.2 km^2) and the

998   smallest population (7.7×10^4). Among the three normal decision alternatives, F1, F2

999   and F5 are highest in S1-3, with values of 3.03×10^9 Chinese Yuan, 9.90×10^8 Chinese

1000 Yuan and 1.12×10^{10} Chinese Yuan, respectively. This indicates that considering the

1001 synergy degree could increase the comprehensive benefit in most sub-regions in the

1002 normal scenario. Among the alternatives in the dry and extremely dry scenarios

1003 (excluding F4 and F5), other objectives are highest in S2-2, with values of 2.84×10^9

1004 Chinese Yuan, 9.63×10^8 Chinese Yuan and 2.67×10^8 Chinese Yuan, respectively. It

1005 suggests that maximizing the unconventional water supply is beneficial for the system

1006 in dry conditions. Additionally, F4 is highest, with a value of 2.29×10^9 Chinese Yuan,

1007 in S2-3 among the three solutions in the dry scenario, and F5 is highest, with a value of

1008 9.17×10^9 Chinese Yuan, in S3-1 in the extremely dry scenario.

1009

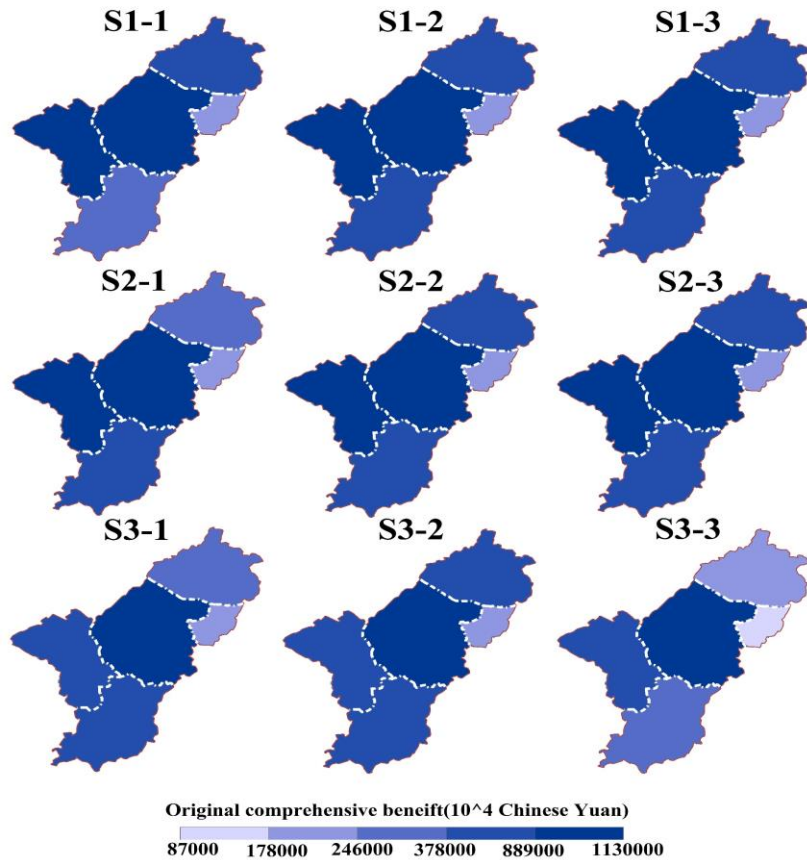



Fig.10. Comprehensive benefit in five sub-regions after the regional collaborative

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)

4.4 Discussion

To assist policymakers in understanding the complex and systemic nature of complex

water resources systems and reveal the dynamic interactions among objectives, network

1022   analysis and optimization were applied. Complex network analysis helps reveal the

1023   interactions among three layers with different dimensions. We determine the level of

1024   synergy in complicated water systems, identify the challenges and opportunities for

1025   sustainable development of water systems in cities with various subregions, and provide

1026   valuable insights and specific action priorities for these regions.. In the networks shown

1027   in Fig. 11, each node represents an individual objective (F1, F2, F3, F4, and F5 represent

1028   the comprehensive benefits in Yibei, Yidong, Yixi, Yinan and the central city,

1029   respectively), and pairwise objectives that are significantly ($P < 0.05$) correlated are

1030   connected by a link, where the strength of each link is related to the Pearson correlation

1031   coefficient. The obtained networks with five nodes were weighted and undirected

1032   (directionality can be estimated only if the direction of causality is known). The size of

1033   the circles in the figure indicates the connectivity of each objective. We considered

1034   trade-offs (i.e., negative correlations wherein one objective improves while the other

1035   worsens) among the objectives. In most scenarios, F5 was the relatively dominant

1036   objective, signifying that other objectives disproportionately deteriorated as progress

1037   was made towards the benefit of the central city, as shown in Fig. 11. It is evident that

1038   the trade-offs are more balanced in the scenarios with the highest degrees of synergy

1039   (S1-3, S2-3, and S3-3), which indicates that the trade-offs and competitions among the

1040   objectives are alleviated when synergy is considered. The links show that the conflicts

1041   of interest between F4 and F5 in scenarios S1-1 and S2-2 are extremely notable,

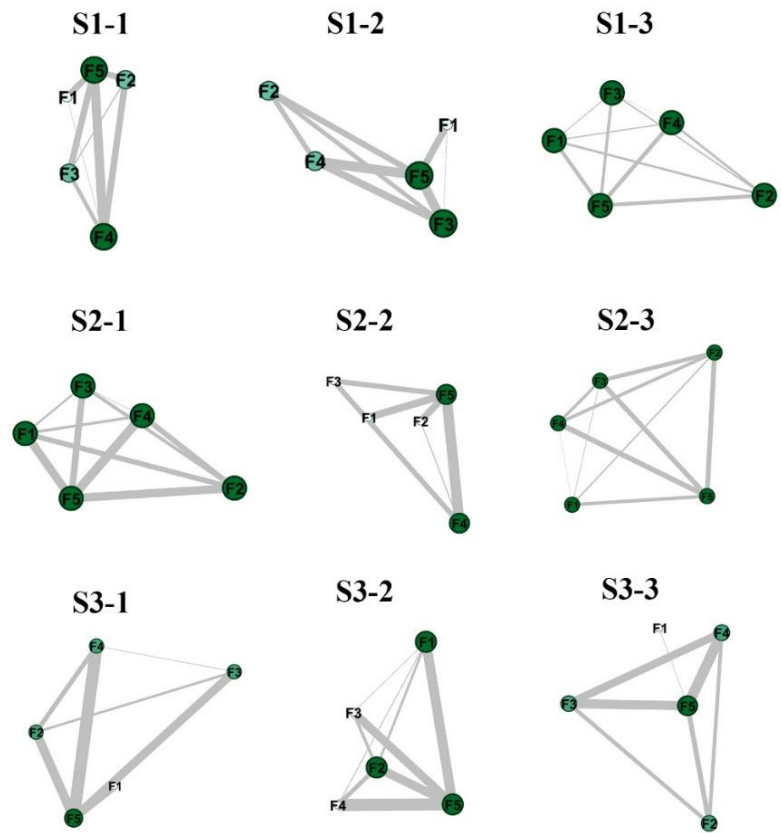
1042   suggesting that the comprehensive benefits in Yinan and the central city correspond to

1043 strong negative interactions in these cases. The connectivity of most objectives was

1044 relatively low in the trade-off network in the extremely dry scenario, but F5 played a

1045 dominant role in terms of negative interactions among objectives.. Moreover, as the

1046 scenario varied from normal to extremely dry, the impact of individual regional targets

1047 on the whole system diminished.

1048

1049 **Fig. 11.** Network analysis of the results of Layer 3

1050 (The circles of F1,F2, F3, F4 and F5 represent the connectivity of each comprehensive

1051 benefit of Yibei, Yidong, Yixi, Yinan and the central city, respectively:S1 represents

1052 normal scenario, S2 represents dry scenario, and S3represents extremely dry

1053 scenarios, S*m*-1 represents the normal scenario with the minimum total amount of

1054   water retained in water works, Sm-2 represents the normal scenario with the

1055   maximum unconventional water supply and Sm-3 represents the normal scenario with

1056   the maximum synergy degree in the second layer, m=1~3)

1057

1058   For comparison, we applied six widely used MOEAs, namely, NSGA-II, SPEA-II,

1059   ε-MOEA, IBEA, MOEA/D and Borg MOEA to solve cases with 3+2+5 mathematical

1060   objectives (3 objectives in the first layer, 2 objectives in the second layer and 5

1061   objectives in the third layer) with the same constraints given previously for Yiwu city

1062   under normal, dry and extremely dry conditions. The constraints and common

1063   parameters, such as the maximum number of model simulations and the simulated

1064   binary crossover (SBX) rate, are set to those used in the PTSOA model. However, it is

1065   difficult to determine feasible decision alternatives with MOEAs, even though the

1066   number of iterations is increased to 20000 (which is far beyond that considered in the

1067   previous modelling) because the complexity of the system overshadows the

1068   optimization capabilities of these traditional models. These results reconfirm the

1069   superiority, efficiency and decoupling capability of the proposed model for optimal

1070   allocation cases involving complex water resources system with multiple stakeholders,

1071   multiple sources, multiple decision-makers and embodied reused systems. By

1072   embedding the targets into hierarchical layers, the excessive abandonment of some

1073   promising alternatives is avoided, and optimal allocation is progressively achieved. In

1074   general, the hierarchical structure of the PTSOA model can simulate complicated

1075   systems with multiple complex objectives and constraints.

1076   In addition, the six MOEAs were used to solve the equations in the third layer of

1077   the PTSOA model, and the overall targets in the first layer were determined based on

1078   these solutions. The necessary parameters and hyper-parameters were consistent with

1079   those used in the third layer of the PTSOA model. Additionally, the benefits in the

1080   current case with no optimization calculated based on the actual water supply are given

1081   for comparison. The current situation was categorized as a normal scenario, and other

1082   models were established with the same conditions to facilitate further comparison and

1083   analysis. There were distinct decision alternatives generated by each model, and the

1084   relevant results are listed based on their value ranges. As shown in Table 4, although

1085   NSGA-II and ε-MOEA yield slightly higher F2 values than PTSOA and F3 generated

1086   by IBEA ($4.8 \times 10^8 \sim 7.2 \times 10^8$ Chinese Yuan) is higher than obtained with PTSOA,

1087   PTSOA performs better than other models in most cases. The PTSOA model is shown

1088   to be the best model for obtaining comprehensive benefits for the sub-regions in Yiwu

1089   in the normal scenario, demonstrating that the PTSOA model offers advantages

1090   including identifying the best alternatives and achieving greater sub-regional benefits

1091   than the other models. The proposed model yields $1.76 \times 10^9 \sim 15.67 \times 10^9$ Chinese Yuan

1092   total comprehensive benefit improvement and can save approximately $3.2 \times 10^7 \sim$

1093 $4.7 \times 10^7 \, \text{m}^3$ of conventional water compared to the current values. It is also evident that

1094   the proposed model yields the highest *TSI* values, reflecting the improvement achieved

1095   by considering the synergy of the system. In terms of the targets in the first layer, except

1096 MOEA/D, other traditional models fail to retain enough water (water requirements for

1097 living under extreme drought conditions of the next configuration period) in the

1098 reservoirs to meet future basic needs. For MOEA/D, although it generates a slightly

1099 higher total water supply benefit, with a value of $2.81 \times 10^8 \sim 3.12 \times 10^8$, the total water

1100 supply shortage and the total amount of reserved water in the reservoirs are worse than

1101 the amounts obtained with the proposed model. Borg MOEA, as an efficient and robust

1102 many-objective optimization tool, is characterized by its use of auto-adaptive multi-

1103 operator search and other adaptive features (Reed et al., 2013). The *TSI* value of Borg

1104 MOEA is lower than PTSOA. Therefore, in the *TSI* dimension, its performance is

1105 slightly worse than the PTSOA model. However, it is noticed that the Borg MOEA

1106 algorithm could save around one-fifth of the computing time of the model (around 7h).

1107 In the future, it would be interesting to figure out how to couple the Borg MOEA

1108 algorithm with our PTSOA model in a more efficient and synergetic way. In this study,

1109 our main focus is to find the most synergetic solution through optimization in a complex

1110 system. Thus, PTSOA has accomplished superior performance in this respect. It trades

1111 some economic benefits for enhanced water supply reliability and sustainable

1112 development, resulting in a decrease in the water supply from conventional water plants.

1113 The consideration of reclaimed water in the proposed model effectively reduces

1114 the use of traditional water and improves the quality of the water environment by

1115 reducing sewage discharge, and other benefits are also achieved (such as meeting the

1116 quality standards for river water and guaranteeing that the ecological water demand of

1117 inland rivers is met). The results obtained by the PTSOA model may help guide both

1118 the government and general public. Our proposed model is superior to traditional

1119 models. It can not only optimize water resource utilization and secure water supplies

1120 but also enhance the synergy and environmental quality of water systems. Considering

1121 synergy across various time scales, the proposed model ensures the synergistic

1122 allocation of water resources at yearly, monthly and daily scales while securing both

1123 present and future water supplies.

1124 **Table 4** Comparison of the comprehensive benefits of the five objectives (F1, F2, F3,

1125 F4, and F5) and the *TSI* values in the current situation and obtained using NSGA-II,

1126 SPEA-II, ε-MOEA, IBEA, MOEA/D, Borg MOEA and PTSOA in the normal

1127 scenario

Comparison	Comprehensive benefits (10^9 Chinese Yuan)					*TSI*
	F1	F2	F3	F4	F5	
NSGA-II	2.72~2.86	0.91~1.03	2.57~2.60	3.21~3.37	7.38~9.95	-3.13~-2.82
SPEA-II	2.84~2.97	0.93~0.99	2.58~3.15	3.02~3.68	8.22~9.99	-2.39~-2.46
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
Borg MOEA	2.95~3.56	0.80~0.98	1.19~2.23	3.11~3.82	12.88~13.90	-2.51~-1.67
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**

1128 **5. Conclusions**

1129 Applying optimal water allocation models to simultaneously enable economic benefits,

1130 water preferences and environmental demands at different decision levels, time scales

1131 and regions is a challenge. In this study, a new process-based three-layer synergistic

1132 optimal allocation model (PTSOA) was developed and applied to a real and complex

1133 water allocation system. The model was divided into three layers to coordinate conflicts

1134 of interest among decision makers at different levels and time scales. Furthermore, the

1135 allocation of reclaimed water was embedded in the proposed model for synergistic

1136 optimal allocation of both conventional and unconventional water. A synergistic index

1137 based on network analysis was put forward to reduce competitions among different

1138 stakeholders and facilitate the positive effects of stakeholder interactions. A hierarchical

1139 optimal algorithm was designed to solve the PTSOA model.

1140   The proposed model was applied to a typical city in Southeast China with scarce

1141 water resources and developed industry. Achieving the optimal allocation of water

1142 resources in this kind of water-scarcity offers a valuable reference for other counties in

1143 China. The key findings of this study are as follows. Firstly, the results demonstrated

1144 that the PTSOA model achieved synergistic allocation among hierarchical decision-

1145 makers across various time scales and in different regions, yielding the highest *TSI* (-

1146 1.66 to -0.89) among the contrast models. Secondly, with a synergistic approach, a

1147 reasonable amount of conventional water is retained for future use in cases with

1148 potentially high risk, with volumes of 3.95×10^7 m³, 3.12×10^7 m³, and 2.43×10^7 m³

1149 retained in normal, dry and extremely dry scenarios, respectively. Moreover, 7.35×10^7

1150 m³, 7.56×10^7 m³, and 7.37×10^7 m³ of conventional water can be saved in the three

1151 scenarios. Thirdly, considering both reclaimed water and conventional water in the

1152 optimization process efficiently improves the quality of municipal water, and more than

1153 1272.21 t/year and 48.81 t/year of COD and ammonia nitrogen emissions are mitigated

1154 compared to those in the current situation. Lastly, distinct from previous models, the

1155 proposed optimal model was implemented with the consideration of spatial dimensions,

1156 which are important but often neglected. The results show that spatial allocation yields

1157 an improvement of 4~95% for the comprehensive benefits in different sub-regions

1158 compared to the benefits achieved with traditional models, and the total comprehensive

1159 benefit increases by 1.76×10^9~15.67×10^9 Chinese Yuan compared to that in the current

1160 situation.

1161 These results and conclusions provide valuable references for the evaluations of other

1162 complicated water allocation systems. The optimal allocation scheme can be

1163 determined for a complex water resources system upon consideration of stakeholder

1164 synergy and various hierarchical decision levels, time scales and regions. More in-depth

1165 studies of synergistic optimal water allocation are needed in the future.

1166

1167 *Data availability.* The data used to support the findings of this study are available from

1168 the corresponding author upon request.

1169

1170 *Author contributions.* JL and YPX designed all the experiments. JL and XZ collected

1171 and preprocessed the data. JL and XZ conducted all the experiments and analysed the

1172 results. JL wrote the first draft of the manuscript with contributions from XZ, SW and

1173   SC. YPX supervised the study and edited the manuscript.

1174

1175   *Competing interests.* The authors declare that they have no conflict of interest.

1176

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