

1 Nested Optimization Approach for the Capacity Expansion of 2 Multiquality Water Supply Systems under Uncertainty

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10 11 12 *Abstract*

13 A nested optimization approach is proposed to solve capacity expansion problems of
14 multiquality water supply systems. The problem to be solved consists of determining the
15 infrastructure that should be built and/or rehabilitated at a specific time. This decision should
16 be taken in a long-term planning perspective. It should consider how the operation will be
17 performed to satisfy demand and water quality requirements by using multiple sources with
18 different water quality at the source, take into account the temporal and spatial distribution of
19 the water resources available and remain aware of the environmental impacts. In addition,
20 decision processes which do not appropriately consider inherent uncertainties (e.g.,
21 hydrological, demographic, and technological uncertainties) can lead to suboptimal solutions.
22 Here, uncertainty is handled using scenario planning with the aim of finding expansion
23 solutions that can be expected to perform well under a set of possible future situations (or
24 scenarios). The solution method combines simulated annealing with nonlinear programming to
25 determine the solution to the nested optimization problem.

26 *Keywords:* Water supply, Capacity expansion, Nested optimization approaches

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1. INTRODUCTION

Nested optimization approaches place one optimization task inside of another. The solution of the outer optimization task, usually referred to as upper level, depends on the solution of the inner optimization task, usually referred to as lower level.

Nested optimization approaches are often associated with bilevel programming or bilevel optimization (Vicente and Calamai 1994; Colson et al. 2007). Bilevel programming emerged from the classic Stackelberg problem (1952) in the field of game theory. The strategic game conceptualized by Stackelberg comprises a hierarchical planning process with a leader and a follower. The leader solves the problem of finding their optimal strategy assuming that they can anticipate the optimal response of the follower to their own actions. In this framework, the leader's optimization problem contains an inner optimization task that corresponds to the follower's optimization problem. Sinha et al. (2013a) give examples of a number of practical bilevel problems studied in the literature in the domain of transportation, economics, management and engineering. The hierarchical structure can introduce difficulties such as non-convexity and disconnectedness, even for simple bilevel linear programming problems (Sinha et al. 2013a).

But nested optimization approaches do not result from a hierarchical planning process as bilevel. Examples in the field of water resources include Schmitz et al. (2007), who presented a nested approach for improving irrigation efficiency where optimizing the irrigation schedule (i.e., number and date of applications) was the "outer task" and optimizing the control of each single water application (i.e., intensity and irrigation time) was the "inner task". The inner optimization task is performed by obtaining the inverse solution of a numerical irrigation model. Ricciardi et al. (2007) developed a nested optimization approach for the design of groundwater remediation systems. Scenario planning is used to represent the uncertainty of hydraulic conductivity. The inner optimization includes a series of deterministic linear

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mathematical programs, one for each scenario, for determining pumping systems that minimize operation and maintenance cost subject to hydraulic-gradient constraints. A penalty value is then added to the cost of the pumping system obtained for each scenario. The penalty term is given by a weighted sum of violation of hydraulic-gradient constraints that occur when the pumping system designed for each scenario is applied to all other scenarios considered to represent the uncertainty of hydraulic conductivity. Finally, the outer optimization examines which pumping system results in the minimum sum of the design cost with the penalty value.

Classic optimization techniques, including the Karush-Kuhn-Tucker approach, Branch-and-Bound techniques and the use of penalty functions, have been employed to solve problems formulated as nested but with limited application to simple cases. Alternatively, modern heuristics or a combination of modern heuristics with classical optimization methods have proved to be successful at handling complex problems formulated as nested (Schmitz et al. 2007; Ricciardi et al. 2009; Sinha et al. 2013a, 2013b).

The nested optimization approach described in this work was developed to support decision-making in the capacity expansion (or redesign) of multiquality water supply systems. In general, the first failures in the desired performance of the water systems caused by increased demand, reduced supply or the imposition of new regulation are handled with corrective actions using the existing infrastructure. However, more serious failures may require the construction of new infrastructure and/or the rehabilitation of what is in place (Hsu et al. 2008). Capacity expansion decisions should be taken in a long term perspective and consider how the systems will be operated in an uncertain environment. It has long been recognized, that failing to incorporate uncertainty in the planning process may result in solutions that do not meet needs in the immediate future, solutions that will become obsolete in the short/medium term or solutions that turn out to be oversized. One common approach to deal with uncertainty in optimization planning models is its representation by a set of scenarios that may be defined

77 as structured representation of the uncertain model parameters. Scenario planning was used for
78 example by Rosenberg and Lund (2009), Kang and Lansley (2013), Ray et al. (2014), or Lan et
79 al. (2015) in recent studies dealing with the development of optimization models for
80 multiquality water-supply systems with explicit representation of uncertainty.

81 But none of the previous optimization models include an explicit representation of water
82 quality as in the nested optimization approach presented in this paper. This aspect can be
83 relevant since different water quality at the source often determines differences in the water
84 quality for the end-users. The explicit representation of water quality introduces nonlinear
85 constraints to reflect the real physical conditions but those nonlinearities difficult the solution
86 of the optimization models (Yang et al. 2000). For solving the nested optimization model
87 detailed in the sections that follow, the authors have also developed a solution method that
88 allows to deal efficiently with scenario planning and the explicit representation of water
89 quality.

90 Section 2 briefly describes the nested optimization approach developed and its solution method
91 to support capacity expansion solutions. Section 3 presents the results of applying it to a real-
92 world case study. Some conclusions are drawn in Section 4. The work presented here is
93 described in more detail in Vieira (2014).

94 **2. NESTED OPTIMIZATION APPROACH**

95 The decision to be taken in each situation corresponds to the infrastructure to be built and/or
96 rehabilitated at a specific time for the capacity expansion of a multiquality water supply
97 system. The nested optimization approach developed is intended to identify capacity expansion
98 solutions provided by solving the outer optimization task and that depend on a set of solutions
99 obtained from the inner optimization task. The solution of each inner optimization task enables
100 us to determine the optimal operation of the redesigned water system in each scenario, which

101 can be defined here as one single realization of the parameters defined as non-deterministic
 102 during the system operation. The consideration of multiple scenarios also makes it possible to
 103 define the approach developed as proactive. The explicit incorporation of some knowledge of
 104 uncertainty during system operation is intended to find capacity expansion solutions that are
 105 less sensitive to the non-deterministic parameters. Mathematically, the capacity expansion
 106 problem to be solved can be defined as follows:

$$\text{Maximize}_Y F(Y, X_1, X_{\dots}, X_{NS}) \quad (1)$$

where $F(Y, X_1, X_{\dots}, X_{NS})$ is the value of a mathematical function determined by
 solving the following NS mathematical programs (one for each scenario)
 with the capacity expansion solution $Y = \{0, 1\}$ as input data

$$\text{Min}_{X_s} f(X_s) \quad (2)$$

subject to (s.t): $g(X_s) = 0$

$$X_s \geq 0$$

where $s = 1, \dots, NS$

107 The optimization problem defined by (1) sets the outer optimization task while the
 108 NS optimization problems defined by (2) set the inner optimization task. The vector Y
 109 represents the capacity expansion solutions, the vectors X_s define the operating decisions in
 110 each scenario s and NS is the total number of scenarios. Section 2.1 and 2.2 describe the
 111 optimization problems included in the two optimization tasks. Section 2.3 presents the method
 112 used to derive the capacity expansion solutions.

113 **2.1 Inner optimization task**

114 The NS optimization problems included in the inner optimization task have the main
 115 characteristics of the model developed by Vieira et al. (2011) to optimize the operation of

116 large-scale multiquality water supply systems dependent on surface water and groundwater
117 sources. The application of the model requires the representation of a given infrastructure as a
118 flow network composed of arcs and nodes, the characterization of the demand and a time series
119 of inflows to reservoirs and of the aquifer recharge. The optimized decisions provided by the
120 solution of the model include the volume of withdrawals from each water source, the operation
121 of the treatment and pumping facilities and the water allocation from each source to the
122 demand nodes. These operating decisions are discretized in monthly periods $t = \{1, 2, \dots, NT\}$
123 over the entire operational planning time horizon, which includes NT time steps. Usually,
124 monthly time steps are adequate for describing in detail the operation of large-scale water
125 supply systems for planning purposes. Such discretization allows describing the most important
126 intra-annual variations in both supply (e.g., storage in reservoirs and piezometric levels in
127 aquifers) and water demand thereby avoiding overly simple representation of phenomena given
128 by annual time steps.

129 Water quality is explicitly represented in the description of the water transport using the
130 multicommodity network flow approach (Fig. 1). This approach requires that water from a
131 different source, or simply of a different quality, is regarded as a separate commodity
132 $k = 1, \dots, NK$ sharing a common distribution network. The water flows are modeled by the
133 variable $x_{pq,t,s}^k$ representing a non-negative flow of water type identified by the index k in the
134 network arc (p,q) from node p to node q in period t in scenario s . Due to their miscibility, it is
135 justifiable to assume that waters modeled as different commodities are perfectly mixed when
136 the time scale used for planning purposes is larger than one day (Yang et al. 2000).

[Insert Fig. 1 approximately here]

138 The objective function $f(\dots)$ in (2) adds the variable operating costs to a set of three penalty
139 functions. The variable operating costs include all the abstraction, treatment and pumping costs

140 that depend on the quantity of water supplied. The penalty functions are used when solving the
141 model to avoid deviations from the objectives of *i*) to satisfy the demand and *ii*) to deliver
142 water of the appropriate quality as specified, in terms of volumetric water blending ratios. One
143 last penalty function is added as an artifice to avoid unnecessary spills from reservoirs. Weight
144 factors in the penalty functions allow prioritization of the objectives for each situation.

145 The constraints $g(\dots)$ in (2) include mathematical functions that simulate the water balance in
146 reservoirs, the groundwater flow in aquifers, and the water flow and quality in a distribution
147 network. Legal water rights and environmental concerns (such as minimum discharges from
148 reservoirs for downstream ecosystem maintenance and minimum piezometric levels in aquifers
149 to prevent problems related to the over-exploitation of the groundwater resources) are also
150 modeled as constraints.

151 The optimization problem is nonlinear. The penalty functions in $f(\dots)$ are quadratic so that
152 greater deviations from the objectives are more heavily penalized. The multiplication of
153 decision variables in the perfect mixing condition (Fig. 1) included in the model constraints
154 introduces a high degree of nonlinearity and may make the solution of the inner optimization
155 task (i.e., the optimal operation of the water system in the different scenarios) quite complex
156 and time consuming.

157 **2.2 Outer optimization task**

158 The mathematical function $F(\dots)$ in (1) integrates two metrics – the performance index (PI) and
159 the total solution cost (PVC) – that are used to evaluate each capacity expansion solution.

160 The performance index (PI) corresponds to the aggregation in a single value of the information
161 given by three performance criteria in the scale [0,1] – reliability (Rel), vulnerability (Vul) and
162 the water quality criterion ($VBld$). Rel and $VBld$ are related to the water quantity and express

163 the general characteristics for these criteria proposed by Hashimoto et al. (1982). Here, Rel is
 164 the volume of water supplied divided by the target demand (also known in the literature as
 165 volumetric reliability), and Vul is the maximum deficit relative to the demand in all time
 166 periods. The use of together Rel and Vul as the two water quantity criteria included in the
 167 performance index should guarantee its suitability for evaluations also related with the
 168 sustainability of the water systems (Kjeldsen and Rosbjerg 2004). $VBlD$ is the water quality
 169 criterion measuring the worst water quality conditions defined in terms of volumetric water
 170 blending ratios at the demand nodes in all time periods. By minimizing the $VBlD$, the worst
 171 water quality conditions should be mitigate and, simultaneously, a higher volume of water with
 172 the best quality to the extent possible should be available *ceteris paribus*. Finally, the value of
 173 the performance index is calculated as the simple average of the three performance criteria:

$$PI = \frac{Rel + (1 - Vul) + (1 - VBlD)}{3} \quad (3)$$

174 The terms $(1 - Vul)$ and $(1 - VBlD)$ are used so that the objective is to maximize Rel and to
 175 minimize Vul and $VBlD$. The value of PI is also a non-negative number taken as one or lower.
 176 Loucks (1997) and Zongxue et al. (1998) had initially proposed two different indexes to
 177 evaluate the performance of water systems and support decision-making. Other authors have
 178 come to examine and propose alternative formulation from those two initial indexes in more
 179 recent studies about the evaluation of performance of water systems (e.g., Sandoval-Solis et al.
 180 2011; Hajiabadi and Zarghami 2014; Ray et al. 2014; Tseng et al. 2015). In any of these studies
 181 water quality is not included as a criterion for evaluating system performance. The inclusion of
 182 a water quality criterion for evaluating the performance of multiquality water-supply systems
 183 can be justified as different water quality at the source often determines differences in the water
 184 quality for the end-users (Yang et al. 2000). Sandoval-Solis et al. (2011) also argue that water
 185 quality criteria can be included in performance indexes for evaluating municipal water use.

186 The total solution cost (PVC) includes initial construction costs for system redesign (CC) and
 187 operating costs (OC) spread over the project lifetime. The operating costs are divided into fixed
 188 and variable costs (FOC and VOC) with the quantity of water supplied:

$$PVC = CC + FOC + VOC \quad (4)$$

189 The PVC reports the total solution cost up to the “present” at a certain discount rate.

190 The function $F(\dots)$ in (1) was inspired by the field of robust optimization introduced by Mulvey
 191 et al. (1995) and followed many others (e.g., Rosenberg and Lund 2009; Kang and Lansey
 192 2013; Ray et al. 2014; Lan et al. 2015). The objective function of the outer optimization task
 193 allows the explicit balancing of the trade-offs between solution robustness and cost. Solution
 194 robustness is defined by a mean-variance formulation of the PI in all the scenarios, and the
 195 objective function $F(\dots)$ can be written as follows:

$$F(\dots) = \underbrace{\sum_{s=1}^{NS} p_s PI_s}_{E(PI_s)} - \varphi \underbrace{\sum_{s=1}^{NS} p_s \left(PI_s - \sum_{s=1}^{NS} p_s PI_s \right)^2}_{\text{Var}(PI_s)} - \omega PVC \quad (5)$$

196 where p_s is the probability of scenario s , $E(PI_s)$ and $\text{Var}(PI_s)$ are the expected value and the
 197 variance of the performance index over all scenarios, and φ and ω are weights representing the
 198 relative importance assigned to the variability of system performance and to the solution cost.
 199 One capacity expansion solution can be obtained from the solution of the nested optimization
 200 problem for each pair of values φ and ω . The mean-variance formulation addresses risk-averse
 201 behavior and higher values of φ reduce the chances of solutions with low performance in some
 202 scenarios being selected. Higher values of ω favor reduced cost solutions. The PVC is also an
 203 expected cost given that VOC are determined by an average value over all scenarios.

204 **2.3 Solution method**

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2 205 The method implemented to find the capacity expansion solutions combines simulated
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4 206 annealing with nonlinear programming (Fig. 2). The basic concept of the solution method is in
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7 207 taking advantage from the nested structure defined in (1)-(2) by decomposing the global and
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9 208 highly complex model (including discrete and continuous variables, and nonlinear constraints)
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11 209 into smaller sub-models with lower level of complexity and that can be efficiently solved
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14 210 independently. The application of decomposition solution methods has a fairly recent origin in
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16 211 the water sector (Cai et al. 2001; Reis et al. 2005, 2006), and has been followed by other
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19 212 authors lately (e.g., Chen et al. 2013; Afshar et al. 2015, Li et al. 2015).

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22 213 [Insert Fig. 2 approximately here]

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26 214 The solution of the nested problem (1)-(2) begins with a random generation of a capacity
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28 215 expansion solution represented in vector Y . This allows to express the binary variables in Y as
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31 216 input data and to define univocally NS nonlinear optimization problems that can be solved
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33 217 independently to determine the optimal operating decisions for each scenario s (i.e., X_s for $s =$
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36 218 $1, \dots, NS$). The value of $F(\dots)$ is determined after obtaining the optimal operating decisions for
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38 219 all scenarios. The solution method proposed here can be implemented using the simulated
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41 220 annealing proposed by Cunha (1999). A stop criterion included in the simulated annealing
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43 221 algorithm determines after calculating the value of $F(\dots)$ at each iteration either the end of the
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46 222 solution process or if a new expansion solution should be generated.

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49 223 The solution method includes a second decomposition when solving each of the nonlinear
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51 224 optimization problems in the inner optimization task. As stated in section 2.1, the perfect
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54 225 mixing condition (Fig. 1) introduces a high degree of nonlinearity and may make the solution
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57 226 of the NS nonlinear optimization problems in the inner optimization task quite complex and
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59 227 time consuming. To reduce the computational burden, the NS nonlinear optimization problems

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228 can be solved with the decomposition approach as described by Vieira and Cunha (2011). In
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2 229 step one, the perfect mixing condition is eliminated from the set of constraints. This set of
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4 230 nonlinear constraints is added only in the second step so that a solution of the complete
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7 231 nonlinear optimization problem is then found. Vieira and Cunha (2011) showed significant
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9 232 reduction of the computation time when solving a nonlinear optimization problem similar to the
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12 233 one handled here in the inner optimization task. Vieira and Cunha (2011) suggested that this
13
14 234 efficiency gain could be extremely useful for reducing the computational burden in capacity
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17 235 expansion problems.

21 236 **3. CASE STUDY**

24 237 The proposed nested optimization approach was implemented to identify potential capacity
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26 238 expansion solutions for the Barlavento Water System (BWS) located in the Algarve region of
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28 239 Portugal. The BWS is regional and supplies water for urban use to 9 of the 16 municipalities in
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30
31 240 the Algarve from surface water and groundwater sources. Surface water is soft and
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33 241 groundwater is naturally hard. Previous studies have demonstrated that a volumetric blend of
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36 242 hard groundwater should be kept below 25% to avoid significant variations in drinking-water
37
38 243 quality (Vieira et al. 2011).

42 244 The current water sources of the BWS are two surface water reservoirs (Odelouca and Bravura)
43
44 245 and two groups of wells (Vale da Vila and Almádena). But the Odelouca reservoir is smaller
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47 246 than was initially planned, as determined by the environmental impact assessment procedure of
48
49 247 this BWS water source. A report by Hidroprojecto and Ambio (2005) for the water utility that
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52 248 manages the BWS, already assumed the reduction in size determined later (in 2006) for the
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54 249 Odelouca reservoir, concluded there would be difficulties in meeting demand for the year 2025
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56 250 (74.7 million m³/year) and suggested that structural solutions were needed to expand the
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59 251 capacity of the BWS.

252 **3.1 Capacity expansion options**

1
2 253 Hidroprojecto and Ambio (2005) singled out two possible surface water transfers from
3
4 254 neighborhood systems and the construction of one seawater desalination plant with three
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6
7 255 possible design sizes for the capacity expansion of the BWS. Vieira (2014) added to those
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9 256 possible options the rehabilitation of six groups of wells and the installation of nanofiltration
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11 257 systems to soften the groundwater in all the well groups (i.e., those in the current sources and
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14 258 those to be rehabilitated as investment options). The typical water recovery rate (i.e., ratio of
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16 259 permeate flow rate to feed flow rate) of the nanofiltration systems would be 85%. Table 1 lists
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18
19 260 the current sources (CS) and the investment options (IO) used in this case study. Each capacity
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21 261 expansion solution results from the selection of one or more investment options. In this case
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24 262 study, there were 589 824 different capacity expansion solutions, given by all the possible
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26 263 combinations of the investment options listed in Table 1. The combination of all possible
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29 264 investment options defines the solution space of this case study. A preliminary evaluation
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31 265 allowed to conclude that it would not be practicable and too much time consuming to solve this
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33
34 266 case study by total enumeration. The final statistics about the computation time are summarized
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36 267 in section 3.3.1.

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40 268 [Insert Table 1 approximately here]

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43 269 The maximum flows indicated in Table 1 depend solely on the pumping and treatment systems
44
45 270 installed/to be installed, whereas the firm quantities also depend on limits set by the authorities.
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47
48 271 The installation of nanofiltration systems can reduce either the maximum flow and/or the
49
50 272 maximum firm quantity of each group of wells. For example, the total pumping capacity of the
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52
53 273 Vale da Vila group as a current source of the BWS is 984 L/s, but in any case the water utility
54
55 274 cannot extract more than 13 million m³/year, as defined by the authorities. The maximum
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57
58 275 values indicated for the investment option H4.O2 result from combining the maximum flow
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60 276 and firm quantity indicated before for the Vale da Vila well group as a current source of the
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277 BWS with the water recovery rate of the nanofiltration systems (85%). In the investment option
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2 278 H4.O1, the maximum flow of 350 L/s corresponds to the 11.05 million m³ (firm quantity for
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4 279 H4.O2) distributed uniformly over one year.
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8 280 Furthermore, the withdrawals from each source are also limited by the simulation of the water
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10 281 balance in each surface reservoir and the simulation of the groundwater flow in each aquifer.
11
12 282 The groups of wells are located in two aquifers. The Almádena group is located in the
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14 283 Almádena-Odiáxere aquifer. All the other groups are located in the Querença-Silves aquifer.
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20 284 **3.2 Hydrological scenarios**

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22 285 The hydrologic scenarios in this test case were generated from a multivariate time series of
23
24 286 monthly precipitation values from a 55 year record (October 1951 - September 2006) for each
25
26 287 surface reservoir and aquifer. The monthly values of precipitation were transformed into
27
28 288 reservoir inflows with a hydrological model, and into aquifer recharge using average recharge
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30 289 rates based on the hydro-geological formations.
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35 290 In this application, ten hydrological scenarios capture some uncertainty associated with the
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37 291 reservoir inflows and the aquifer recharge. Each scenario corresponded to a five year
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39 292 multivariate data block sampled from the historic multivariate time series. Nine of the ten
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41 293 scenarios were sampled randomly using the moving blocks bootstrap method with partial block
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43 294 overlap while one scenario was chosen specifically as detailed next. The moving blocks
44
45 295 bootstrap method (Vogel and Shallcross 1996) is a simple nonparametric method. Avoiding
46
47 296 defining assumptions regarding the marginal probability distributions of the variables and the
48
49 297 spatial and temporal covariance structure of the variables, one simply resamples randomly, with
50
51 298 replacement, a set of multivariate data blocks sampled from the historic multivariate time
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53 299 series. The challenge is to resample the records in such a way as to assure that the temporal and
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55 300 spatial covariance structure of the original time series is preserved as well as also that the first
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301 values and the last values of each block are be nearly independent (Vogel and Shallcross 1996;
302 Buishand and Brandsma 2001). The other scenario was chosen specifically so that the serious
303 drought that afflicted the Algarve in 2004 and 2005 would have to be included covering the period
304 October 2001 – September 2006. In a reference paper, Watkins and McKinney (1999) had
305 previously used an approach similar to this by combining scenarios selected randomly and
306 drought scenarios chosen specifically to generate a finite number of scenarios in a planning
307 model.

308 As described above, nine of the ten scenarios were sampled randomly from a historic time
309 series in line with the hypothesis of stationary conditions. But this assumption is opened to
310 wide discussion in recent times from the announced climate change scenarios. Many authors
311 have discussed the “death” of stationary of the hydrologic processes (Milly et al. 2008; Matalas
312 et al. 2012; Salas et al. 2012). In recent papers, Kasprzyk et al. (2012, 2013) and Herman et al.
313 (2016) developed different approaches that include a special attention to drought scenarios and
314 their impact on water resources planning given that these phenomena could become more
315 frequent under climate change. In this paper, one used a simple approach by giving to all
316 scenarios the same probability p_s in Eq. (5), including to the drought scenario. This represents
317 giving to the drought scenario an importance higher than that related directly to its frequency
318 from the historic time series, and envisaging some non-stationary about the hydrological
319 processes in testing the nested optimization approach presented in this paper.

320 ***3.3 Results and discussion***

321 **3.3.1. Solution robustness and cost**

322 The capacity expansion solutions presented next allow to explicit balancing the trade-offs
323 between solution robustness and cost. The results presented next were obtained after solving the
324 nested problem (1)-(2) with five different pair of values φ and ω [Eq. (1) is detailed in (5)]. The

325 best solution for each pair of values φ and ω was found in tens of hours by searching always
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2 326 just less than 0.5% of the solution space. The statistics about the computation time and the
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5 327 search of the solution space confirmed that it would not be practicable and too much time
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7 328 consuming to solve this case study by total enumeration.

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10 329 The five pair of values φ and ω in Eq. (5) were defined after setting $\varphi = 1$, $\omega = \omega^* / PVC_{Sup}$, and
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13 330 and $\omega^* = 0.1, 0.5, 1, 5, 10$. The PVC_{Sup} corresponds to the total cost defined by Eq. (4) of a
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16 331 particular capacity expansion solution designated as *Sup*. In this case study, the solution *Sup* was
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18 332 the one with the highest fixed costs ($CC + FOC$) in Table 1 (i.e., the solution *Sup* included the
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21 333 selection of investment options H1, H2, H3.O3, H4.O2, H5.O2, H6.O3, ... , H10.O3). The
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23 334 discussion that follows also includes the analysis of the results obtained in Solution \emptyset , the “do
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26 335 nothing” solution that retains the current sources. The results for Solution \emptyset and Solution *Sup*
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29 336 were obtained in a single iteration of the solution process described in section 2.3.

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32 337 Table 2 shows that the expansion solutions determined with the three highest values of the
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35 338 weight balancing the cost ($\omega^* = 1, 5$ and 10) do not include any of the investment options found
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37 339 by Hidroprojecto and Ambio (2005). In these three cases, the capacity expansion of the BWS is
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40 340 achieved by rehabilitating the groups of wells, with or without including the installation of
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42 341 nanofiltration systems to soften groundwater. Table 3 shows that the cost of those three
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44 342 solutions is lower – total cost between 158.6 and 177.6 million euros (€) – but there is less
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47 343 impact on the system performance, as $E(PI_s)$ is lower and $Var(PI_s)$ is higher. These results are
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49 344 due to two main factors. First, apart from the Almádena group of wells, all the groups are
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52 345 located in the Querença-Silves aquifer. This means that too often the withdrawals in the
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54 346 Querença-Silves aquifer are limited by model constraints that become active because of
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57 347 minimum piezometric levels in selected locations. Second, the rehabilitation of groups of wells
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59 348 may not be enough to reverse reductions in the maximum flows and/or total firm quantity from
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349 the installation of nanofiltration systems in the Vale da Vila and/or Almádena groups of wells
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2 350 (see section 3.1). Both factors contribute to the demand not being fully met in more than one
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4 351 scenario. The results also show that the poorest values of the performance criteria and the
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6
7 352 performance index are for the scenario specifically included here (i.e., scenario 2001-2006 –
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10 353 see section 3.2), thus the serious drought that afflicted the Algarve in 2004 and 2005 was
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12 354 always included in this case study.

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15 355 [Insert Table 2 approximately here]

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19 356 [Insert Table 3 approximately here]

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21
22 357 Table 2 also shows that the same capacity expansion solution was found with $\omega^* = 0.1$ and 0.5.
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24
25 358 It corresponds to the capacity expansion of the BWS by prescribing new infrastructure for the
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27 359 transfer of surface water from the Santa Clara system. Table 3 shows that for this capacity
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30 360 expansion solution $E(PI_s)$ almost equals one (i.e., maximum) and $\text{Var}(PI_s)$ is virtually null
31
32 361 indicating a nearly optimal system performance in all scenarios.

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36 362 All metrics [CC , PVC , $E(PI_s)$ and $\text{Var}(PI_s)$] are in the range defined by the values for Solution
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38 363 \emptyset and Solution *Sup* (Table 3). These results support the hypothesis that Solution \emptyset and
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41 364 Solution *Sup* should be those of minimum and maximum robustness, respectively.

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44 365 In brief, and as expected, the variation of ω^* allowed the identification of a trade-off between
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46
47 366 solution robustness and cost. Lower cost solutions were found by increasing ω^* as this weight
48
49 367 corresponds to a cost penalty. But lower cost solutions are also less robust solutions as $E(PI_s)$
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52 368 decreased and $\text{Var}(PI_s)$ increased when ω^* was increased. Significant improvements in solution
53
54 369 robustness necessarily imply higher costs. A robust solution was found with a reduced
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56
57 370 penalization of cost.

371 3.3.2. Detailed evaluation of system performance

372 A more detailed evaluation about system performance can be drawn from Table 4. This table
373 shows besides the average value of the performance index (*PI*) over all scenarios (already in
374 Table 3) its minimum and maximum value between all scenarios as well as the same statistics
375 for the three performance criteria (*Rel*, *Vul* and *VBl*) that define the performance index. The
376 last two performance criteria are represented in Table 4 by $(1 - Vul)$ and $(1 - VBl)$ such that
377 for all the performance indicators the minimum corresponds to the worst value and the
378 maximum to the best value, respectively.

379 From section 2.2, the *PI* is defined by Eq. (3); the reliability *Rel* represents the volume of water
380 supplied divided by the target demand; the vulnerability *Vul* is the maximum deficit relative to
381 the demand in all time periods; and *VBl* is the water quality criterion representing the worst
382 water quality conditions at all demand nodes in all time periods. *PI*, *Rel*, *Vul* and *VBl* are
383 non-negative taken as one or lower. From the introduction to this case study, the ratio
384 *HGW/TW* [hard groundwater supplied/total water (soft + hard) supplied] should be kept below
385 0.25 (or 25%) to avoid significant variations in drinking water quality. In this case study, the
386 *VBl* measured specifically the difference between the highest ratio *HGW/TW* at all demand
387 nodes in all time periods and the volumetric blending objective of 0.25, but only above that
388 value: $VBl = \max[(HGW/TW - 0.25), 0]$.

389 From Table 4, the minimum value of *Rel* in the hypothesis “do nothing” (Solution \emptyset)
390 represents that the satisfaction of the demand at the system level (given by the ratio total water
391 supplied/total water demand) has the minimum value of 0.818 or 81.8% in one of the ten
392 scenarios. Also for Solution \emptyset and from the minimum value of $(1 - Vul) = 0.738$, it is
393 possible to conclude that there is at least one time period in which the ratio total water
394 supplied/total water demand is not higher than 73.8%. Finally, the minimum value of

395 $(1 - VBl_d)$ reveals that there is at least one demand node and one time period in which all the
1
2 396 water supplied has a ratio HGW/TW equal to 1 or 100%. [here, when the ratio $HGW/TW = 1$,
3
4 397 $VBl_d = 0.75$, and $(1 - VBl_d) = 0.25$]. All the minimum values of the performance criteria
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6
7 398 were recorded in the same scenario (the scenario October 2001 – September 2006 that covers
8
9
10 399 that the serious drought that afflicted the Algarve in 2004 and 2005) whereby the minimum value
11
12 400 of the PI in all scenarios for Solution \emptyset ($= 0.602$) can be determined directly from the
13
14
15 401 minimum values of the performance criteria shown in Table 4.
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18 402 The increase in the value of $E(PI_s)$ from Solution \emptyset to the expansion solution found with
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20
21 403 $\omega^* = 10$ (in Table 3 or Table 4) is more closely related with the evolution of $(1 - VBl_d)$. The
22
23 404 VBl_d is the water quality criterion, and the installation of nanofiltration systems (NFS) in
24
25
26 405 Almádena wells group (option H5.O2 – see Table 2) has a significant impact in this
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28 406 performance criteria. On the contrary, there is no significant improvement in the performance
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31 407 criteria related with water quantity (Rel or Vul). In Solution \emptyset , the withdrawals from the
32
33 408 Querença-Silves aquifer were too often limited by minimum piezometric levels in the inner
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36 409 optimization task. In the capacity solution found with $\omega^* = 10$, there are new water sources in
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38 410 the Querença-Silves aquifer (options H7.O1 and H10.O1) but it is not possible to increase
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41 411 significantly the total abstractions in that aquifer.
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44 412 The installation of NFS in Vale da Vila wells group for hardness removal in the capacity
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47 413 expansion solutions found with $\omega^* = 1$ and 5 (option H4.O1 – see Table 2) contributes
48
49 414 significantly to guarantee good water quality in any scenario as $(1 - VBl_d)$ is always maximum
50
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52 415 (Table 4). But the installation of the NFS decreases the statistics of the performance criteria
53
54 416 related with water quantity in comparison with the capacity solution found with $\omega^* = 10$. This
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57 417 happens given that it is not possible to use all the water pumped from the aquifer but only 85%
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59 418 which is the water recovery rate of the NFS (section 3.1).
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419 In the capacity expansion solution found $\omega^* = 0.1$ or 0.5 , the target demand would be totally
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2 420 satisfied in any scenario, and there would be only a minimal deviation to the objective of
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5 421 supplying water with a volumetric blending of hard groundwater lower than 25%. The
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7 422 maximum volumetric blending of hard groundwater was 26.7% in the already mentioned
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10 423 serious drought scenario.

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13 424 Finally, Fig. 3 shows the variation of the *PI* in all scenarios for Solution \emptyset and for the capacity
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16 425 expansions solutions identified in Table 2. The scenario that covers the serious drought that
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18 426 afflicted Algarve in 2004 and 2005 is scenario #10. But other scenarios lead to a lower system
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21 427 performance in Solution \emptyset and in the lower cost solutions found $\omega^* = 1, 5$ and 10 , particularly,
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23 428 in scenarios #2, #4, #7 and #8. These scenarios include other less serious droughts that afflicted
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25
26 429 the Algarve in 1950s, 1970s, 1980s and 1990s (Vieira 2014). As shown in Fig. 3, only in the
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28 430 solution found with $\omega^* = 0.1$ or 0.5 and that implies a higher investment, it would be possible
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30
31 431 to have nearly optimal performances in all scenarios, thereby reducing some impact about the
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33 432 uncertainty associated to the natural hydrology.

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36 433 [Insert Fig. 3 approximately here]
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41 434 **4. CONCLUSIONS**

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43 435 The application of the nested optimization approach to the selected case study indicated that it
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46 436 could potentially support decision-making in real-world problems. The modeling approach
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48 437 presented here allows the evaluation of the trade-offs between system robustness and cost,
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51 438 explicitly considering uncertain factors during the system operation. The capacity expansion
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53 439 solution identified here as robust is associated with an initial investment of 28.3 million euros
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56 440 and a total cost of less than 200 million euros. That capacity expansion solution costs more than
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58 441 other solutions that show a good performance in some historic scenarios but that fail in other
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60 442 historic scenarios. Even without considering other sources of uncertainty (e.g., non-stationarity
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443 of hydrologic series, population growth, cost factors) arriving at a definitive decision on the
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2 444 capacity expansion solution of the BWS will never be straightforward. In general, if the
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4 445 decision taken is to make significant investments in the capacity expansion of the water
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7 446 systems and extreme situations do not then occur, it can be always claimed that unnecessary
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10 447 investments were made. However, relatively modest investments might not be enough to limit
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12 448 the negative impacts of extreme events to an acceptable level. The ability of the proposed
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14 449 modeling approach to generate a restricted set of potential capacity expansion solutions that can
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17 450 be studied in more detail before reaching a final decision has been effectively demonstrated.
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550 **LIST OF FIGURES**

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- 551 **Fig. 1** Conceptual representation of a multicommodity flow network with $NK = 2$ and perfect
552 mixing condition at node p
- 553 **Fig. 2** Simplified representation of the solution method
- 554 **Fig. 3** Variation of the performance index in all scenarios for Solution \emptyset and solutions found
555 with $\omega^* = 0.1, 0.5, 1, 5$ and 10

556 **LIST OF TABLES**

557 **Table 1** Summary of the current sources (CS) and the investment options (IO)

Water source	Investment ID	Firm quantity (× 10 ⁶ m ³ /year)	Costs				
			CC (×10 ⁶ €)	FOC (×10 ³ €/year)	VOC (€/m ³)		
CS		257.20	NA	NA	0.106		
	Odelouca reservoir						
	Bravura reservoir	6.00	NA	NA	0.190		
	Vale da Vila wells group*	13.00	NA	NA	0.090		
	Almádena wells group+	3.47	NA	NA	0.023		
	Inter-system water transfer						
	Santa Clara	H1	20.00	28.31	443.3	0.122	
	Sotavento	H2	18.42	35.45	348.1	0.113	
	Sea-water desalination plant	H3.O1/ H3.O2/H3.O3	7.88/ 15.77/23.65	23.03/ 41.60/56.37	1152.8/ 2004.7/2847.7	0.266/ 0.263/0.261	
	Installation of nanofiltration systems (NFS) in current wells group						
Vale da Vila	H4.O1/H4.O2	11.05/11.05	6.67/16.14	135.1/202.1	0.137/0.133		
Almádena	H5.O1/H5.O2	1.61/1.95	1.09/1.96	34.2/39.7	0.140/0.137		
IO	Rehabilitation of wells groups with local disinfection (LD) or installation of nanofiltration systems (NFS)						
	Paderne*	LD	H6.O1/	7.27/	1.41/	100.0/	0.037/
		NFS	H6.O2/H6.O3	3.09/6.18	3.37/5.35	112.6/148.3	0.150/0.147
	Torrinha*	LD	H7.O1/	3.15/	0.18/	16.4/	0.023/
		NFS	H7.O2/H7.O3	1.34/2.68	1.03/1.89	44.0/54.3	0.141/0.137
	Marco*	LD	H8.O1/	6.53/	0.73/	56.9/	0.029/
		NFS	H8.O2/H8.O3	2.78/5.55	2.48/4.26	79.0/104.5	0.143/0.140
	Ferrarias*	LD	H9.O1/	1.86/	0.12/	9.7/	0.023/
		NFS	H9.O2/H9.O3	0.79/1.58	0.62/1.13	36.3/43.1	0.145/0.140
	Medeiros*	LD	H10.O1/	2.52/	0.17/	12.9/	0.023/
NFS		H10.O2/H10.O3	1.07/2.14	0.85/1.54	40.0/48.7	0.145/0.138	

559 Note: * – Wells group locate in Querença-Silves aquifer; + – Wells group located in Almádena-Odiáxere aquifer

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580 **Table 2** Solutions obtained with $\varphi = 1$ and $\omega^* = 0.1, 0.5, 1, 5$ and 10

Weight φ	Weight ω^*	Investment options selected
1	10	H5.O2, H7.O1, H10.O1
	5	H4.O1, H5.O1, H10.O1
	1	H4.O1, H5.O1, H7.O3, H9.O3, H10.O1
	0.5	H1
	0.1	H1

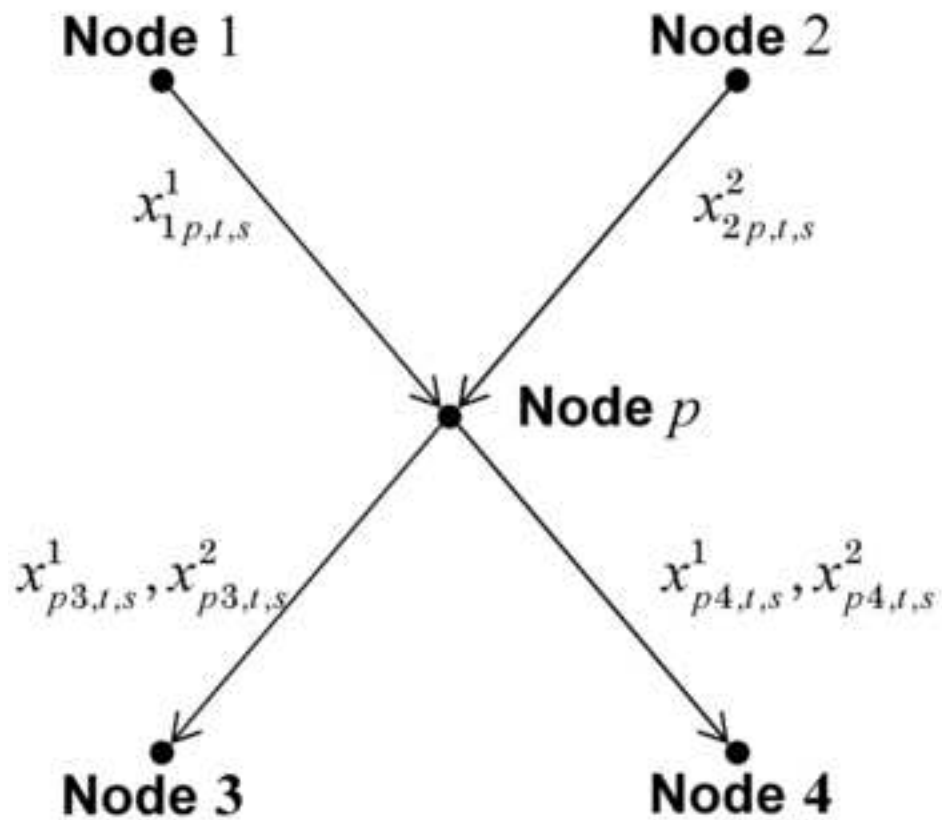
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 582 **Table 3** Summary of results for Solution \emptyset , Solution *Sup* and solutions found with
 583 $\omega^* = 0.1, 0.5, 1, 5$ and 10 (indicated in Table 2)

Solution	$E(PI_s)$	$Var(PI_s)$	$CC (\times 10^6 \text{ €})$	$PVC (\times 10^6 \text{ €})$
\emptyset	0.861	0.233	0	154.7
$\omega^* = 10$	0.929	0.135	2.31	158.6
$\omega^* = 5$	0.966	0.024	7.93	169.7
$\omega^* = 1$	0.980	0.015	10.94	177.6
$\omega^* = 0.5$ and 0.1	0.999	≈ 0	28.31	194.7
<i>Sup</i>	1	0	152.4	389.4

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 586 **Table 4** Minimum (min.), average (E) and maximum (max.) values of the performance index
 587 and the performance criteria for Solution \emptyset , Solution *Sup* and solutions found with $\omega^* = 0.1,$
 588 $0.5, 1, 5$ and 10

Solution	PI_s			Rel_s			$(1-Vul_s)$			$(1-VBld_s)$		
	min.	$E(\dots)$	max.	min.	$E(\dots)$	max.	min.	$E(\dots)$	max.	min.	$E(\dots)$	max.
\emptyset	0.602	0.861	1.000	0.818	0.972	1.000	0.738	0.950	1.000	0.250	0.663	1.000
$\omega^* = 10$	0.649	0.929	1.000	0.876	0.984	1.000	0.822	0.973	1.000	0.250	0.829	1.000
$\omega^* = 5$	0.844	0.966	1.000	0.806	0.964	1.000	0.726	0.935	1.000	1.000	1.000	1.000
$\omega^* = 1$	0.878	0.980	1.000	0.849	0.978	1.000	0.785	0.961	1.000	1.000	1.000	1.000
$\omega^* = 0.5$ and 0.1	0.994	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	0.983	0.998	1.000
<i>Sup</i>		1.000			1.000			1.000			1.000	

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Perfect mixing condition
at node p :

$$\left[\begin{array}{l} \frac{x_{p3,t,s}^1}{x_{p3,t,s}^1 + x_{p3,t,s}^2} = \frac{x_{p4,t,s}^1}{x_{p4,t,s}^1 + x_{p4,t,s}^2} \\ \frac{x_{p3,t,s}^2}{x_{p3,t,s}^1 + x_{p3,t,s}^2} = \frac{x_{p4,t,s}^2}{x_{p4,t,s}^1 + x_{p4,t,s}^2} \end{array} \right.$$

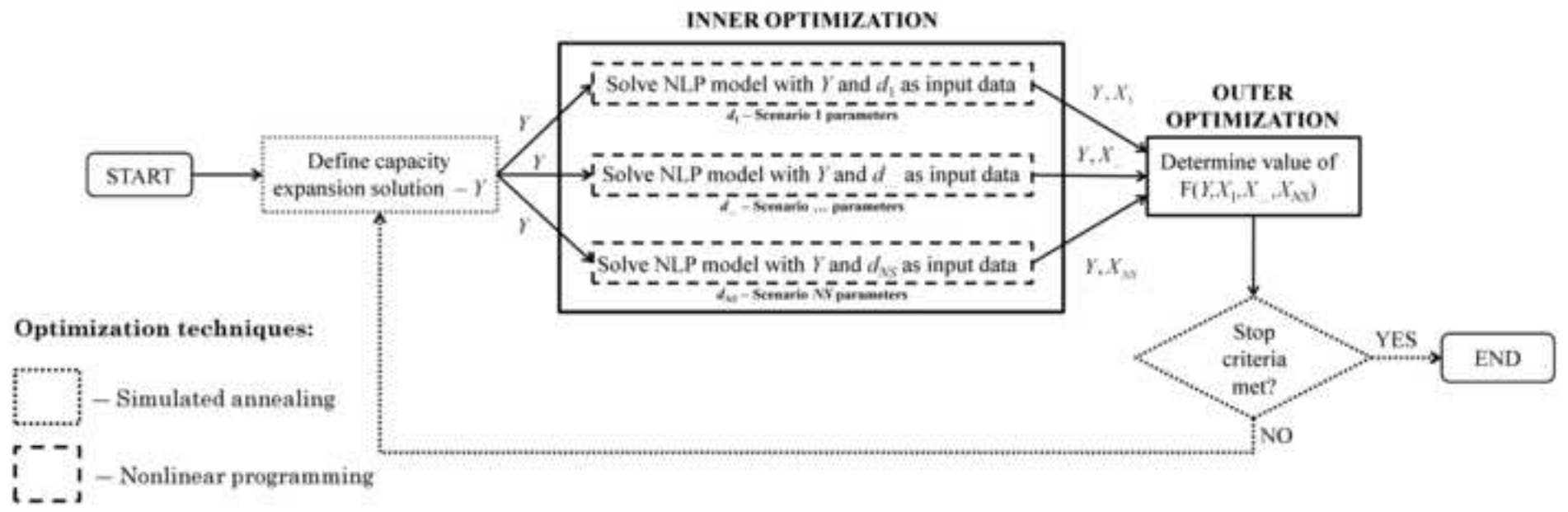


Fig3

