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1 **Potential of Interactive Multiobjective Optimization in Supporting the**
2 **Design of a Groundwater Biodenitrification Process**

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19 **Abstract:**

20 The design of water treatment plants requires simultaneous analysis of technical, economic and
21 environmental aspects, identified by multiple conflicting objectives. We demonstrated the advantages
22 of an interactive multiobjective optimization (MOO) method over a posteriori methods in an unexplored
23 field, namely the design of a biological treatment plant for drinking water production, that tackles the
24 process drawbacks, contrarily to what happens in a traditional volumetric-load-driven design procedure.
25 Specifically, we consider a groundwater denitrification biofilter, simulated by the Activated Sludge
26 Model modified with two-stage denitrification kinetics. Three objectives were defined (nitrate removal
27 efficiency, drawbacks on produced water, investment and management costs) and the interactive
28 method NIMBUS applied to identify the best-suited design without any a priori evaluation, as for
29 volumetric-load-driven design procedures. When compared to an evolutionary MOO algorithm, the
30 interactive solution process was faster, more understandable and user-friendly and supported the
31 decision maker well in identifying the most preferred solution (main design/operating parameters) to
32 be implemented. Approach strength has been proved through both sensitivity analysis and positive
33 experimental validation through a pilot scale biofilter operated for three months. In synthesis, without
34 any “a priori” evaluation based on practical experience, the MOO design approach allowed obtaining a
35 preferred Pareto optimal design, characterized by volumetric loading in the range $0.85\text{-}2.54 \text{ kg}_N \text{ m}^{-3} \text{ d}^{-1}$
36 ¹ (EBCTs: 5-15 min), a carbon dosage of $0.5\text{-}0.8 \text{ g}_{C,dos}/\text{g}_{C,stoich}$, with SRTs in the range 4-27 d.

37

38 **Keywords:** Water treatment; Interactive method; NIMBUS method; IND-NIMBUS; Decision support;
39 Pareto optimality.

40

41 **1. Introduction**

42 Designing a water treatment plant involves selecting the best process and defining the optimal
43 configuration to guarantee the required removal efficiency at the lowest global cost, standing for
44 economic and environmental costs at the same time. An effective plant design should manage multiple
45 aspects, such as water quality, available treatment technologies, operational constraints, construction
46 challenges, regulatory requirements, consumer/environmental concerns and economic feasibility

47 (Crittenden et al., 2012). Even when considering only the last aspect, one must balance between
48 treatment efficacy, investment and operational costs for treatment unit realization and running, and both
49 investment and operational costs for additional treatment units that could be required as a consequence
50 of specific drawbacks of the selected process (such as water pH variation, biomass leakage, biological
51 or chemical reactions by-products in the treated effluent) (AWWA and ASCE, 2005). Experience-based
52 design approaches, such as volumetric-load-driven procedures for biological treatment processes, do
53 not optimize design cases from both investment and management points of view, as they are based on
54 average behavior considerations (Rivas et al., 2008).

55 Thus, designing a water treatment plant represents a complex decision problem involving multiple
56 conflicting criteria (Crittenden et al., 2012). Indeed, decision support tools and methods (Hakanen et
57 al., 2013; Hamouda et al., 2009; Hartikainen et al., 2015; Maier et al., 2014; Nicklow et al., 2010; Poch
58 et al., 2004; Reed et al., 2013) are needed to support the choice of the best design highlighting the trade-
59 offs involved. Despite the broad literature on applying decision support tools for water management
60 problems (Brown et al., 2015), tools to support treatment unit design are limited and most references
61 focus on water resource systems and wastewater treatment applications. However, drinking water
62 treatment design has specificities that do not allow the direct application of results from the wastewater
63 field. For instance, adopting a biological process for drinking water treatment requires the careful
64 evaluation of typical process drawbacks that are usually neglected in the wastewater field, such as by-
65 products of (incomplete) biological reactions or biomass leakage in treated water.

66 An example of applying a biological process for drinking water production is contamination of the
67 water supply source by nitrate. Pollution by nitrate endangers public health (Dahab and Lee, 1988;
68 Kapoor and Viraraghavan, 1997; Soares, 2000; Shrimali and Singh, 2001; Magram, 2010, Sharma and
69 Sobti, 2012) and regulation limits have been imposed by US Environmental Protection Agency (US
70 EPA) and the European Commission: in Italy, the regulatory limit is set at 50 mg/L for nitrate and
71 0.5 mg/L for nitrite in drinking water. Nitrate removal is attainable through different treatment
72 processes, as catalysis, reverse osmosis, ion exchange, and heterotrophic denitrification (Kapoor and
73 Viraraghavan, 1997; Soares, 2000; Shrimali and Singh, 2001). Among the full-scale applied
74 alternatives, bionitrification is the most cost-effective, as operational costs are minimized by the

75 absence of any brine to be disposed of or treated (Soares, 2000; Shrimali and Singh, 2001; Aslan, 2008).
 76 Bionitrification exploits the bacteria ability to reduce nitrates to gaseous nitrogen in an anoxic
 77 environment, given the presence of biodegradable organic carbon which ensures anoxic conditions and
 78 acts as the electron donor (Rittman and McCarty, 2001). The main weakness of bionitrification
 79 applied to drinking water production is the sensitivity to variations in feeding and operating conditions,
 80 which can affect the overall process performance, enhancing the accumulation of nitrite. Besides, two
 81 aspects have to be considered in the risk of bacterial regrowth in distribution networks, which are
 82 usually neglected in case of wastewater: the release of biomass and the presence of readily
 83 biodegradable organic carbon in the effluent from the biological reactor. These two represent further
 84 parameters to be considered in process evaluation.

85 Tools that support optimization of multiple conflicting objectives belong to the field of multiobjective
 86 optimization (MOO). MOO methods optimize mathematical models involving multiple conflicting
 87 objective functions and allow the identification of so-called Pareto optimal solutions, reflecting the
 88 trade-offs among the conflicting objectives. A solution is called Pareto optimal if none of the objective
 89 function values can be improved without impairing at least one of the other objectives. When
 90 considering two solutions P_1 and P_2 , P_1 is said to be dominated by P_2 if P_2 is better than P_1 with respect
 91 to at least one objective and not worse than P_1 with respect to all other objectives. Thus, a Pareto optimal
 92 solution is not dominated by any other solution.

93 A MOO problem can be formulated as (Miettinen, 1999):

$$\text{minimize}\{z_1(\underline{x}), \dots, z_j(\underline{x}), \dots, z_m(\underline{x})\} \quad (1)$$

94 subject to

$$\underline{x} = (x_1, \dots, x_i, \dots, x_n) \in S, \quad (2)$$

95 where

$$S = \{\underline{x} \in \mathbb{R}^n \mid (lb_i \leq x_i \leq ub_i, i = 1, \dots, n) \text{ and } (p_k(\underline{x}) = 0, k = 1, \dots, eq) \text{ and } (q_h(\underline{x}) \leq 0, h = 1, \dots, ieq)\}. \quad (3)$$

96 The real-valued objective functions $z_j: S \rightarrow \mathbb{R}$ are simultaneously optimized in the feasible region $S \subset$
 97 \mathbb{R}^n , which is a set in the design space defined by the lower (lb_i) and upper (ub_i) bounds for the n design

98 variables x_i as well as equality (p_k) and inequality (q_h) constraints. By mapping a design variable vector
99 with the objective functions, objective vectors in the m -dimensional objective space are obtained. In
100 what follows, we use the terms solution and design as synonyms. The whole set of Pareto optimal
101 solutions is referred to as a Pareto front. Because the objective functions in MOO problems are typically
102 conflicting, there exist several different Pareto optimal solutions and additional preference information
103 from a human decision maker (DM) is needed to identify the most preferred solution.

104 Many MOO methods have been developed to solve complex design optimization problems and the
105 choice depends on the characteristics of the problem to be solved (Miettinen, 1999; Miettinen et al.,
106 2008; Miettinen and Hakanen, 2017); such as the number and the form of objective functions, design
107 variables and the type of preference information available from the DM (e.g., desired values of
108 objectives or acceptable trade-offs).

109 MOO methods can be classified on how they involve the DM's preferences (Miettinen, 1999): before
110 running the optimization algorithm ("a priori" methods), after having found a set of Pareto optimal
111 solutions ("a posteriori" methods) or during an iterative optimization process where the DM's
112 preferences are used to find more preferred solutions (interactive methods). Brown et al. (2015) reported
113 a dramatic increase in the use of a posteriori methods in water systems in recent years. In particular, so-
114 called evolutionary multiobjective optimization (EMO) algorithms have been assessed in water
115 resource management considering algorithmic performance evaluation and identifying future research
116 challenges (Maier et al., 2014; Reed et al., 2013). In the above-mentioned papers, decision making and
117 interactive approaches are briefly mentioned as future challenges (e.g. support through visualization).

118 Additionally, Brown et al. (2015) summarized the short history of water resource systems and
119 highlighted the use of progressive articulation of preference information in MOO (Singh et al., 2008)
120 and indicated it as an emerging research area. An example of an interactive approach is the Modelling
121 to Generate Alternatives (MGA) method and related approaches (Brill et al., 1990; Zechman and
122 Ranjithan, 2007) that have reached main stream in environmental decision making with a nice
123 connection between interactive MOO and sensitivity analysis (Reed et al., 2013). In the MGA method,
124 a small amount of solutions is given to the DM, who can provide additional information not modeled
125 or quantified. In interactive MOO methods, such information is assumed to be the preferences of the

126 DM. Brill et al. (1990), showed that “human-machine decision-making system will perform better when
127 the human is presented with a few different alternatives than when presented with a homogeneous set
128 of alternatives, as might result from sensitivity analysis”. Similarly, interactive MOO methods have
129 been seen to perform better than generating a large set of Pareto optimal solutions for the DM (Miettinen
130 et al., 2008). However, literature of drinking water treatment design rarely focuses on applying
131 interactive methods or do not consider Pareto optimality of the obtained results (Monarchi et al., 1973).
132 This paper is focused on the optimization of the design of a biological treatment plant for drinking water
133 production that tackles the process drawbacks, contrarily to what happens in a traditional volumetric-
134 load-driven design procedure. In detail, a groundwater biodenitrification filter is considered as a case
135 study for nitrate removal, taking into account two important drawbacks: effluent quality, requiring
136 specific monitoring and post-treatments, and investment and management costs. Indeed, as for the
137 former aspect, products of incomplete biological reactions and biomass leakage in treated water cannot
138 be neglected in a biofilter design for drinking water treatment. To find an optimal design to our case
139 study by active guidance of the DM, we applied the interactive NIMBUS method (Miettinen and
140 Mäkelä, 2006), implemented in the IND-NIMBUS software (Miettinen, 2006). The reason for using
141 IND-NIMBUS is that it is one of the few available implementations of interactive MOO methods and
142 it has been successfully applied to practical problems in various domains (Hakanen et al., 2013;
143 Hartikainen et al., 2015; Ojalehto et al., 2014; Steponavičė et al., 2014). In addition, we compared the
144 efficacy of IND-NIMBUS and an EMO algorithm NSGA-II (Deb et al., 2002) with its implementation
145 NGPM (Lin, 2011) to see the effect of incorporating DM’s preferences into the optimization process
146 and could identify several benefits. The biological process was modelled modifying the Activated
147 Sludge Model 1 (ASM1) (Henze et al., 2000) to take into account nitrite formation, which is usually
148 neglected in biological processes for wastewater treatment. A pilot scale biofilter, managed for about
149 three months, gave data for the validation of the optimization outputs. This work explores the
150 application of interactive MOO methods as supporting tools for process design in a novel field: drinking
151 water treatment. This application lead to new insights on the integration of MOO approaches with
152 conventional process design which can be extended to similar problems, highlighting advantages and
153 helping the choice of the most appropriate decision support tool.

154 **2. Material and Methods**

155 2.1 Design problem definition

156 The design of the denitrification biofilter has been tailored to remove nitrate from groundwater pumped
157 by Milan city supply wells, characterized by the simultaneous presence of organic pollutants, mainly
158 volatile organic compounds and pesticides. Table 1 reports the main characteristics of groundwater
159 observed during a 70 days monitoring period (three analyses per week).

160 As for the design problem, an upflow submerged biofilter (influent flow rate of 0.6 m³/h) was
161 considered, with the dosage of sodium acetate as organic carbon source to support biomass growth,
162 with stoichiometric carbon requirements of 0.70 g_C/g_{DO}, 1.69 g_C/g_{NO₃-N} and 1.27 g_C/g_{NO₂-N} (C: total
163 organic carbon, DO: dissolved oxygen, NO₃-N: nitrate, NO₂-N: nitrite), as recommended by Henze et
164 al. (2008). Analyses were performed according to Standard Methods (APHA, 2012).

165

166 **Table 1.** Main characteristics of groundwater to be treated in a biofilter. Active biomass, described as
167 suspended mg_{COD}/L (COD: Chemical Oxygen Demand), is calculated based on VSS (Volatile
168 Suspended Solids) measures considering biomass molecule as C₅H₇O₂N according to bioenergetic
169 evaluation by Henze et al. (2008).

	Symbol	Unit	Number of data	Mean	Standard Deviation	Minimum	Maximum
Temperature	T	°C	31	17.4	1.08	14.6	18.8
pH	pH	-	31	7.3	0.12	7.0	7.5
Dissolved Oxygen (DO)	S _{o,in}	mg _{DO} /L	29	6.2	0.55	5.0	7.2
Nitrate	S _{NO₃,in}	mg _{NO₃-N} /L	30	8.9	0.65	7.7	10.0
Nitrite	S _{NO₂,in}	mg _{NO₂-N} /L	24	0.01	0.025	0.00	0.09
Total Organic Carbon (TOC)	S _{S,in}	mg _C /L	4	< 1	-	-	-
Active biomass	X _{BH,in}	mg _{COD} /L	19	0.81	0.090	0.00	0.28

170

171 The design optimization was performed through an iterative procedure involving the biofilter simulation
172 model (Section 2.2), the optimizer (Section 2.3) and two data exchanger tools (Supporting Information
173 S1). After system initialization (Section 2.4), MOO methods were applied. By systematically varying
174 the design variable values, the optimizers generated different designs whose performance was evaluated

175 by the simulation model in terms of the objective and constraint function values, finally, leading to a
176 Pareto optimal design.

177 A pilot scale groundwater denitrification biofilter was built for the validation of MOO outputs: a
178 biological upflow submerged filter (Biofor®, Degrémont; $V = 0.2 \text{ m}^3$) with expanded clay as biomass
179 support (Biolite®, Degrémont; $d_{50} = 3.5 \text{ mm}$). The flow rate was maintained constant at $0.6 \text{ m}^3/\text{h}$,
180 implying an upflow rate of 8.3 m/h . In addition to organic carbon dosage, phosphorus (P) was dosed
181 setting the phosphorus to nitrogen (N) ratio at 0.05 gP/gN , to consider both aerobic and anoxic
182 metabolism requirements (Tang et al., 2011). Thus, the validation of the optimization results was done
183 through data collected during tracer tests (Supporting Information S2) and during a stationary phase of
184 the biological processes that lasted about three months.

185 2.2 Biofilter simulation model

186 The modeling of the denitrification biofilter was performed through AQUASIM 2.0 - EAWAG
187 (Reichert, 2008). Biofilter hydraulics was modeled through a series of eight Continuously Stirred Tank
188 Reactors (CSTRs), which permits easy simulation of a Plug Flow Reactor with a low to moderate axial
189 dispersion ($d = 0.05 - 0.07$) (Tchobanoglous et al., 2014). Each CSTR had the same constant volume
190 (V_{cstr}) 12.5% of the reactor volume (V_r). A fraction (Q_{rec}) of the influent flow rate was assumed to be
191 recirculated to simulate biomass retention in each compartment and calculated from V_r and sludge
192 retention time (SRT) as:

$$Q_{\text{rec}} = \frac{V_r}{\text{SRT}} \quad (4)$$

193 Biological processes occurring in the reactor were modeled through a modification of ASM1. They are
194 biological growth in aerobic and anoxic conditions (both on nitric and nitrous nitrogen), biomass decay
195 and organic compounds hydrolysis, as reported in Supporting Information S3 together with
196 stoichiometric coefficients, process rates and parameters.

197 The ASM1 process rates were modified with 2-step denitrification kinetics from Magrì and Flotats
198 (2008) and Kornaros and Lyberatos (1998), describing respectively a denitrifying biomass with a nitrite
199 reduction rate considerably greater than the nitrate reduction rate and a nitrite accumulating biomass
200 (nitrite reduction kinetic inhibited by nitrate presence). The modified model was formulated to predict

201 incomplete denitrification both in terms of nitrate residuals with complete degradation of nitrite and
202 nitrite accumulation. Once having set influent water inflow (Q) and characteristics (Table 1), design
203 and operating parameters, the model calculates the state variable values of the biological system at the
204 stationary phase. The state variables were the concentration of dissolved nitrate (S_{NO_3}), nitrite (S_{NO_2}),
205 oxygen (S_O) and organic substrate (S_S) as well as the content of active biomass (X_{BH}), particulate non-
206 biodegradable products arising from biomass decay (X_P) and slowly biodegradable substrate arising
207 from particulate decay (X_S).

208 2.3 Multiobjective design optimization problem

209 The aim of the optimization of the biofilter design was minimizing nitrate concentration in the effluent,
210 investment and maintenance costs and effluent quality, in terms of carbon and nitrite concentration, in
211 order to contain post-treatment requirements. To formulate this problem, three design variables (DVs)
212 and three objective functions (OBJs) were identified.

213 The design variables represent design and operating parameters most significantly affecting the design
214 performances:

- 215 - DV₁: reactor volume V_r (ranging between 50 L and 1200 L),
- 216 - DV₂: readily biodegradable substrate being externally added C_{dos} (dosed carbon, as COD, ranging
217 between 0 mg_{COD}/L and 200 mg_{COD}/L),
- 218 - DV₃: sludge retention time SRT (ranging between 1 d and 100 d).

219 The objective functions are:

- 220 - OBJ₁: nitrate removal efficiency, as the residual concentration in the effluent (NO_3-N_{out}),
- 221 - OBJ₂: total cost of the plant considering both investment and operating costs ($Costs$),
- 222 - OBJ₃: quality of the biofilter effluent, both in terms of organic carbon and nitrite concentration
223 (COD_{out}).

224 A detailed description of their definition is reported in Supporting Information S4.

225 Functions OBJ₁ to OBJ₃ to be minimized are respectively expressed as nitric nitrogen concentration in
226 the effluent:

$$OBJ_1 = NO_3 - N_{out} \left[\frac{mg_N}{L} \right] = S_{NO_3}, \quad (5)$$

227 as the sum of costs of reactor realization, reagent consumption for carbon supply, energy consumption
 228 for backwashing and sludge disposal:

$$\begin{aligned}
 OBJ_2 &= Costs[\text{€}] \\
 &= 0.8 \frac{\text{€}}{L} \cdot V_R + 10yr \\
 &\cdot \left(C_{dos} \cdot 27.92 \frac{\text{€} \cdot L}{yr \cdot mg} + \frac{1}{t_{cycle}} \cdot 160.3 \frac{\text{€} \cdot h}{yr} + \frac{\Delta M_{TOT,bw}}{t_{cycle}} \cdot 1.314 \right. \\
 &\left. \cdot 10^{-3} \frac{\text{€} \cdot h}{yr \cdot mg} \right)
 \end{aligned} \tag{6}$$

229 and as the sum of organic carbon and nitrous nitrogen concentrations in the effluent as COD:

$$OBJ_3 = COD_{out} \left[\frac{mg_{COD}}{L} \right] = S_S + S_{NO_2} \cdot 1.71 \frac{mg_{COD}}{mg_N}. \tag{7}$$

230 The symbols used have already been introduced, except for $\Delta M_{tot,bw}$, in (6) which is sludge removal for
 231 a single backwashing and t_{cycle} which is the treatment cycle duration, both calculated from the definition
 232 of SRT and the backwashing procedure reported by Richard (Richard, 1989) on real scale Biofor^(R)
 233 through equations detailed in Supporting Information S4.

234 Constraints were set on state variables influencing the biological system and the OBJ values to consider
 235 two conditions that cannot be violated, but that are not already stated in the simulation model:

236 - CONSTR₁: maximum acceptable particulate matter accumulation:

$$CONSTR_1: \overline{X_{TOT}} \leq 6750 \frac{mg_{COD}}{L} \tag{8}$$

237 - CONSTR₂: maximum acceptable value for nitric nitrogen concentration in the effluent:

$$CONSTR_2: S_{NO_3} \leq 8.5 \frac{mg_N}{L}. \tag{9}$$

238 The first constraint limits particulate matter concentration under the value corresponding to 75% of
 239 reactor voids filled by particulate matter; while the second constraint assures a nitric nitrogen
 240 concentration lower than 75% of the regulation limit on drinking water.

241 It has to be noted that no constraint has been set on nitrous nitrogen and organic carbon concentrations
 242 in the effluent, even though a regulation limit does exist especially for nitrous nitrogen. This is because
 243 no drinking water treatment plant would supply the effluent of a bionitrification unit as it is: post-
 244 treatments have to be provided, at least for safety reasons in case of malfunctioning. Thus, nitrite and

245 organic carbon concentrations in the biofilter effluent have to be minimized rather than keeping below
246 regulation limits to minimize costs of the required post-treatments. Consequently, this evaluation is
247 integrated in the optimization problem in OBJ₃ instead of adding specific constraints.

248 2.4 Multiobjective optimization methods

249 To solve the design problem, the interactive MOO method NIMBUS was applied and its performance
250 compared to an EMO algorithm. Typically, interactive methods calculate few Pareto optimal solutions
251 based on the preference information specified by a human DM and iteratively support the DM in finding
252 the most preferred solution. The synchronous NIMBUS method (Miettinen and Mäkelä, 2006) was
253 applied, implemented in the IND-NIMBUS software framework (Miettinen, 2006; Ojalehto et al.,
254 2014).

255 NIMBUS starts by computing the ranges of the OBJ values in the Pareto front and an initial Pareto
256 optimal solution, which is shown to the DM. If the DM is satisfied, the most preferred solution has been
257 found. Otherwise, the DM is asked to express preferences on how the solution should be changed to get
258 a more preferred solution. This is done through a classification of the OBJs, indicating whether their
259 values at the current Pareto optimal solution:

- 260 1. should be improved as much as possible,
- 261 2. should be improved up to a given bound,
- 262 3. are acceptable as they are,
- 263 4. are allowed to impair till a given bound, or
- 264 5. may change freely at the moment.

265 Because of Pareto optimality, if some OBJ is improved, some others should be allowed to impair. The
266 classification information of the DM is considered when new Pareto optimal solutions are computed
267 (up to four in the synchronous NIMBUS method). These solutions are then shown to the DM who can
268 select the most preferred of them and either stop or classify again. This iteration continues until the DM
269 is satisfied and is convinced that better solutions do not exist. The interaction is enabled through a
270 graphical user interface of IND-NIMBUS (see an example screenshot in Supporting Information S5).
271 Pareto optimal solutions are computed by converting the MOO problem with the preference information
272 into single objective optimization sub-problems, which are solved with appropriate optimizers. In the

273 present work, they were solved with the differential evolution optimizer (Storn and Price, 1997) (with
274 6000 maximum iterations allowed, with maximum 400 generations, crossover rate of 0.9, and F factor
275 of 0.8).

276 Contrary to interactive methods, EMO algorithms operate with a set of solutions (called a population)
277 whose evolution through different iterations (called generations) selects nondominated solutions
278 providing an approximation of the Pareto front after a number of generations. No expression of
279 preferences is required from the DM up to the final choice of the most preferred solution from the final
280 nondominated set. As an EMO algorithm, the commonly used NSGA-II algorithm (Deb et al., 2002)
281 and its Matlab implementation NGPM (Lin, 2011) were used. In NSGA-II, a population of solutions
282 is initialized randomly. Then, for each generation, the population evolves by using genetic operators
283 (selection, crossover and mutation) that include randomness to obtain a new population that is both
284 closer to the Pareto front and as diverse as possible. After the maximum number of generations, the
285 output is a set of nondominated solutions that is used to approximate the Pareto front (the parameters
286 for NGPM were: population size 100 points with 100 generations, crossover rate 1.2 and mutation
287 probability 0.5).

288 2.5 Sensitivity analysis

289 A sensitivity analysis was performed to test the robustness of the solutions and generalize the efficacy
290 of the MOO method in solving the design problem: case-study specific parameters and the adopted
291 biofilter simulation model were changed and the obtained MOO solutions were compared.

292 First, the variability of the optimization results was assessed due to the variation of four parameters,
293 with considered values in parentheses:

- 294 - nitric nitrogen concentration in raw water ($\text{NO}_3\text{-N}_{\text{in}}$, tested values: 4.5 mg_N/L, 20 mg_N/L,
295 30 mg_N/L);
- 296 - influent flow rate (Q, tested values: 0.3 m³/h, 1.2 m³/h, 1.8 m³/h);
- 297 - biomass concentration in backwashing water ($X_{\text{TOT,bw}}$, tested values: 100 mg_{COD}/L, 400 mg_{COD}/L,
298 600 mg_{COD}/L);
- 299 - dispersion in the biofilter simulated through a different number of CSTRs in series (*n*, tested values:
300 4 and 6).

301 Then, the effect of simulation model variation was studied considering two different simulation models
302 presented in Kornaros and Lyberatos (1998) and Magrí and Flotats (2008), characterized by process
303 rates and parameters described in Supporting Information S6.

304 **3. Results and Discussion**

305 A preliminary assessment of the MOO problem was performed through a feasible region investigation
306 by generating 3000 random points between the upper and lower bounds of the DVs and simulating the
307 system for each point. The feasibility of the points was checked by evaluating the corresponding
308 constraint function values and the ratio of feasible points was calculated to identify which constraint
309 was limiting. Results are summarized in Supporting Information S7. This analysis permits to highlight
310 the conflicts among OBJs: while a reduction of COD_{out} (OBJ_2) and costs (OBJ_1) can be achieved
311 concurrently, both OBJs conflict with $\text{NO}_3\text{-N}_{\text{out}}$ concentrations (OBJ_3). The conflict is especially critical
312 in case of desired OBJ_3 values below $0.2 \text{ mg}_\text{N}/\text{L NO}_3\text{-N}_{\text{out}}$. The DM's role, hence, is to find the preferred
313 balance of such conflicting objectives.

314 3.1 Multiobjective optimization through IND-NIMBUS

315 The optimization applying IND-NIMBUS was started by evaluating the ranges of the OBJs (so-called
316 nadir and ideal objective vectors) (Miettinen, 1999) and a first Pareto optimal solution, reported in Table
317 2 (iteration 1). Then, an iterative solution process guided by the DM's preference information (as
318 classification, see Section 2.4), was conducted resulting in Pareto optimal solutions reported in Table 2
319 (iterations 2-4). All the solutions generated are shown in Figure 1.

320 The ideal and the nadir objective vectors showed that solutions do exist that are able to perform
321 complete $\text{NO}_3\text{-N}$ removal (ideal $\text{OBJ}_1 = 0$) or to assure almost no worsening of effluent quality (ideal
322 $\text{OBJ}_3 = 0$), but not simultaneously.

323 The first Pareto optimal solution (solution 1) allows an 87% nitrate nitrogen removal with 7202 euro
324 costs ($12003 \text{ euro}\cdot\text{m}^{-3}\cdot\text{h}$) and COD effluent concentration of about $1.16 \text{ mg}_{\text{COD}}/\text{L}$. Higher nitrogen
325 removal efficiencies are reported in the literature for full scale drinking water biodenitrification units
326 (Richard, 1989), and an efficiency higher than 90% is reported for pilot scale units (Matějů et al., 1992).
327 Furthermore, the low level of COD_{out} limits post-treatment requirements but it can correspond to a
328 dramatic contribution of nitrous nitrogen considering the low value of dosed carbon (49% of

329 stoichiometric requirements). Thus, further optimization was needed and the DM started providing
 330 preference information to find more preferable solutions.

331

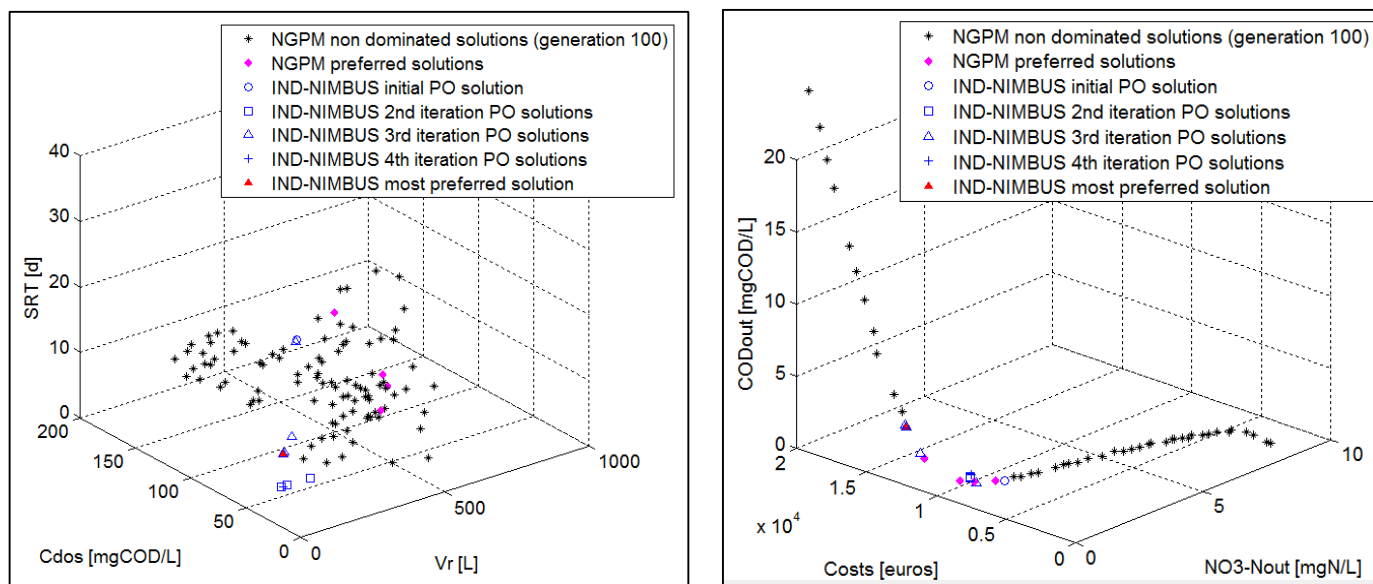
332 **Table 2.** Pareto optimal solutions generated by IND-NIMBUS and DM's preference information at
 333 different iterations. The most preferred Pareto optimal solution is highlighted in grey.

NIMBUS iteration	Pareto optimal solution	DM's Preference Information					DV1	DV2	DV3	OBJ1	OBJ2	OBJ3
		MOO Starting Point	OBJ that should improve	OBJ acceptable as it is	OBJ allowed to impair	OBJ that may change freely	V _r	C _{dos}	SRT	NO ₃ -N _{out}	Costs	COD _{out}
							[L]	[mg _{COD} /L]	[d]	[mg _N /L]	[euros]	[mg _{COD} /L]
1	Nadir	-	-	-	-	-	-	-	-	8.89	56,100	158
	Ideal	-	-	-	-	-	-	-	-	0	41.3	0.2
	1	-	-	-	-	-	83	25.4	26.8	1.13293	7,202	1.16173
2	2	1	OBJ3 (as much as possible)	OBJ1	-	OBJ2	52	31.4	4.1	0.71954	8,921	1.12766
	3						151	31.3	4.1	0.73631	8,961	1.12750
	4						73	31.3	4.1	0.72356	8,909	1.12768
3	5	4	OBJ1 (as much as possible)	-	-	OBJ2 OBJ3	101	42.8	7.5	0.00019	12,169	4.07301
	6						107	42.9	7.6	0.00017	12,214	4.17777
	7						117	39.0	10.2	0.00117	11,115	2.56437
	8						89	27.9	26.1	0.40238	7,898	1.27773
4	9	1	OBJ1 (up to 0.89 mg _N /L)	-	OBJ2 (up to 10000€) OBJ3 (up to 2 mg _{COD} /L)	-	57	31.3	4.1	0.75324	8,875	1.27357

334

335 To demonstrate the DM's role in the solution process, we discuss here some particular aspects. At the
 336 second iteration, the DM accepted the OBJ₁ value as it is, asking to improve as much as possible OBJ₃
 337 and letting OBJ₂ change freely. Three Pareto optimal solutions were computed with a negligible
 338 difference in performances. A little improvement was obtained in OBJ₃ (2.9% reduction of COD_{out}
 339 value) thanks to a higher carbon dosage (61% of stoichiometric requirements), that implied an
 340 improvement in OBJ₁ (36% reduction). As the dosed carbon was still lower than stoichiometric
 341 requirements, the risk of incomplete denitrification still existed and the nitrous nitrogen contribution to
 342 COD_{out} could be relevant. Thus, the DM started iteration 3 from solution 4. After the preferences had
 343 been expressed, four more Pareto optimal solutions were computed, with almost complete NO₃ removal,
 344 higher costs and higher values of COD_{out}. The results suggested to the DM that a 90% NO₃ removal

345 (0.89 mg_N/L NO₃-N_{out}), with costs around 10,000 euros and COD_{out} concentration around 2 mg_{COD}/L
 346 could be a good trade-off.
 347



348 **Figure 1.** Nondominated solutions found with NGPM (generation 100) and Pareto optimal solutions
 349 found with IND-NIMBUS in the design space (a) and in the objective space (b).

350
 351 The obtained Pareto optimal solutions were few and thus easy to compare, but carrying relevant
 352 information supporting the choice of the most preferred design and insight about the feasibility of the
 353 preferences expressed.
 354 Indeed, some trade-offs clearly appeared to the DM. First of all, the iterations guided by the DM's
 355 preference information rapidly reached solutions assuring almost complete nitrate removal (solutions 2
 356 - 9) at acceptable costs, but also that the lowest OBJ₃ value for Pareto optimal solutions is 1.13 mg_{COD}/L.
 357 It also showed that Pareto optimal solutions can be obtained with a dosed carbon lower than the
 358 stoichiometric requirements, since the simulation model takes into account the organic carbon available
 359 from biomass decay (endogenous organic carbon). However, supplying carbon under the stoichiometric
 360 level does not assure the complete removal of nitrous nitrogen, which can represent an important
 361 fraction of the OBJ₃ value. Therefore, the iterative comparison of solutions showed to the DM a critical
 362 issue: obtained values for OBJ₃ are difficult to be fully evaluated: the minimum value of OBJ₃

363 corresponded to an acceptable concentration of residual carbon ($0.42 \text{ mg}_C/\text{L}$), in case of complete
364 denitrification, but it corresponded also to an unacceptable value of $\text{NO}_2\text{-N}$ ($0.66 \text{ mg}_N/\text{L}$), in case of
365 incomplete denitrification. Thus, the iterative process revealed a difficulty in identifying the acceptable
366 level of impairment for OBJ_3 , as it aggregates the concentrations of $\text{NO}_2\text{-N}$ and TOC in the effluent
367 water. The results suggested that further studies should be performed, with the implementation of a
368 fourth OBJ (splitting OBJ_3 in two), which offers a more informative optimization model.

369 Considering what has been outlined so far, solution 5 represented the most preferred design to be
370 implemented. Compared to other Pareto optimal solutions, it involves a higher COD_{out} value. However,
371 it assures a high removal of nitric nitrogen ($>90\%$, $\text{NO}_3\text{-N}_{\text{out}} < 0.89 \text{ mg}_N/\text{L}$) with a SRT value that
372 implies good biomass retention, good endogenous carbon and carbon dosage equal to 83% of the
373 stoichiometric requirements that, together, are more likely to involve complete denitrification with a
374 high TOC contribution and almost zero $\text{NO}_2\text{-N}$ contribution to the COD_{out} value (accepted to be around
375 $4 \text{ mg}_{\text{COD}}/\text{L}$). Overall, the interactive solution process enabled the DM to learn about the
376 interdependencies of the objectives and the feasibility of expressed preferences and get convinced of
377 the goodness of the solution found.

378 Finally, considering the calculation time, 8 hours were needed for the problem initialization but only 2
379 hours were necessary for each optimization. This calculation time was still regarded as acceptable but
380 it would have also been possible to employ an approach directed to computationally expensive problems
381 as e.g. in Steponavičė et al. (2014).

382 Despite the calculation time, the application of IND-NIMBUS was intuitive and user-friendly from the
383 DM's point of view, since she was not asked to understand the working principles of the optimization
384 algorithm. The limited number of solutions to compare helped the DM in the choice of the best suited
385 one. Lastly, the iterative procedure gave a deeper insight on relationships among objectives, increasing
386 the ability and the confidence in choosing the optimal design to be implemented, without neglecting
387 potentially interesting portions of the Pareto front.

388 3.2 Multiobjective optimization through NGPM

389 The NGPM software, where no preferences are considered, was also applied to study the effect of
390 including DM's preferences into the optimization. The NGPM optimization took 10.35 hours and

391 generated 100 nondominated points with an increasing ratio of feasible points for each population
 392 (reaching 100% at generation 3). As it is typical of EMO methods, Pareto optimality of solutions is not
 393 assured and it is only known that they are nondominated. In this sense, the population obtained at
 394 generation 100 represented an approximation of the Pareto front. Smallest and largest values for each
 395 objective in the final population are reported in Table 3.

396

397 **Table 3.** Main descriptive statistics of nondominated solutions produced by NGPM (generation 100).

	DV₁	DV₂	DV₃	OBJ₁	OBJ₂	OBJ₃
	V_r	C_{dos}	SRT	NO₃-N_{out}	Costs	COD_{out}
	[L]	[mg_{COD}/L]	[d]	[mg_N/L]	[euro]	[mg_{COD}/L]
Minimum	75	5	5	$2 \cdot 10^{-6}$	1,619	0.3
Maximum	984	200	34	8.50	56,409	158

398

399 When considering the aim of the optimization, a single Pareto optimal design to be implemented had to
 400 be found among the 100 nondominated solutions obtained and therefore a choice by the DM was needed
 401 based on her experience. In fact, it should be stressed that EMO methods do not give any additional
 402 information to help the DM's choice. The NGPM optimization gave indications on the most suitable
 403 range of values for V_r and SRT design variables (Table 3), but no suggestion could be deduced about
 404 C_{dos}, which involves a wide range of design performances. The choice could be made by visually
 405 analyzing the objective space in a 3D plot, because the problem had only three objectives (this is no
 406 more possible if the number of OBJs is higher). Thus, in this case, the most preferred solution could be
 407 sought among solutions with NO₃-N_{out} lower than 1 mg_N/L and COD_{out} lower than 5 mg_{COD}/L. This
 408 corresponded to the four preferred solutions that are shown in Figure 1, characterized by V_r, SRT and
 409 C_{dos} respectively equal to 231 - 444 L, 11 - 28 d and 26 - 37 mg_{COD}/L (corresponding to C_{dos}/C_{stech} equal
 410 to 50-70%). The carbon dosage of these solutions is too low since with a carbon dosage lower than
 411 stoichiometric requirements, the risk of incomplete denitrification increases as C_{dos}/C_{stech} ratio
 412 decreases. However, it appeared to be complicated to find a proper solution among the NGPM solutions
 413 with a lower COD_{out}, which is obtained through a higher dosage of carbon and acceptable values of the
 414 other two objectives.

415 3.3 Discussion and validation of optimization results

416 The presented results showed that MOO is a valuable tool for drinking water treatment design
417 optimization, with strengths and weaknesses depending on the applied method. When comparing
418 solutions found with the two optimization methods, one must keep in mind that NGPM solutions are
419 only nondominated while IND-NIMBUS solutions are assured to be Pareto optimal (if the single
420 objective optimizer guarantees optimality). Then, a comparison can be done by checking if the IND-
421 NIMBUS solutions belong to the region of design and objective spaces where NGPM solutions are
422 concentrated. Considering results reported in Tables 2 and 3, all IND-NIMBUS solutions have reactor
423 volume values on a different range compared to NGPM and the same can be said about SRT values of
424 solutions 1 and 9. This indicates that Pareto optimal solutions found with IND-NIMBUS do not overlap
425 with nondominated solutions found with NGPM. Thus, NGPM did not find solutions that the DM found
426 with IND-NIMBUS, as visualized in Figure 1 in both design and objective spaces.

427 General considerations on biofilter optimal design can be drawn by normalizing IND-NIMBUS results:
428 Pareto optimal solutions resulted to be characterized by volumetric loading in the range 0.85-
429 $2.54 \text{ kg}_N \text{ m}^{-3} \text{ d}^{-1}$ (with EBCTs in the range 5-15 min) and a carbon dosage of 0.49-0.83 $\text{g}_{C,dos}/\text{g}_{C,stoich}$,
430 with SRTs in the range 4-27 d. Pareto optimal solutions in these ranges are expected to involve a nitric
431 nitrogen removal efficiency of 87-100%, with 809-1573 $\text{€g}_{N,removed}$ and $0.04 \pm 0.097 \text{ g}_{COD,out}/\text{g}_{COD,in}$, with
432 the COD content in the effluent being made up both by residual carbon and nitrite.

433 Considering the performances of the pilot scale biofilter built for the validation of the MOO results
434 (data not shown), it has to be reported that applying the suggested carbon dosage for volumetric loadings
435 and EBCTs led to lower nitric nitrogen efficiencies (40-75%) with average COD_{out} equal to
436 $4.8 \text{ mg}_{COD}/\text{L}$, but with peaks of nitrous nitrogen up to $5.4 \text{ mg}_N/\text{L}$. On the contrary, higher efficiencies
437 (55-100%) were obtained for volumetric loadings and EBCTs in the proposed ranges but with a carbon
438 dosage of 1.05-1.34 $\text{g}_{C,dos}/\text{g}_{C,stoich}$ with average COD_{out} equal to $7.4 \text{ mg}_{COD}/\text{L}$ but composed by residual
439 organic carbon for 87% on average. These observations confirm the need of splitting the third objective
440 in two, for a better optimization of nitrous nitrogen concentration in the effluent as a function of the
441 dosed carbon.

442 When comparing the applied optimization methods, the reported results proved that NGPM can be
443 applied to get an approximation of the Pareto front, keeping in mind that the distance from the real
444 Pareto front is unknown and decreases only by increasing the number of generations. Thus, it can be
445 applied if the purpose of the optimization is the estimation of possible trade-offs. However:

- 446 - If the purpose is finding the most preferred Pareto optimal solution as the design to be
447 implemented, NGPM is not able to identify it and further optimizations or analyses are needed.
- 448 - NGPM results can give some indications to help the DM's choice of the most preferred solution,
449 but an unsupported choice has to be made mainly based on the DM's experience.
- 450 - The evaluation of the NGPM results has to be done by plotting them in the design and objective
451 spaces. However, this is possible only for up to three dimensions and in higher dimensions
452 other visualizations are needed (Miettinen, 2014).

453 On the contrary, IND-NIMBUS has not been intended for studying the whole Pareto front but to help
454 the DM in finding her/his preferred Pareto optimal solution. IND-NIMBUS proved to be well suited for
455 the design problem considered:

- 456 - It allowed obtaining Pareto optimal solutions, whose evaluation was supported by an easy
457 visualization of the results. This enables also the consideration of a higher number of objectives.
- 458 - It allowed performing multiple optimization iterations that increased DM's knowledge on the
459 MOO problem in the areas of interest. It also showed the best and the worst design
460 performances in terms of defined objectives and revealed the need for a better MOO problem
461 formulation (i.e., by splitting the third objective into two distinct ones for a better evaluation of
462 required post-treatments).
- 463 - The DM's choice was effectively supported to find the most preferred design to be implemented
464 and the DM was not overloaded by having to study too much information at a time.

465 3.4 Sensitivity analysis results

466 A sensitivity analysis was performed evaluating the variation of the feasible region, NGPM and IND-
467 NIMBUS results and detailed outputs are available in Supporting Information S8.

468 The feasible region analysis appeared to be affected mainly by nitric nitrogen concentration in the
469 influent: increasing values of $\text{NO}_3\text{-N}_{\text{in}}$ decreased the number of feasible solutions, because of an
470 increasing number of points violating constraint 2 (adequate nitrate removal).

471 As for IND-NIMBUS, the sensitivity analysis was conducted performing five steps of the interactive
472 method to identify the most preferred design, for each different MOO problem. The obtained results
473 revealed that the greatest variations of DVs and OBJ values for the most preferred design, were
474 associated with $\text{NO}_3\text{-N}_{\text{in}}$ variation (+736% DV_1 value), and the application of 4-CSTRs model (+698%
475 DV_3 value) and Magrì and Flotats (2008) model (+654% DV_1 value and 1105% DV_3 value).

476 As for NGPM, the highest variations were observed varying influent flow rate that led to reactor volume
477 variation up to +255%, involving a cost variation of +208%. However, the nondominated solutions
478 were also significantly affected by $\text{NO}_3\text{-N}_{\text{in}}$: increasing values increased both the reactor volume (up to
479 +95%) and the dosed carbon (up to 198%) leading to designs with higher costs (up to 196%) but also
480 higher residual concentrations in the effluent of $\text{NO}_3\text{-N}$ (up to +56%) and COD (up to +189%). Lower
481 but remarkable variations were observed increasing hydraulic dispersion (e.g. for lower number of
482 CSTRs in series) and applying the simulation model of Magrì and Flotats (2008): the former involved
483 higher values of SRT (up to +126%), while the latter identified designs with higher reactor volumes (up
484 to +174%) and higher values of $\text{NO}_3\text{-N}_{\text{out}}$ (up to +63%).

485 The presented results allowed generalizing the efficacy of the proposed MOO approach indicating that
486 $\text{NO}_3\text{-N}_{\text{in}}$ is the most important parameter affecting the optimization results, together with influent flow
487 rate, hydraulic dispersion in the reactor and the considered simulation model.

488 **4. Conclusions**

489 Reported results show that it is beneficial to formulate a denitrification biofilter design problem as a
490 multiobjective optimization problem. We demonstrated that applying an interactive MOO method
491 offers advantages over a widely used a posteriori evolutionary algorithm and, thus, it is necessary to
492 choose the correct MOO method to find the most preferred Pareto optimal design to be implemented.
493 Considering the specific design problem of a pilot scale biofilter for groundwater biodenitrification,
494 results showed that:

- 495 - The interactive method was the most suitable one, effectively supporting the design process up
 496 to the identification of the final, most preferred, Pareto optimal design.
- 497 - General considerations on biodenitrification designs can be drawn by normalizing IND-
 498 NIMBUS results: Pareto optimal designs resulted to be characterized by volumetric loading in
 499 the range $0.85\text{-}2.54 \text{ kg}_N \text{ m}^{-3} \text{ d}^{-1}$ (with EBCTs in the range 5-15 min) and a carbon dosage of
 500 $0.49\text{-}0.83 \text{ g}_{C,dos}/\text{g}_{C,stoich}$, with SRTs in the range 4-27 d. These values are expected to involve a
 501 nitric nitrogen removal efficiency of 87-100% with $809\text{-}1573 \text{ €g}_{N,removed}$ and
 502 $0.044\pm 0.097 \text{ g}_{COD,out}/\text{g}_{COD,in}$ and the COD content in the effluent made up by residual carbon
 503 and nitrite.
- 504 - Observations on a pilot scale biofilter validated the identified Pareto optimal designs. However,
 505 they also confirmed the need of splitting the third objective in two, for a better optimization of
 506 nitrous nitrogen concentration in the effluent as a function of the dosed carbon.

507 In general, the presented MOO design approach with the aid of the IND-NIMBUS software allowed
 508 obtaining a Pareto optimal design without any “a priori” evaluation based on practical experience, as in
 509 the case of volumetric-load-driven design procedures. In order to narrow and improve the range of the
 510 Pareto optimal designs, further studies should be done adopting a four-objective model by splitting the
 511 “effluent water quality” objective in two, considering nitrite and carbon concentrations separately. In
 512 that case, the efficiency of the EMO software NPGM applied would suffer further but IND-NIMBUS
 513 would still be applicable.

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 515 Causal Models and Multiobjective Optimization (DEMO), jyu.fi/demo, of the University of Jyväskylä.

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