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1 **Stochastic hydro-economic modeling for optimal management of**
2 **groundwater nitrate pollution from agricultural under hydraulic**
3 **conductivity uncertainty.**

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9 **Abstract:** In decision-making processes, reliability and risk-aversion play a decisive role. This
10 paper presents a framework for stochastic optimization of control strategies for groundwater
11 nitrate pollution from agriculture under hydraulic conductivity uncertainty. The main goal is to
12 analyze the influence of uncertainty in the physical parameters of a heterogeneous groundwater
13 diffuse pollution problem on the results of management strategies, and to introduce methods
14 that integrate uncertainty and reliability in order to obtain strategies of spatial allocation of
15 fertilizer use in agriculture. A hydro-economic modeling approach is used for obtaining the
16 allocation of fertilizer reduction that complies with the maximum permissible concentration in
17 groundwater while minimizes agricultural income losses. The model is based upon nonlinear
18 programming and groundwater flow and mass transport numerical simulation, condensed on a
19 pollutant concentration response matrix. The effects of the hydraulic conductivity uncertainty
20 on the allocation of nitrogen reduction among agriculture pollution sources is analyzed using
21 four formulations: Monte Carlo simulation with pre-assumed parameter field, Monte Carlo
22 optimization, stacking management, and mixed-integer stochastic model with predefined
23 reliability. The formulations were tested in an illustrative example for 100 hydraulic
24 conductivity realizations with different variance.

25 The results show a high probability of not meeting the groundwater quality standards when
26 deriving a policy from just a deterministic analysis. To increase the reliability several
27 realizations can be optimized at the same time. By using a mixed-integer stochastic
28 formulation, the desired reliability level of the strategy can be fixed in advance. The approach
29 allows deriving the trade-offs between the reliability of meeting the standard and the net
30 benefits from agricultural production. In a risk-averse decision-making, not only the reliability
31 of meeting the standards counts, but also the probability distribution of the maximum pollutant
32 concentrations. A sensitivity analysis was carried out to assess the influence of the variance of
33 the hydraulic conductivity fields on the strategies. The results have shown that larger the
34 variance, greater the range of maximum nitrate concentrations and the worst-case (or maximum
35 value) that could be reached for the same level of reliability.

36 **Key words** groundwater; fertilizer allocation; nitrates; uncertainty; optimization; stochastic management model

37

38 **1. Introduction**

39 Agricultural activities are often the main source of elevated nitrate concentrations in
40 groundwater (e.g., Oyarzun et al., 2007). Moreover, in the last decades the nitrate
41 concentrations in groundwater increased due to the intensive use of fertilizers in agriculture
42 (e.g., Candela et al., 2008). The need of controlling of groundwater diffuse pollution has given
43 rise to the development of an extensive legal framework in several countries. In Europe, the
44 requirements for agricultural nonpoint pollution in Europe are being ruled by a series of
45 European Directives. The Nitrates Directive (Directive 91/676/EEC), which was established in
46 1991 to reduce nitrate water pollution from agricultural sources, involves the declaration of
47 Nitrate Vulnerable Zones in which constraints are placed on inorganic fertilizer and organic
48 slurry application rates. The Drinking Water Directive (80/778/EEC and its 98/83/EC revision)
49 sets a maximum allowable concentration for nitrate of 50 mg/l, while the EU Water Framework

50 Directive (Directive 2000/60/EC; WFD), enacted in 2000, establishes a legal framework to
51 protect and restore clean water across Europe and ensure its long-term sustainable use. The
52 WFD includes groundwater in its river basin management planning, and sets clear milestones
53 for groundwater bodies in terms of delineation, economic analysis, characterization (analysis of
54 pressures and impacts), monitoring, and the design of programs of measures to ensure a good
55 status of quantity and chemical groundwater status by 2015. In addition, significant upward
56 trends in the concentration of pollutants should be identified and reversed (Directive 2006/
57 118/EC, Groundwater Directive).

58
59 In order to control and improve groundwater quality, it is necessary to implement often costly
60 management decisions, and here computer models has a basic role for simulating the impact of
61 different policies and get insight into the best options according to the objectives and
62 constraints of our problem. Modeling of nitrate contamination of groundwater in agricultural
63 watersheds has mostly been addressed in a deterministic way (e.g., Martínez and Albiac, 2004;
64 Almasri and Kaluarachchi, 2005; Candela et al., 2008; Peña-Haro et al., 2009). However,
65 because of the heterogeneous nature of most groundwater bodies and the inherent uncertain, the
66 errors involved in the predictions of future pollutant concentration can be considerable.
67 Stochastic models may provide additional insight into the risk and probability of achieving
68 groundwater standards.

69
70 One of the most difficult issues in groundwater management modeling is dealing adequately
71 with the effect of model uncertainty in optimal decision making (Wagner and Gorelick, 1987).
72 The uncertainty stems from a wide variety of factors ranging from partial knowledge about
73 aquifer properties, its boundary conditions, land use practices, on-ground pollutant loading, soil
74 characteristics, depth to water table, flow and transport parameters affecting pollutant fate and

75 transport in groundwater, to economic, regulatory and political factors. The effect of these
76 uncertainties on groundwater management at contaminated sites has been widely reported in
77 the literature, mostly for pumping remediation strategies (Freeze and Gorelick, 1999). The
78 main approaches to deal with these uncertainties can be divided into classic chance-constrained
79 programming and Monte Carlo-based methods. Chance-constrained programming allows for
80 constraints' violations up to preassigned probability levels, based on the derivation of
81 deterministic equivalents of the chance-constraints (Charnes et al., 1958; Charnes and Cooper,
82 1963). This often involves an a priori assumption of the statistical distribution of the random
83 variable (e.g. Tung, 1986; Wagner and Gorelick, 1987). For cases involving numerical models
84 of complex hydrogeology, an alternative is to generate a set of equally likely multiple
85 realizations of the hydraulic conductivity field, using then Monte Carlo analysis to assess
86 uncertainty regarding the achievement of the environmental objectives with the optimal
87 strategy (e.g., Wagner and Gorelick, 1989; Morgan et al., 1993; Feyen and Gorelick, 2004).
88 Monte Carlo methods can be further subdivided into the following simulation-optimization
89 techniques: stacking management models, Monte Carlo optimization, and mixed-integer
90 stochastic optimization with predefined reliability. All these approaches will be subsequently
91 discussed in the methodology section.

92
93 Most previous applications of these four approaches have focuses on “pump and treat”
94 alternatives for optimal remediation of contaminated aquifers. Most of these studies deal with
95 uncertainty on the hydraulic conductivity or the regional boundary conditions (e.g., Wagner
96 and Gorelick, 1989; Feyen and Gorelick, 2004), although other sources of uncertainty have
97 been also considered (eg. Van den Brink et al., 2008)

98

99 This paper presents a stochastic hydro-economic modelling framework for analyzing fertilizer
100 management strategies to control groundwater nitrate pollution under groundwater parameter
101 uncertainty. It does not intend to discuss the choice of different policy instruments for efficient
102 pollution control, topic for which an extensive literature already exists (e.g., Shortle and Griffin,
103 2001; Batie and Horan, 2004). Instead, the main contribution of this research is to analyze the
104 influence of uncertainty in the physical parameters of a heterogeneous groundwater diffuse
105 pollution problem on the results of fertilizer management strategies, and to introduce methods
106 that integrate uncertainty and reliability in order to obtain strategies of spatial allocation of
107 fertilizer use in agriculture (fertilizer standards) to meet the groundwater nitrate concentration
108 limits required by law (e.g., EU Water Framework Directive) .

109 The paper is organized as follows. First, we describe the proposed hydro-economic framework
110 and analyze four different approaches (based on Monte Carlo analysis of multiple stochastic
111 realizations) to deal with uncertainty in the pollutant concentration predictions due to uncertain
112 in the spatial variability of the hydraulic conductivity. Then, a 2D synthetic case study is used
113 to illustrate the application of the methodology.

114

115 **2. Methods**

116 The heterogeneity of hydraulic conductivity field has a strong influence on the migration and
117 evolution in time and space of the pollutant concentration in groundwater and therefore on the
118 optimal fertilizer application. The K of an aquifer can vary spatially by several orders of
119 magnitude (see, e.g., Salamon et al, 2007). To the important variability of the parameter we
120 have to add the lack of data in most practical cases. Given the uncertainty in the conductivity,
121 our groundwater flow and mass transport predictions, based on the conductivity fields, will be
122 uncertain. Therefore, the uncertainty of the K spatial variability should be incorporated into the
123 decision process in order to derive a strategy to control groundwater nitrate pollution with

124 certain reliability. This paper presents a systematic stochastic framework, using four different
125 formulations, to explicitly incorporate the effects of uncertainty through to the design of
126 reliable groundwater quality schemes. The stochastic hydro-economic modeling framework has
127 been designed for determining groundwater nitrate pollution from agriculture, considering the
128 uncertainty in the conductivity field and the reliability in the optimal strategy designed. All the
129 stochastic formulations are based upon the deterministic framework presented by Peña-Haro et
130 al. (2009). A brief description of the method is provided in the next section.

131
132 The stochastic approaches for dealing with uncertainty require the generation of multiple
133 equiprobable spatial K fields (realizations), which can be obtained by means of an appropriate
134 geostatistical approach (such as interpolation methods, sequential Gaussian or indicator
135 simulation, conditional K fields obtained from inverse models, etc.). Obviously, the uncertainty
136 in the results will be strongly influenced by the variance of the hydraulic conductivity
137 probability distribution and the spatial correlation structure. Therefore, the aquifer should be
138 characterized as adequately as possible in order to obtain reliable results. Moreover, a
139 sensitivity analysis with regard the uncertain parameters should accompany a work like this.

140

141 **2.1. Deterministic hydro-economic management model**

142 The deterministic management model for groundwater pollution control was formulated in
143 Peña-Haro et al. (2009). A holistic optimization model is used to determine the spatial and
144 temporal fertilizer application rate that maximizes the net benefits in agriculture constrained by
145 the quality requirements in groundwater at specified control sites. In accordance with the WFD,
146 the maximum concentrations at these control sites are the policy targets, which are defined by
147 imposing legal upper bounds on the concentration level of specified pollutants in water, based
148 on specific criteria such as adequate margins of safety for human or ecological health. A

149 coupled agronomic and flow and transport-groundwater modeling approach is used to quantify
 150 the relationship between emissions (i.e., nitrogen loading rates) and groundwater quality
 151 impacts at regulatory control sites. Specifically, Pena-Haro et al. (2009) compute unit response
 152 functions for each source-well pair, which is generated by simulating long-term nitrate
 153 concentration evolution at the control sites in response to uniform source loading with unit
 154 stress. The integration of the response matrix in the constraints of the management model
 155 allows simulating by superposition the evolution of groundwater nitrate concentration over
 156 time at different points of interest throughout the aquifer resulting from multiple pollutant
 157 sources distributed over time and space. Linearity of the system is required to apply
 158 superposition; therefore groundwater flow has to be considered as steady-state. The approach
 159 explicitly simulate the fate and transport of nitrates within the aquifer in the optimization
 160 model, unlike methods that use black-box statistical models such as artificial neural networks
 161 or genetic algorithms to relate on-ground nitrogen loadings with nitrate concentrations (Almasri
 162 and Kaluarachchi, 2007; Aly and Peralta, 1999; Ritzel et al., 1994).

163 The benefits in agriculture were determined through crop prices and crop production functions,
 164 being the management model for groundwater pollution control formulated as follows:

$$165 \quad \text{Max } \Pi = \sum_{s=1}^n \sum_{t=1}^T \frac{1}{(1+r)^y} A_s (p_s \cdot Y_{s,y} - p_n \cdot N_{s,y} - p_w \cdot W_{s,y}) \quad (1)$$

166

167 subject to:

$$168 \quad \sum_s RM_{cxt,sxy} \cdot cr_{sxy} \leq q_{cxt} \quad \forall c,t,y \quad (2)$$

169 where Π is the objective function to be maximized and represents the present value of the
 170 net benefit from agricultural production (€) defined as crop revenues minus fertilizer and water
 171 variable costs (fixed costs are not included); A_s is the area cultivated for crop located at source
 172 s ; p_s is the crop price (€/kg); $Y_{s,y}$ is the production yield of crop located at source s at planning

173 year y (kg/ha), that depends on the nitrogen fertilizer and irrigation water applied; p_n is the
174 nitrogen price (€/kg); $N_{s,y}$ is the fertilizer applied to crop located at source s at year y (kg/ha), p_w
175 is the price of water (€/m³), and $W_{s,y}$ is the water applied to crop located at source s at each
176 planning year y (m³); r is the annual discount rate, \mathbf{RM} is the unitary pollutant concentration
177 response matrix where each column is the nitrate concentration for each crop area (s) times de
178 number of years within the planning horizon (y), the number of rows equals the number of
179 control sites (c) times the number of simulated time steps (t) in the frame of the problem; \mathbf{q} is a
180 vector of water quality standard imposed at the control sites over the simulation time (kg/m³);
181 \mathbf{cr} is a vector representing the nitrate concentration recharge (kg/m³) reaching groundwater
182 from a crop located at source s , which is obtained dividing the nitrate leached over the water
183 that recharges the aquifer. Both nitrate leached and crop production are represented by
184 polynomial regression equations depending on the water and fertilizer use (see Peña-Haro et
185 al., 2009). These equations can be derived from the results of agronomic simulations models
186 like EPIC (Williams, 1995; Liu et al., 2007; Peña-Haro et al., 2010)

187 This modeling approach was developed under several assumptions:

- 188 ▪ No crop rotation, changes in farm management practices or changes in crop patterns are
189 considered. This issue is very important for irrigation districts and crops in which
190 farmers may react to input regulations with changes in crop patterns and crop rotation
191 practices. Rotation with crops like alfalfa is a useful management practice for
192 controlling the soil nitrate content (e.g. Toth and Fox, 1998). Changes in management
193 practices and cropping patterns are less likely in the short run than changes in the input
194 levels (Helfand and House, 1995).
- 195 ▪ The data on leaching corresponds to average water application rates. No dynamic
196 changes of irrigation applications and rainfall over time are considered.

- 197 ▪ Only restrictions on fertilizer use are considered; irrigation cutting could be also a way
198 of decreasing nitrate leaching.
- 199 ▪ The cost of the policies for controlling nitrate pollution is simplified as the direct costs
200 to the users, in terms of net income losses. Transaction costs associated with
201 introducing and maintaining a policy instrument are not considered, although they
202 might be significant in certain cases.

203 As mentioned, this formulation assumes fixed water applications and crop locations; therefore,
204 the word “optimal” is used hereinafter to refer just to the fertilization rates resulting from the
205 optimization problem defined for controlling groundwater nitrate pollution and not to better
206 irrigation plans or the most environmentally appropriate locations for growing crops.

207

208 The optimization problem is coded in GAMS, a high-level modeling system for mathematical
209 programming problems (GAMS, 2008a).

210

211 **2.2. Stochastic hydro-economic approaches**

212 The framework allows considering four different stochastic approaches to analyze groundwater
213 quality management under parameter uncertainty:

214

215 **2.2.1. Reliability of deterministic optimization. Monte Carlo simulation with pre-assumed** 216 **(“true”) parameter field.**

217 The objective is to evaluate the reliability of the optimal fertilizer application for an aquifer
218 with a pre-assumed heterogeneous hydraulic conductivity field. This is carried out by assuming
219 one of the multiple K fields generated as the “true” hydraulic conductivity field (e.g., Bark et
220 al., 2003; Ko and Lee, 2008), and determining the corresponding optimal fertilizer application.

221 The reliability of meeting the standard (or probability of not failure) and the uncertainty of the

222 pre-assumed optimal application are evaluated by simulating the resulting fertilizer allocation
223 for the series of random fields stochastically generated, and testing whether the maximum
224 concentrations are reached or not.

225

226 **2.2.2. Uncertainty on optimal fertilizer application. Monte Carlo optimization**

227 Monte Carlo management models solve the nonlinear simulation-optimization problem
228 individually for each one of a series of multiple equiprobable realizations obtained using an
229 appropriate geostatistical model. Because of its simplicity, this approach has been widely
230 applied to the design of optimal groundwater remediation strategies (e.g., Gorelick 1983;
231 Wagner and Gorelick, 1989; Freeze and Gorelick 1999; Feyen and Gorelick, 2004; Lacroix et
232 al., 2005; Ko and Lee, 2008; Van den Brink et al., 2008). In this approach, a series of individual
233 optimization problems are solved, each for a single realization of hydraulic conductivity. Each
234 one of the fertilizer applications obtained represents a random sampling from the cumulative
235 density function (CDF) of optimal fertilizer application rates. Therefore, the results of the
236 Monte Carlo hydro-economic modeling can be used to characterize the probability distribution
237 of the optimal fertilizer application rates.

238

239 **2.2.3. Multiple realizations or stacking management approach**

240 In the multiple realization or stacking approach the nonlinear simulation-optimization problem
241 is simultaneously solved for a set of different scenarios representing uncertainty, e.g., by using
242 a sampling of hydraulic conductivity realizations generated using geostatistical techniques
243 (e.g., Wagner and Gorelick, 1989; Aly and Peralta, 1999; Feyen and Gorelick, 2004 and 2005;
244 Ko and Lee, 2009). However, this approach does not allow a priori definition of the system
245 reliability. The reliability is determined through post-optimization Monte Carlo analysis on a

246 much larger set of realizations that were used in the stack. The mathematical formulation of the
247 multiple realization groundwater quality management model consist of maximize (1) subject to:
248

$$249 \quad \sum_s RM_{(c \times t, s \times y)_i} \cdot cr_{(s \times y)_i} \leq q_{(c \times t)} \quad \forall i, c, t, y \quad (3)$$

250
251 where an additional component (i) is added to the **RM** matrix considered in the deterministic
252 hydro-economic management model. This component is made up of as many elements as
253 realizations of the random conductivity field are simultaneously considered in the management
254 model. That is, the optimization problem is solved for $i = 1, \dots, s_n$, where i represents a hydraulic
255 conductivity realization, and s_n is the stack size, i.e, the number of hydraulic conductivity
256 realizations included in the stochastic management model. The optimization problem retains
257 the same number of decision variables as the deterministic model, but the number of
258 concentration constraints is increased by a factor of i . The reliability is determined through
259 post-optimization Monte Carlo analysis on a much larger set of realizations that were used in
260 the stack.

261
262 **2.2.4. Mixed-integer stochastic optimization with predefined reliability**
263 Morgan et al. (1993) introduced a mixed-integer approach to solve the problem of optimal
264 groundwater remediation design with a certain degree of reliability. The approach combines the
265 advantages of the simulation-optimization models with those of the chance-constrained models.
266 In this case, the user selects the desired degree of reliability, which is accomplished by
267 allowing a certain number of the Monte Carlo realizations to fail. Other authors have also
268 applied this technique to groundwater remediation (e.g., Ritzel et al., 1994;, Dhar and Datta,
269 2007; Ng and Eheart, 2008), which has also been termed as mixed-integer-chance-constrained
270 programming (MICCP) (Morgan et al., 1993).

271 We have reformulated the approach presented by Morgan et al. (1993) to deal with nitrate
 272 pollution abatement in order to meet certain groundwater quality standards, like the ones ruled
 273 by the EU Water Framework Directive. The proposed stochastic management problem was
 274 defined as finding the optimal fertilizer allocation (for a certain crop distribution) that
 275 maximizes the welfare from crop production that meet the groundwater quality constraints with
 276 a certain reliability.

277
 278 The chance-constrained problem is reformulated as a Mixed Integer Non-Linear Programming
 279 (MINLP). As in Morgan et al. (1993), the stochastic nature of the conductivity field is analyzed
 280 through Monte Carlo realizations, and multiple realizations make up the constraint sets of the
 281 optimization model (in this case, represented by pollutant concentration response matrices, as
 282 in Peña-Haro et al., 2009). The desired reliability of the system is predetermined by fixing the
 283 number of constraints that may be violated, which is done by replacing equations (1) and (2)
 284 with equations (4) to (7).

285
 286 The stochastic method is formulated as follows:

$$287 \quad \text{Max } \Pi = \sum_s \sum_y \frac{1}{(1+r)^y} A_s (p_s \cdot Y_{s,y} - p_n \cdot N_{s,y} - p_w \cdot W_{s,y}) - M \cdot \sum_i F_i \quad (4)$$

288
 289 subject to:

$$291 \quad \sum RM_{(c \times t, s \times y)_i} \cdot cr_{(s \times y)_i} - M \cdot f_{(c \times t)_i} \leq q_{(c \times t)_i} \quad \forall i, c, t, y \quad (5)$$

$$292 \quad \sum_{c,t} f_{(c \times t)_i} \leq M \cdot F_i \quad \forall i \quad (6)$$

294

295
$$\sum_i F_i \geq NF \quad i = 1, \dots, NR \quad (7)$$

296

297 where:

298 M is a large positive number;

299 i is the hydraulic conductivity realization number,

300 NR is the total number of realizations;

301 f is a matrix of binary integer variables, where i is the realization number, c refers to control
 302 site, t stands for simulated time step, and y is the planning year. The matrix represents the
 303 individual failures, and its components take the value 1 if the quality standard is exceeded at
 304 any time in any control site, and 0 otherwise;

305 F is a binary vector with i elements showing realization failures. It takes the value 1, thus
 306 representing a failure, if the quality standard is exceeded in at least one time step at any control
 307 site for a certain realization i , and 0 otherwise.

308 NF is the number of realization failures that are allowed, defined in accordance with the desired
 309 reliability level, R , which is given by,

310

311
$$R = 1 - \frac{\sum_i F_i}{NR} \quad (8)$$

312

313 Therefore, reliability is maintained by constraining the number of failures allowed. Note that
 314 with this formulation for each realization i , a failure ($F_i=1$) is considered when the quality
 315 standard is not met, independently on how many times or in how many control sites the quality
 316 standard is exceeded. Therefore, for a single realization i , f may exceed the quality standard in
 317 several times steps or control sites, thus leading to define F_i as a failure, i.e., $F_i = 1$. Finally,
 318 failures are penalized in the objective function as shown in (4).

319

320 Unlike the classic chance-constrained applications (e.g., Tung, 1986; Wagner and Gorelick
321 1987; McSweeney and Shortle, 1990; Wagner 1999), this formulation considers uncertainty in
322 the response matrix coefficients and does not require a priori definition of the distribution, as it
323 is required in the “classic” chance-constrained programming (Charnes et al., 1958; Charnes and
324 Cooper, 1963), in which the problem has been usually solved by transforming the probabilistic
325 constraints to deterministic equivalents given knowledge. The deterministic equivalent-based
326 methods can be solved by linear or nonlinear programming methods (e.g., Charnes and Cooper,
327 1963; Kataoka, 1963). Nevertheless, they entail a series of drawbacks such as requiring
328 assumptions of parameter distributions that may induce to errors (for mathematical
329 convenience, the most widely used statistical model is the normal distribution, e.g., Tung,
330 1986; Wagner and Gorelick, 1987), or to be unsuitable for complex nonlinear problems where
331 the deterministic equivalent may be difficult or even impossible to establish. Furthermore, they
332 become cumbersome whenever reliability is defined as the probability of meeting a set of
333 constraints simultaneously, rather than one or more (Ng and Eheart, 2008). All these problems
334 are avoided with the approach here presented. However, the chance-constrained approach has
335 also the advantage of requiring less computational effort than the multiple realization model or
336 the mixed-integer models.

337

338 **3. Illustrative example**

339 The aquifer system configuration is the same that the one used by Peña-Haro et al. (2009),
340 which apply the deterministic formulation to a 2D homogeneous synthetic aquifer. In this case,
341 however, we consider heterogeneous hydraulic conductivity.

342 The aquifer has impermeable boundaries and steady-state flow from top to bottom of the
343 domain. The finite difference grid is 500×500 meters, and the domain has 58 rows and 40

344 columns. A confined aquifer has been modeled with a thickness of 10 meters, effective porosity
345 of 0.2, and dispersivity of 10 meters. The natural recharge is 500 m³/ha. There are 70 stress
346 periods, each of one year (365 days). Seven different crop zones (pollution sources or just
347 sources in our model formulation) with five different crops are considered. For each crop a
348 quadratic production function and a leaching function have been defined (Peña-Haro et al.,
349 2009). Each source is related to a crop as shown in Figure 1. Three control sites with
350 concentration upper bounds of 50 mg/l of nitrates, as established by the EU water legislation,
351 are imposed.

352

353 [Figure 1]

354

355 The four different stochastic formulations described in section 2 were considered in order to
356 analyze the effect of parameter uncertainty on “optimal” groundwater management and
357 reliability in meeting the water quality standards. A 40 year planning horizon was considered
358 for each scenario, with a constant annual fertilizer application during the 40 years. All the
359 optimization models are coded in GAMS (GAMS, 2008a). The nonlinear optimization models
360 were solved using CONOPT (Drud, 1985), which is based on the Generalized Reduced
361 Gradient algorithm designed for large programming problems. The optimization problem
362 reformulated as a MINLP is also coded in GAMS, using the SBB solver (GAMS, 2008b),
363 combination of the standard Branch and Bound method and a standard nonlinear programming
364 solver (CONOPT in this case). The preprocessing of all the required information in the format
365 required by the GAMS code for the optimization models, including the simulations of the K
366 fields and the generation of the pollutant concentration response matrices, has been automated
367 by means of a “batch” file.

368

369 **3.1. Simulation of K fields**

370 The different stochastic optimization management formulations require the generation of
371 multiple K fields. The simulation of these K fields, in the 2D synthetic case stated above, has
372 been performed by means of a sequential Gaussian simulation using the computer code
373 GCOSIM3D (Gómez-Hernández and Journel, 1993). The stochastic structure is assumed to be
374 common for all simulated K fields, which simplifies the analysis avoiding the uncertainty on
375 the stochastic structure. Because of this, all K fields are equally likely realizations, and
376 therefore, are plausible representations of reality because they are conditional to the same data
377 and display the same degree of spatial variability.

378
379 The stochastic structure has been defined by using a spherical variogram with a range
380 approximately equal to 1/5 of the aquifer size, 0.5 of nugget effect, and sill of 4. The effect of
381 different degrees of heterogeneity of the parameters in the aquifer has been studied.
382 Specifically, a sensitivity analysis by considering two different variances of the hydraulic
383 conductivity distribution has been carried out, both with a normal distribution with mean 40
384 m/day and with variances of $15 \text{ m}^2/\text{day}^2$ (referred as “case 1”) and $60 \text{ m}^2/\text{day}^2$ (“case 2”). A
385 hundred realizations were generated for each case. We assume that this set is large enough to
386 provide a significant representation of the variability of the parameter. Figure 2 illustrates the K
387 field for the realization #1, while Figure 3 shows the frequency distribution and univariate
388 statistics for all K realizations.

389
390 [Figure 2]

391
392 [Figure 3]

393

394 **3.2. Pollutant concentration response matrices**

395 Once the different conductivity fields were generated the pollutant concentration responses
396 from unit recharge rates at the sources were simulated. The pollutant response matrix describes
397 the influence of pollutant sources upon concentrations at the control sites over time. The
398 simulated time horizon corresponds to the time for the solute to pass all the control sites, and it
399 is independent of the length of the planning period. To construct the pollutant concentration
400 response matrix the flow and transport governing equations must be solved. MODFLOW
401 (McDonald and Harbough, 1988), a finite difference groundwater flow model, and MT3DMS
402 (Zheng and Wang, 1999), a solute transport model were used. A pollutant concentration
403 response matrix was generated for each k field realization.

404

405 **3.3. Reliability of the deterministic optimization. Monte Carlo simulation.**

406 The purpose is to assess the probability of meeting the quality standard for a policy that has
407 been designed without taken into account hydraulic conductivity uncertainty. For this case, one
408 of the realizations (realization 14) was chosen as the “true” K field. The resulting optimal
409 fertilizer application is then tested on the random fields generated to check the reliability of
410 meeting the water quality standard (Monte Carlo simulation). Figure 4 shows the reliability or
411 probability of not exceeding certain nitrate concentration level for the two cases with k fields
412 with different variances, obtained from the maximum concentration values simulated at each
413 conductivity field for the optimal fertilizer application of the “true” parameter field. The
414 reliability level of the pre-assumed optimal policy for meeting the quality standard was only a
415 14% for case 1 (i.e., only in 14 realizations out of the 100 simulated nitrate concentrations did
416 not exceed the limit of 50 mg/l), and 24% for case 2. It is clear, however, that this reliability
417 levels will highly depend on the realization chosen to find the optimal management (the chosen
418 “true” field). With a larger variance, although the reliability of meeting the standard is higher

419 the range of probable maximum concentrations increases, what can be relevant for the design
420 of risk-averse policies.

421 Reducing the fertilizer application rate, the reliability level can be increased up to 100%. For
422 case 2, the mean application rate has to be reduced by 20% to obtain a global 100% reliability
423 when checked with the 100 realizations. This result was obtained by lowering the constraining
424 quality standard (to 30.6 mg/l), as proposed by Ko and Lee (2008) for the analysis of the
425 optimal remediation design of a contaminated aquifer. Although this fertilizer management
426 achieves 100% reliability, it is important to note that this strategy is not necessarily the
427 “optimal” policy for 100% reliability. This fact will be further discussed in the section of the
428 mixed-integer stochastic approach. The alternative with a 24% reliability level produces a total
429 annual net benefit of 20.8 M€. With 100% reliability (20% fertilizer reduction), the total annual
430 net benefits is reduced to 19.7 M€.

431

432 [Figure 4]

433

434 **3.4. Uncertainty on optimal fertilizer application. Monte Carlo optimization**

435 In this formulation, the uncertainty is considered by solving the hydro-economic optimization
436 model for each of the 100 individual realizations and comparing the corresponding results. This
437 approach can be used to characterize the probability distribution of the optimal fertilizer
438 application rates (Figure 5). The mean for the case 1 (variance of $15 \text{ m}^2/\text{day}^2$) is 138.3 kg/ha,
439 the standard deviation is 2.9, and the mean fertilizer rates range from 131.4 to 148.5 kg/ha.
440 However, it cannot be assured that all these strategies would have a high probability of meeting
441 the standard, what limits the applicability to make decisions. In order to estimate the reliability
442 of meeting the objectives of any of the specific strategies that we obtain, we have to simulate
443 the strategy with the complete set of realizations (post-optimality Monte Carlo simulation). For

444 example, for the strategy that corresponds to the mean fertilizer application, the reliability of
445 meeting the standard is 33%.

446 For case 2 (variance of $60 \text{ m}^2/\text{day}^2$), the mean value is similar (138.9 kg/ha), while the standard
447 deviation goes up to 5.3. The reliability of the strategy corresponding to the mean rate is 35%.
448 The results show more dispersivity and a broader range of possible values of the mean fertilizer
449 rates obtained from a single-realization optimization, and therefore, a greater variability of the
450 economic impact of the strategy for a larger variance in the K fields.

451

452 [Figure 5]

453

454 **3.5. Stacking approach for optimal fertilizer allocation**

455 For this formulation, the hydro-economic management model is solved only once,
456 simultaneously for the complete stack of 100 realizations of the random conductivity field;
457 therefore, only one optimal fertilizer application is obtained. Chang (1993) investigated the
458 number of realizations to be included in the staking in order to achieve a certain level of
459 reliability, using a Bayesian framework. He obtained the following relationship between stack
460 size (number of realizations, NR) and reliability (R):

461

$$462 \quad R = \frac{NR + 1}{NR + 2} \quad (9)$$

463

464 Feyen and Gorelick (2004) concluded that the previous relationship obtained by Chan (1993)
465 overestimates the reliability for different stack sizes, and presents a formula that provides
466 expected reliability as a function of the number of realizations in the stack and the variance of
467 the log hydraulic conductivity σ^2 as:

468

469
$$R = \frac{NR - 0.5}{NR + 2(\sigma^2 + 1)} \quad (10)$$

470

471 For our case, the application of equations, (9) and (10) yields the same reliability for the 100
472 realizations, 99%. Therefore, the size of the stack is considered big enough to assess reliability
473 levels.

474 As expected, the groundwater quality standard is not exceeded when simulating the optimal
475 strategy for all the realizations of the stack (Figure 6). The reliability will be therefore 100%,
476 assuming the 100 set of realizations as a representative measure of k variability. The total net
477 benefit of the optimal solution with a 100% reliability is higher for case 1 (20.22 M€/year) than
478 for the case with a larger variance (19.89 M€/year), since in the latter the fertilizer application
479 has to be lower in order to meet the standards. However, the use of this approach does not
480 allow for prespecification of the desired system reliability. Since the reliability of the system
481 management is not explicitly considered in the optimal solution, the method can lead to
482 conservative (and more expensive) solutions.

483

484 [Figure 6]

485

486 Figure 7 shows the influence of the stack size in the reliability of the resulting strategies. Post-
487 optimization Monte Carlo reliability analyses were carried out by simulating each optimal
488 solution against the set of a hundred different hydraulic conductivity realizations. As expected,
489 the reliability of the optimal solution increases with the stack size. The values of reliability
490 versus stack size are in agreement with the findings of other authors (Wagner and Gorelick,
491 1989; Chan 1993 and Ko and Lee, 2009) for the optimal remediation design to control

492 groundwater pollution, and Feyen and Gorelick (2004) for controlling groundwater outflow in
493 wetlands. The results also show that a high reliability can be achieved with a stack of a reduced
494 number of realizations.

495

496 [Figure 7]

497

498 **3.6. Mixed-integer stochastic approach with predefined reliability**

499 In this formulation, the stochastic nature of the conductivity field is considered in the decision-
500 making process by integrating the complete set of Monte Carlo realizations through the
501 response matrix of the optimization management model. The method guarantees the optimal
502 solution for a pre-specified reliability level by using simultaneously all the generated
503 realizations and fixing the number of constraints that may be violated. Different reliability
504 levels were tested. The range of the maximum concentration values that are reached decreases
505 with increasing reliability of meeting the standard, and a steeper slope of the probability curve
506 is observed (Figure 8). The worst-case (upper value) of the maximum nitrate concentrations
507 increases with decreasing reliability (Figure 9). The larger the variance, the greater the range
508 and the worst-case (maximum concentration values). These results tell us that with a high
509 variance, a risk-averse decision-maker would prefer a more costly strategy with higher
510 reliability of meeting the standard than in the case of low variance, in order to reduce the risk of
511 a reaching a high nitrate concentration exceeding by far the standard (which will implies higher
512 economic impacts in terms of environmental and resource costs).

513

514 [Figure 8]

515

516 [Figure 9]

517

518 The objective function (the total net benefit) increases nonlinearly with decreasing reliability
519 (Fig. 10). This implies that a larger amount of net benefit has to be sacrificed when a more risk-
520 averse management is considered.

521

522 [Figure 10]

523

524 For the same reliability level, the total net benefit is greater for a lower variance. A high
525 variance also implies that some critical realizations further limit the fertilizer application rate
526 for that reliability level. As the reliability level gets lower, the total net benefit for both K
527 variance fields gets closer, since the fertilizer rate moves toward the optimal application that
528 yields the maximum benefits. For each realization, the influence of the different sources upon
529 the concentration at the control sites is different, and the corresponding benefits from crop
530 production will differ. Table 1 shows the percentage of fertilizer reduction that produces the
531 maximum crop yield that is required to meet the groundwater quality standards for different
532 levels of reliability. These results are relevant for the design of optimal land use policies to
533 control groundwater nitrate pollution. From the table we can see that no fertilizer reduction is
534 need in certain areas, while in the other areas the reduction has to be greater in order to achieve
535 a higher reliability of meeting the standards. The pattern of the spatial fertilizer reduction is
536 maintained for the different reliability levels, showing the robustness of the solution.

537

538 [Table 1]

539

540 **4. Discussion**

541 The four stochastic modeling approaches aforementioned have been applied to analyze how
542 uncertainty of hydraulic conductivity leads to different reliability levels of meeting the quality
543 standards. Eventually, this is translated into different optimal fertilizer application rates, and
544 therefore, different net benefits (or reduction of income losses). The four approaches tackle this
545 problem from different points of view. Some important insights can be drawn from the results
546 above presented.

547 First, we have assessed the reliability of the policy derived from the deterministic optimization
548 for a pre-assumed parameter field. The chosen K field is not necessarily true, and therefore, the
549 obtained optimal fertilization scheme could succeed or fail in meeting the groundwater
550 concentrations standards when applied to random K fields by means of Monte Carlo
551 simulations. As it has been shown, this formulation may lead to low reliability levels. Hence,
552 this formulation is not recommended to derive reliable policies (especially in very
553 heterogeneous aquifers) and should be discarded in the decision making process. Although we
554 can artificially reduce the constraining quality standard in order to achieve a higher reliability
555 in meeting the 50 mg/l of groundwater nitrate concentration, it has been proved that this
556 solution does not necessarily yield the maximum for the objective function (total net benefits).

557 The Monte Carlo optimization approach can be used to characterize the probability distribution
558 of the mean optimal fertilizer application rates. A post-optimality Monte Carlo simulation is
559 required to estimate the reliability of meeting the standards. Results from these post-
560 simulations have shown that the mean value of the probability distribution can lead, again, to
561 low reliability levels regardless of the variance of the K fields. The different strategies of
562 fertilizer application rates may have a high probability of not meeting the standard, what limits
563 the applicability to make decisions. On the other hand, a choice of a more restrictive fertilizer
564 application (e.g., the lower quartile value of the distribution) could result in too conservative
565 (and more expensive) solution.

566 Contrary, in the stacking approach, the fertilizer standard resulting from the optimization model
567 fulfills the quality standards for all the realizations (Figure 6); therefore, the reliability level is
568 equal to 100%, assuming that the set of K realizations used in the stacking is large enough to
569 provide a significant representation of the parameter variability. The literature has provided
570 formulas that relate the number of realizations to include in the staking in order to achieve a
571 certain level of reliability. Our results are in line with those presented by other works related to
572 pumping remediation of aquifer pollution (e.g., Chan, 1993; Feyen and Gorelick, 2004). By
573 means of a post-optimization Monte Carlo analysis, the results show that high reliability levels
574 (greater than 90%) can be reached with a small stack sizes (Figure 7). However, since the
575 reliability of the system management is not explicitly considered in the optimal solution, the
576 method can lead to conservative and less economic efficient solutions.

577 This problem is overcome by resorting to a mixed-integer stochastic approach with an a priori
578 defined reliability level, allowing a certain number of simulations to fail the standards. The
579 higher the predefined reliability level and the lower variance, the lower the minimum
580 concentration that can be reached (Figure 8 and Figure 9). In addition, the lower the variance,
581 the higher the benefits (Figure 10). As a result, this approach leads to less costly and more
582 reliable solutions than in the staking approach, guaranteeing the “optimal” strategy of spatial
583 fertilizer application (maximum total benefit) for a fixed reliability level.

584

585 **5. Conclusions**

586 A stochastic hydro-economic modeling framework for optimal management of groundwater
587 pollution under K uncertainty has been presented. A holistic optimization model determines the
588 spatial and temporal fertilizer application rate that maximizes the net benefits in agriculture
589 constrained by the groundwater nitrate concentration standards at various control sites. The
590 stochastic management framework presented allows to derive least-cost fertilizer plans in order

591 to meet the groundwater quality standards ruled by the EU Water Framework Directive or any
592 other water legislation under conditions of parameter uncertainty. As shown in the results,
593 parameter uncertainty leads to different management policies with clear implications in
594 reliability levels, costs and benefits. The study of the least-cost alternative for meeting the
595 environmental objectives is also important in order to justify potential time and objective
596 derogation when disproportionate costs are identified (WFD, art. 4).

597 Four different formulations (Monte Carlo simulation with preassumed parameter field, Monte
598 Carlo optimization, stacking approach, and mixed-integer stochastic optimization with
599 predefined reliability level) have been applied in order to analyze the influence of the
600 uncertainty of the spatial variability of the hydraulic conductivity upon the optimal
601 management of groundwater nitrate pollution from agricultural sources. All the approaches use
602 a Monte Carlo-type analysis involving a series of realizations of the uncertain parameter, in
603 order to assess reliability and uncertainty of different fertilizer application strategies. These
604 results represent an upper bound or benchmark comparison to possible second-best solutions
605 for controlling nitrate pollution, like economic taxes or incentives either on inputs or ambient
606 standards.

607 The framework has been applied to a controlled 2D synthetic aquifer system, offering insights
608 into the impacts of uncertainty in the optimal management strategies. Given the uncertainty in
609 the pollutant concentration predictions due to uncertain spatial variability of the hydraulic
610 conductivity, the solution of the optimization of a single realization does not guarantee a high
611 reliability in meeting the groundwater quality standards. A stochastic analysis that considers
612 uncertainty in the performance of the system allows providing more reliable management
613 strategies than deterministic models.

614 In order to increase the reliability, we can simultaneously optimize for a sampling or stack of
615 hydraulic conductivity realizations (stacking approach). The reliability of the optimal solution

616 increases with the stack size. However, this approach does not allow for pre-specification of the
617 desired system reliability, and the method can lead to too conservative solutions.

618 In decision-making processes, reliability and risk-aversion play a decisive role. By using a
619 mixed-integer stochastic formulation, an a priori reliability level of the strategy can be
620 explicitly fixed. As the mixed-integer stochastic model includes the complete set of
621 realizations, it guarantees the best optimal strategy (maximum total net benefit) for that level of
622 reliability, as shown by the results. This approach also allows deriving the trade-off curve
623 between the reliability level and the net benefits.

624 In a risk-averse decision-making, not only the reliability of meeting the standards counts, but
625 also the probability distribution of the maximum pollutant concentrations. A risk-averse
626 decision-making is specially justified when dealing with well-capture zones for drinking water
627 supply (health risk) or sensitive areas of groundwater dependent ecosystems. A sensitivity
628 analysis was conducted to assess the influence of the variance of the hydraulic conductivity
629 fields on the optimal strategies. The results have shown that the larger the variance, the greater
630 the range of maximum nitrate concentrations and the worst-case (or maximum value) that could
631 be reached for the same level of reliability of meeting the standard.

632 In the reliability versus net benefit trade-off, for the same reliability level, the total net benefit
633 is greater when the variance is lower. Note that by assuming uncertainty in the random function
634 (e.g., Llopis-Albert and Capilla, 2009) or by considering higher variances of the K , a greater
635 influence in the results than in the analyzed cases should be expected.

636 The uncertainty can be reduced by improving the site characterization, providing more realistic
637 and reliable management schemes. For that purpose, a promising extension of the present work
638 is the integration of a stochastic inverse model in the described framework, in which the
639 stochastic simulations are constrained to data such as hydraulic conductivity, piezometer head,
640 solute concentrations, travel times or secondary data obtained from expert judgment and

641 geophysical surveys. The influence of the K uncertainty is only analyzed for a fertilizer
642 standards policy. There is a broad range of policies for controlling nitrates in the literature
643 (standards or economic instruments on inputs, emissions or ambient concentrations) (Shortle
644 and Griffin, 2001). A further extension of this work is to incorporate these different policies
645 into the hydro-economic formulation in order to compare their effectiveness in controlling
646 nitrate pollution as second-best solutions.

647 Besides groundwater hydraulic conductivity, there are many other sources of uncertainty,
648 ranging from partial knowledge about the aquifer properties and boundary conditions, land use
649 practices, on-ground nitrogen loading, nitrogen soil dynamics, soil characteristics, depth to
650 water table, to the diverse economic, regulatory and political factors. The analysis of
651 uncertainty and risk can be also extended to the derived health risk problem (Lichtenberg et al.,
652 1989; Innes and Cory, 2008). Further research is required in order to represent the diversity of
653 potential on-farm management decisions and other policy options rather than fertilizer use, and
654 to extend the analysis to other sources of uncertainty.

655 Finally, the method can be extended to consider other sources of nitrate pollution such as
656 animal farming, landfills, and septic tanks. Although the method and tools are suitable for
657 simulating the effects of these sources on nitrate concentration at the control sites, further
658 research would be required for modeling the economics of abating the pollution from these
659 other sources.

660

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817

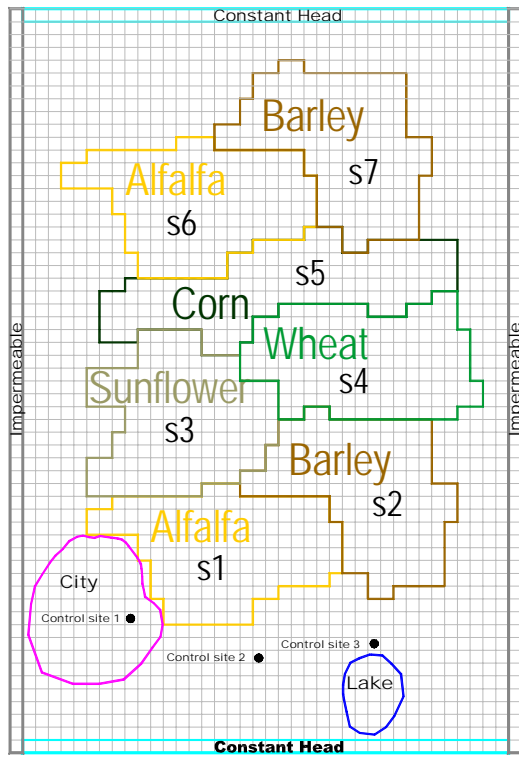


Figure 1. Aquifer system

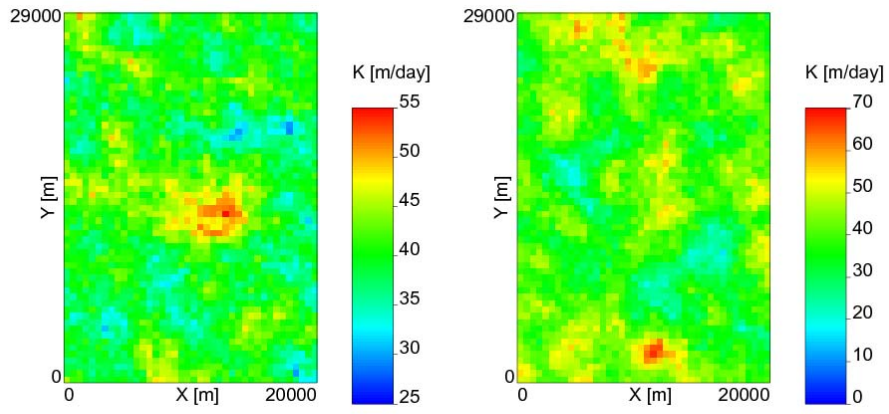


Figure 2. K field for realization #1 and variances of 15 (left) and 60 (right)

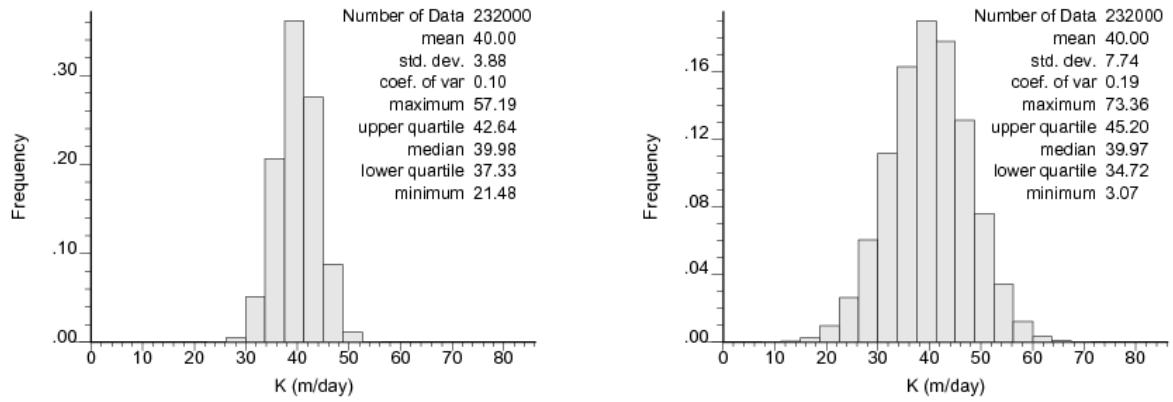


Figure 3. Frequency distribution and univariate statistics for all K realizations and variances of 15 (left) and 60 (right)

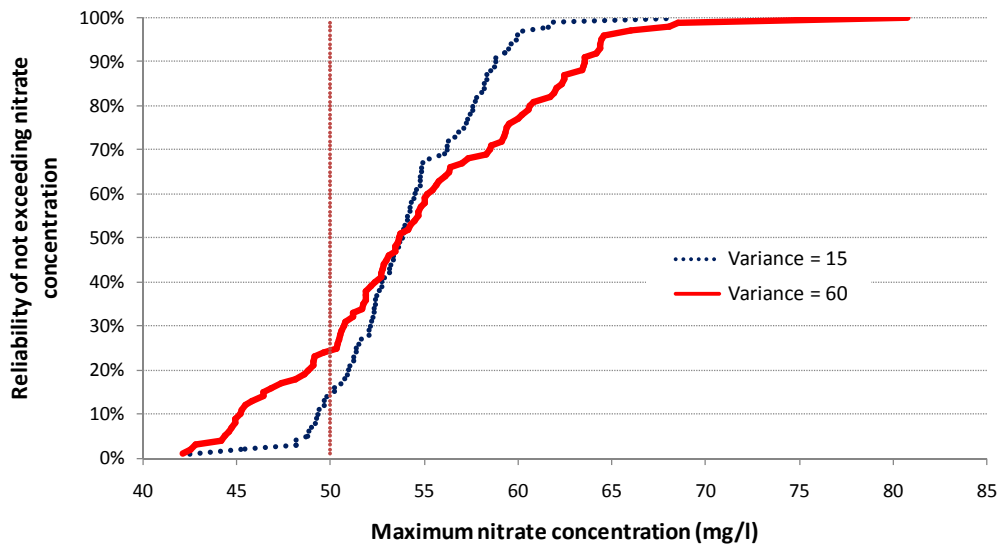


Figure 4. Reliability (probability of not exceeding the maximum nitrate concentration) of the optimal fertilizer application for realization 14 with variances of 15 and 60.

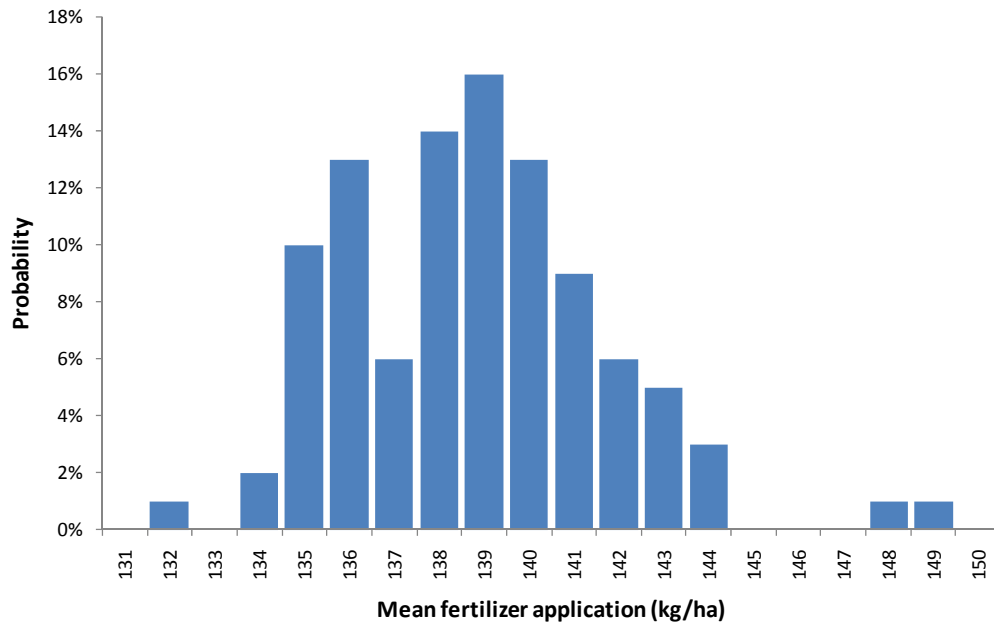


Figure 5. Probability distribution of the mean fertilizer application, case 1.

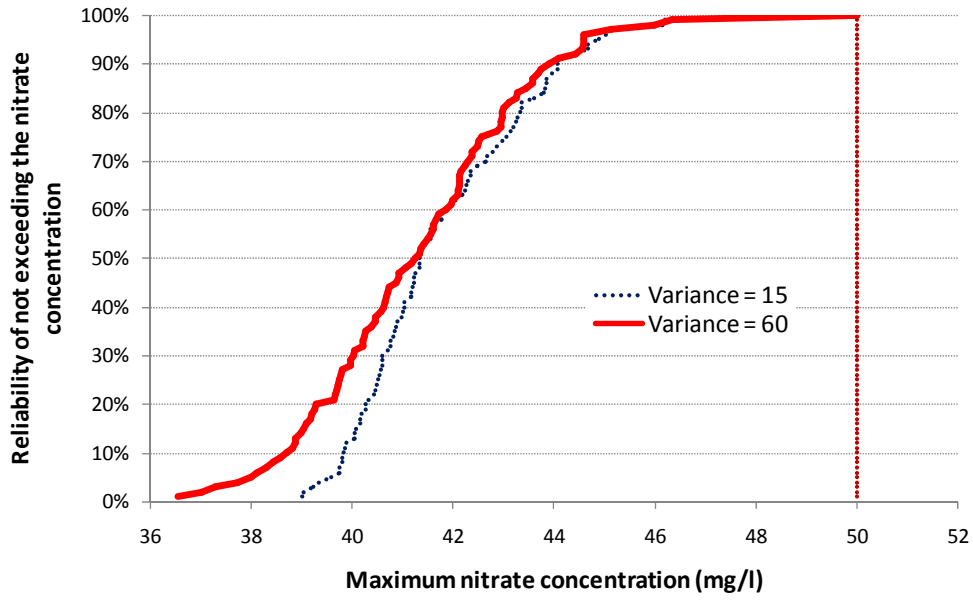


Figure 6. Maximum nitrate concentration vs. reliability of not exceeding the nitrate concentration (post Monte Carlo simulation).

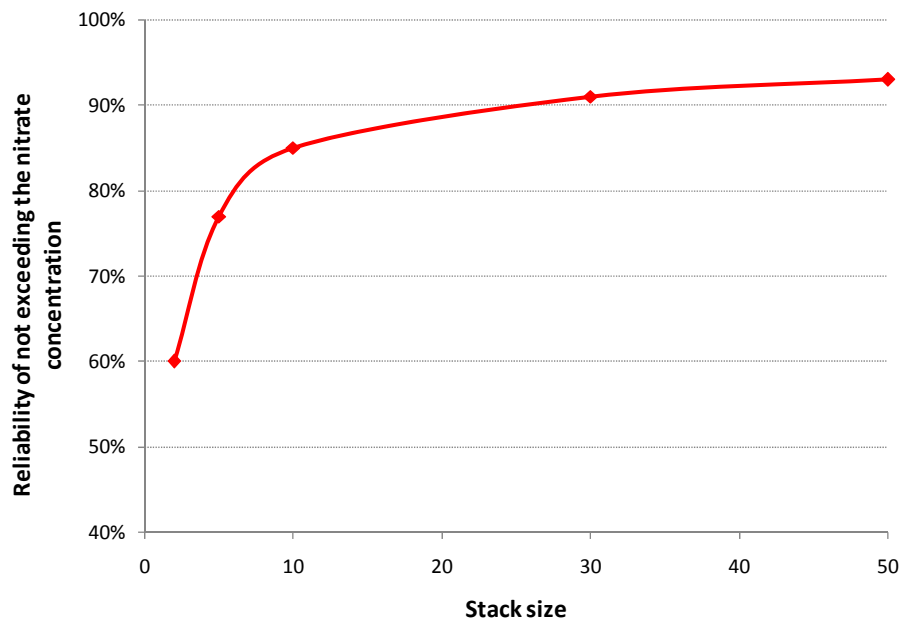


Figure7. Mean reliability (post Monte Carlo simulation) vs. stack size.

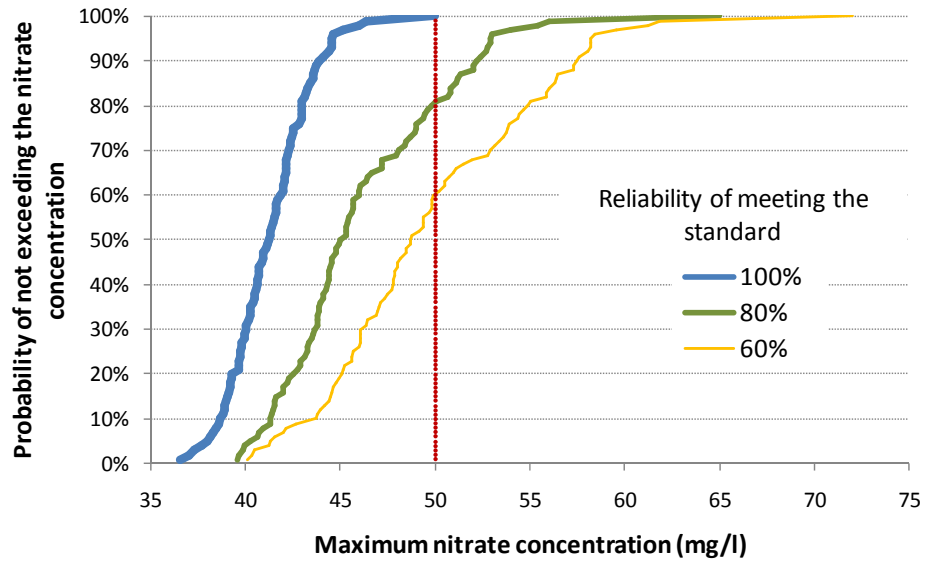


Figure 8. Probability of not exceeding the nitrate concentration for different reliability levels.

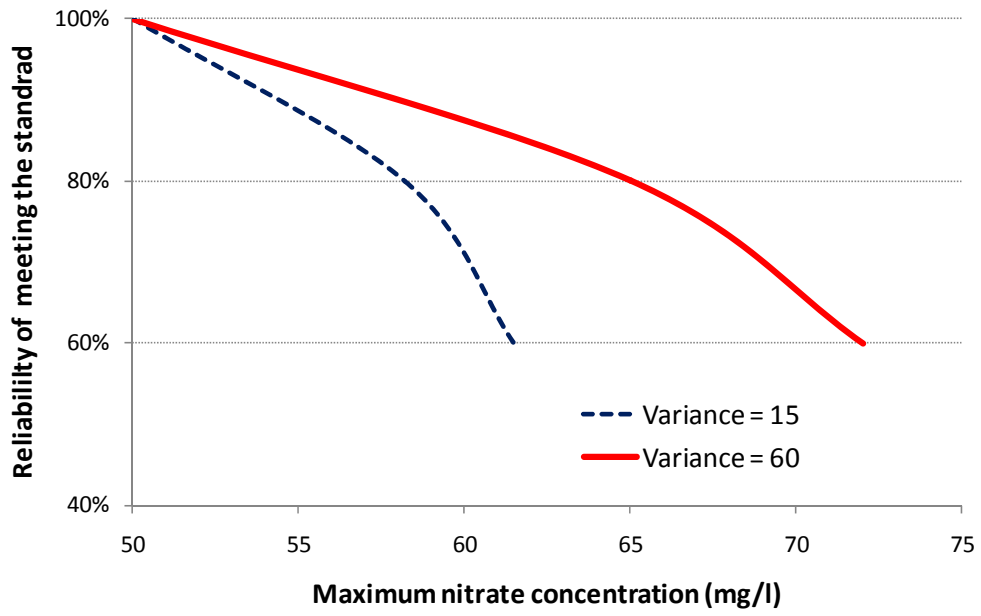


Figure 9. Reliability vs. upper value of maximum nitrate concentrations

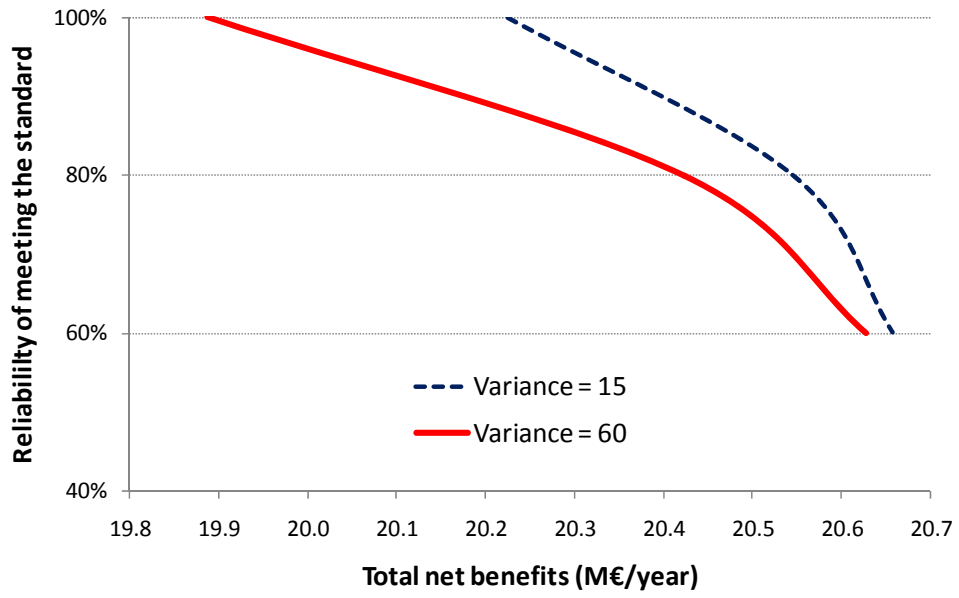


Figure 10. Trade-off between reliability and benefits

Table 1. Percentage of spatial fertilizer reduction for different levels of reliability

Crop Area	Reliability		
	100%	80%	60%
s1	3.29%	2.58%	2.12%
s2	0.00%	0.00%	0.00%
s3	43.07%	29.22%	22.17%
s4	0.00%	0.00%	0.00%
s5	17.99%	14.00%	11.48%
s6	2.75%	2.15%	1.76%
s7	0.00%	0.00%	0.00%