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MULTI-OBJECTIVE OPTIMIZATION FOR THE DESIGN OF GROUNDWATER SUPPLY SYSTEMS UNDER UNCERTAIN PARAMETER DISTRIBUTION*

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Abstract: The design and management of groundwater supply systems may be formulated as an optimization problem, where a pumping scheme is sought that minimizes the system cost and, at the same time, complies with a series of constraints of technical, economical, and environmental nature. Due to uncertainties in the characterization of subsurface parameter distributions, the solution to the management problem must consider the trade off between cost optimality and the risk of not meeting the management constraints. In this work, the risk is quantified either as the probability of violation of management constraints, or as the expected intensity of violation. The solution to the trade-off problem is addressed by combining a multi-objective evolutionary algorithm with a model simulating groundwater flow in confined aquifers. In order to avert the direct inclusion of the simulation flow model into the optimization algorithm, a stochastic response-matrix approach is used. The computational efficiency of the devised framework is such that it can be applied to problems characterized by large numbers of decision variables. The comparison of the two alternative trade-off formulations, expected cost vs. probability of failure and expected cost vs. expected intensity of violation, indicates that the latter has the advantage of providing more complete information on the risk associated with any given pumping scheme, along with the advantage of producing a more dispersed ranking of the pumping strategies and, ultimately, a larger set of optimal trade-off pumping schemes.

Key words: *groundwater management, stochastic multi-objective optimization, risk*

Mathematics Subject Classification: *Primary: 90C29, 60G10; Secondary: 90C56*

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1 Introduction

The design and operation of groundwater supply systems that comply with technical, economic, environmental, and social constraints is often an expensive and challenging process given the typical complexity of hydrogeological settings. A typical groundwater management problem considers the placement of a number of pumping wells, and the determination of flow rate schedules in order to identify the best management alternatives while accounting for management objectives and constraints.

In the case of groundwater supply systems, objectives can be related, for example, to the total production cost or to the total amount of pumped water, whereas constraints may be imposed on pumping rates, hydraulic head distributions and water demands. When management problems are characterized by multiple competing objectives, optimal management solutions can be represented by trade-off sets, which may offer valuable support to stakeholders in the decision making process.

The typical modeling approach to groundwater planning and management considers the coupling of optimization algorithms with groundwater simulation models. Extensive literature reviews on these methodologies are provided by [1], [27], and [57]. The literature offers also several case studies in which optimization has proven effective in assisting a groundwater informed decision making (e.g. [4, 3, 12, 16, 25, 41, 42, 47, 54]).

However, the application of combined optimization-simulation tools is often limited by

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uncertainties characterizing the subsurface system (e.g. heterogeneous geological settings, hydrogeological parameter distributions, boundary conditions), which directly reflect on uncertainties in the response predicted with groundwater simulation models, and ultimately may lead to management strategies that are sub optimal and/or violate the management constraints. Thus, under conditions of uncertainty, the groundwater supply management problem acquires a stochastic nature, whose goal is to determine robust pumping strategies that, for example, minimize production costs, while guaranteeing adequate levels of reliability.

In the last decades, significant research has been conducted on stochastic optimization applied to the design of groundwater systems. Detailed reviews of stochastic groundwater optimizations models are provided in [5, 7, 21, 28, 39, 50]. Chance-constrained (CC) techniques constitute one of first attempts to incorporate uncertainty into the optimization model. With these techniques, the solution to an optimization problem subject to stochastic constraints is addressed by imposing the probability of constraint violation to be below a prescribed acceptable level. In groundwater management problems, CC optimization has been applied, among others, by [48] for aquifer development, [51, 52] for remediation of polluted aquifers, and [31] for the planning of extraction/injection systems in connected stream-aquifer systems. One limitation of CC techniques is that they can control at most the probability of constraint violation without assessing the magnitude of violations.

The importance of accounting for the intensity of constraint violations was shown by [53], who presented an optimization model for groundwater remediation under conditions of parameter uncertainty, where the objective was to minimize the cost of well operation, which included also a penalty term, called "recourse", proportional to the amount of violation of a prescribed clean-up target constraint. This method was also applied by [44] in a context of planning of groundwater supplies. [43] advanced a stochastic programming formulation referred to as "robust optimization", which was subsequently applied by [55] to groundwater remediation problems. In robust optimization, a solution is optimality-robust if it remains close to optimal under most scenarios used to model the uncertain parameters, whereas it is feasibility-robust it is meets the constraints under most scenarios. Of related interest are applications of decision analysis concepts to the management of groundwater resources under uncertain parameters [22, 21]. In this case, the enforcement of stochastic constraints is achieved by considering, in addition to the total cost of the system under design, a "risk cost" directly proportional to the probability of not complying with prescribed management targets. In principle, the role played by the risk cost in decision analysis is very similar to the role of recourse in robust optimization.

In all of the methods presented by [22, 43, 53, 55] the optimization problem takes on multi-criteria form that implicitly addresses the trade off between optimality and reliability, with the latter explicitly accounting for constraint violations. Note that with these methods the groundwater management is formulated as a single-objective (SO) problem, which requires the definition of penalty costs associated with constraint violations. The specification of these penalties often represents a shortcoming of these formulations, since it requires direct involvement of stakeholders in the management of the groundwater system.

In this study, we advance an optimization framework that may be applied to assist the design and the management of groundwater supply systems in confined aquifers known with uncertainty. The focus is on the hydraulic conductivity distribution, which is often the most uncertain hydrogeological parameter to characterize due to its inherent spatial heterogeneity. This methodology is developed and applied to one of the groundwater management benchmark problems formulated by [39], which, in recent years, have been utilized by several researchers in the optimization community [18, 19, 20, 29, 32, 33, 38].

In this methodology, the SO constrained optimization problem of [39] is modified into a multi-objective (MO) optimization problem by substituting the constraint inequalities with an additional objective function representing, in a probabilistic sense, the violation of the constraints in the optimization formulation. Two formulations of the additional objective function are here investigated. In one case, this is quantified by the probability of constraint violation, whereas, in another, this is represented by the average intensity of constraint violation, *i.e* the expected value of its statistical distribution.

The goal of the MO optimization problems is the determination of the set of pumping schemes that trade off cost optimality against the risk of not complying with the management constraints. The MO approach may be particularly advantageous in the decision making process. In one case, where the reliability theme is considered in terms of probability of constraint violation, the MO problem constitutes a generalization of CC methods [48, 51, 52, 31] and provides trade-off sets that directly address the increase in cost necessary to design more reliable pumping systems. In another, when stochastic constraints are expressed in terms of average intensity of violation, the MO approach is able to produce trade-off sets without requiring the definition of penalty coefficients [43, 53, 55] that would be otherwise necessary, within a SO approach, to commensurate violations to the groundwater supply cost.

These optimization problems are solved using a MO evolutionary algorithm. This class of algorithms is particularly indicated to deal with problems involving non-linear and discontinuous objective functions. [13] provide a detailed review of MO evolutionary algorithms and their applications in science and engineering fields. In this work, we utilize a Niche-Pareto Genetic Algorithm (NPGA) [17, 34] in combination with a stochastic groundwater flow model relying on a stochastic simulation (or Monte Carlo) technique.

In general, combined optimization-simulation frameworks may be computationally overwhelming when the evaluation of the objective functions requires the use of "expensive" simulation models. In these instances, methodologies are needed that allow for averting the direct inclusion of the stochastic simulation model within the optimization loop. Over the years, several works have been presented where "surrogate" objective functions are developed in order to reduce the computational burden at the expense of model accuracy [2, 5, 11, 14, 37, 42, 46, 49, 56].

In this work, instead of calibrating surrogates of the objective functions, a substitute of the simulation model is developed. Indeed, the nature of the flow in confined aquifers makes it possible to determine linear functions providing a response identical to that of the groundwater flow model, at a much lower computational cost. By using this technique, the stochastic flow simulation model is used to calculate the so-called response matrix [27] for each hydraulic conductivity scenario prior to the optimization loop. The optimization algorithm is thus linked to a stochastic response-matrix simulator, which drastically improves the computational performance of the optimization process and ultimately allows for considering large numbers of decision variables.

2 Methodology

The major components of the framework presented in this work are: a MO management problem addressing the optimal design of groundwater systems under parameter uncertainty; a response-matrix approach to predict the response of the aquifer system to pumping stress; and a MO optimization algorithm that identifies sets of optimal pumping schemes trading off cost optimality against reliability.

2.1 Multiobjective Management Problem

In [39], the groundwater supply management is formulated as a SO optimization problem, where a solution is searched for that minimizes the cost of the system, subject to a series of constraints:

$$\min_{\mathbf{Q}} \left[\mathrm{Cost}\left(\mathbf{Q}, \widetilde{\mathbf{s}}\right)\right] \tag{2.1}$$

$$\widetilde{\boldsymbol{\chi}} = \boldsymbol{\chi}\left(\mathbf{Q}, \widetilde{\mathbf{s}}\right) \leq \boldsymbol{\chi}_c \tag{2.2}$$

The components of the vectors $\boldsymbol{\chi}$ and $\boldsymbol{\chi}_c$, are respectively generic functions and coefficients used to represent constraint inequalities. The variables upon which the objective function (2.1) and the constraint inequalities (2.2) depend are: the vector of the decision variables, $\mathbf{Q}$, *i.e* the pumping rates at a number of potential pumping well locations; and the vector of the state variables, $\widetilde{\mathbf{s}}$, *i.e* the hydraulic head distribution in the aquifer. The state variables depend upon the pumping scheme $\mathbf{Q}$, the boundary conditions, and the parameter distribution in the aquifer.

Due to uncertainty, the distribution of hydraulic conductivity in the aquifer, $\widetilde{\mathbf{K}}$, is here thought of as a stochastic process. The symbol "$\widetilde{\ }$" denotes stochasticity. Consequently, state variables, the total cost and the constraint functions are themselves stochastic variables. Following a stochastic simulation approach, uncertainty is dealt with by generating a large number, N_{MC}, of equally likely realizations of the stochastic parameters $(\mathbf{K}_k; k = 1, 2, .., N_{MC})$.

The goal of the management problem is to (a) optimize the expected value of the groundwater supply cost calculated over this series of realizations:

$$Cost\,(\mathbf{Q}) = \mathrm{E}\,[\mathrm{Cost}\,(\mathbf{Q}, \widetilde{\mathbf{s}})] \cong \sum_{k=1}^{N_{MC}} \frac{\mathrm{Cost}\,(\mathbf{Q}, \mathbf{s}_k)}{N_{MC}} \tag{2.3}$$

while (b) probabilistically enforcing the specified constraints over the considered ensemble of realizations. In Equation (2.3), $\mathbf{s}_k$ indicates the vector of the state variables under the pumping scheme $\mathbf{Q}$ and the generic parameter realization $\mathbf{K}_k$.

In this study, two methods are considered to address the constraint inequalities under uncertain parameters. In the first of these two methods, constraint inequalities (2.2) are "relaxed" but penalized according to the frequency with which their violation occurs. For any given pumping strategy, $\mathbf{Q}$, such a frequency is quantified by the probability of failure [30]:

$$P_{fail}\,(\mathbf{Q}) \cong \frac{n_v\,(\mathbf{Q}) - 0.5}{N_{MC}} \tag{2.4}$$

where n_v represents the number of hydraulic conductivity realizations in which at least one of the constraints (2.2) is not met. By introducing P_{fail}, the SO and constrained optimization problem (2.1-2.2) is transformed into the two-objective problem:

$$\begin{aligned} &\min_{\mathbf{Q}} \{Cost\,(\mathbf{Q})\} \\ &\min_{\mathbf{Q}} \{P_{fail}\,(\mathbf{Q})\} \end{aligned} \tag{2.5}$$

In the second method, constraint inequalities (2.2) are relaxed but penalized according to the expected value of the intensity of violation:

$$Violation\,(\mathbf{Q}) = \mathrm{E}\,[\mathrm{Violation}\,(\mathbf{Q}, \widetilde{\mathbf{s}})] \cong \sum_{k=1}^{N_{MC}} \frac{\max\{0, \| \boldsymbol{\chi}\,(\mathbf{Q}, \mathbf{s}_k) - \boldsymbol{\chi}_c \|\}}{N_{MC}} \tag{2.6}$$

where $\| \cdot \|$ is an arbitrary norm used to quantify the violation associated with multiple constraints. Therefore, the constrained-optimization problem (2.1-2.2) is transformed into the two-objective problem:

$$\begin{aligned} &\min_{\mathbf{Q}} \{Cost\,(\mathbf{Q})\} \\ &\min_{\mathbf{Q}} \{Violation\,(\mathbf{Q})\} \end{aligned} \tag{2.7}$$

It must be mentioned that, in a statistical sense, the cost and violation objectives may be considered in terms of a generic representative value obtained from their respective probability distribution functions, the choice of which is ultimately related to the general conditions of risk aversion [6, 10, 21]. The assumption of the expected value of the distributions adopted in (2.7) corresponds to the case of risk-neutral decision making, in which stakeholders assign, in terms of cost and violation, the same "weight" to all parameter scenarios. On the other hand, in the case of risk-aversion, management strategies should be ranked based upon representative values that are larger than the expected values of the pdf's, since stakeholders would be more worried about, and assign a larger weight to, parameter scenarios that produce larger cost and drawdowns.

The goal of both problems (2.5) and (2.7) is the determination of the "Pareto-optimal" set of pumping strategies that trade off cost optimality against the risk of not meeting the management constraints. A pumping strategy is Pareto optimal if there is no other strategy that performs at least as well in both objectives and strictly better in at least one objective.

In the groundwater benchmark problem outlined by [39], the domain is represented by a 1000×1000 (m×m), 30-m thick, horizontal, and confined aquifer. The aquifer bottom and its top are at elevations, z_{bot} and z_{top}, of 0 and 30 m, respectively. The bottom of the aquifer is chosen as the hydraulic head datum. The aquifer is uniformly recharged at its top at a constant rate of 1.903×10^{-8} m/s (0.6 m/year). Groundwater flow is subject to the lateral boundary conditions represented in Figure 1a. The bottom of the aquifer is impermeable. A detailed description of all hydrogeological parameters may be found in [39].

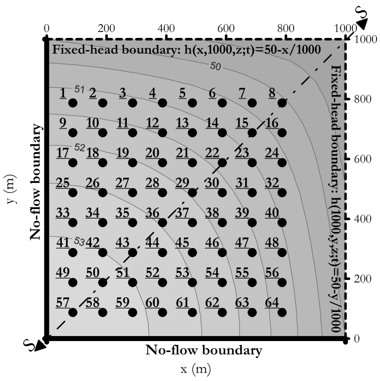

Figure 1: Horizontal projection of the confined aquifer hypothesized by [39] along with the location of 64 potential pumping wells used to identify optimal groundwater withdrawal strategies. The contour lines in the background represent the expected value of the hydraulic head (m) in the aquifer prior to groundwater pumping.

As is typical in groundwater hydrology [15], the heterogeneous distributions of hydraulic conductivity is modeled according to a geostatistical conceptual model [36], in which $\widetilde{\mathbf{K}}$ is represented as spatially distributed random process. In particular, a stationary, anisotropic, log-normal process with an exponential covariance function is adopted:

$$\begin{aligned} &\text{(a)} \qquad \log \widetilde{K} = Y_{\widetilde{K}} = N\left(\mu_{Y_{\widetilde{K}}}, \sigma_{Y_{\widetilde{K}}}\right) \\ &\text{(b)} \qquad cov_{Y_{\widetilde{K}},Y_{\widetilde{K}}}(\mathbf{d}) = \sigma^2_{Y_{\widetilde{K}}} \cdot \exp\left(-\sqrt{\frac{d_x^2}{\lambda_x^2} + \frac{d_y^2}{\lambda_y^2} + \frac{d_z^2}{\lambda_z^2}}\right) \end{aligned} \tag{2.8}$$

where: $\mu_{Y_{\widetilde{K}}}$ and $\sigma_{Y_{\widetilde{K}}}$ are the mean and the standard deviation of the normal log-K distribution, indicated by $N\left(\mu_{Y_{\widetilde{K}}}, \sigma_{Y_{\widetilde{K}}}\right)$; (d_x, d_y, d_z) are the components of the distance vector $\mathbf{d}$; and $(\lambda_x, \lambda_y, \lambda_z)$ are the spatial correlation scales along the coordinate directions. The random process (2.8) considered here is characterized by the geostatistical parameters of the random field III provided by [39], which are reported in Table 1. To represent the uncertainty in the hydraulic conductivity spatial distribution, an ensemble of equally-likely realizations $\mathbf{K}_k$ $(k = 1, 2, .., N_{MC})$ fitting to the process (2.8) is generated using the sequential Gauss simulation algorithm developed by [7].

Table 1: Geostatistical parameters characterizing the hydraulic conductivity spatial distribution [39].

$\mu_{Y_{\widetilde{K}}}$ log(m/s)	$\sigma_{Y_{\widetilde{K}}}$ log(m/s)	λ_x (m)	λ_y (m)	λ_z (m)
-4.3	1	50	50	7.5

In [39], the groundwater supply cost is a non-linear, discontinuous function of the decision variables (well number, locations and pumping rates) and state variables (hydraulic heads):

$$\text{Total Cost}\,(\mathbf{Q},\mathbf{s}) = \sum_{i=1}^{n_{ext}+n_{inj}} c_0 \cdot d_{w,i}^{b_0} \;+\; \sum_{i=1}^{n_{ext}} c_1 \cdot |Q_i^m|^{b_1} \cdot (z_{gs} - h_{min})^{b_2}$$
$$+\int_{t_{in}}^{t_{fin}} \left[\sum_{i=1}^{n_{ext}} c_2 \cdot Q_i \cdot (h_i - z_{gs})\right] \cdot dt \;+\; \int_{t_{in}}^{t_{fin}} \left[\sum_{i=n_{ext}+1}^{n_{ext}+n_{inj}} c_3 \cdot Q_i\right] \cdot dt \tag{2.9}$$

where: n_{ext} is the number of extraction wells, and n_{inj} is the number of injection wells; Q_i is the pumping rate for the i-th well (m^3/s) (the i-th component of the decision variable vector $\mathbf{Q}$); Q_i^m is the design extraction rate for well i, equal to -6.4$\times$10^{-3} m^3/s ($\sim$-550 m^3/day); h_i and h_{min} represent the hydraulic head in well i (m) and its minimum allowable value, respectively; z_{gs} indicates the ground surface elevation, located at 60 m above the datum, whereas $d_{w,i}$ (m) is the depth of well i below the ground surface (60 m); t_{in} and t_{fin} are the initial and final time for groundwater pumping (s). The coefficients b_i's and c_i's associated with the objective function (2.9) are provided in Table 2 The four terms at the right-hand

Table 2: Groundwater supply cost function coefficients [39].

Coefficient	Value	Unit
b_0	0.3	(/)
b_1	0.45	(/)
b_2	0.64	(/)
c_0	5.5×10^3	\$/m^{b_0}
c_1	5.75×10^3	\$/[(m^3/s)$^{b_1}\cdot$m^{b_2}]
c_2	2.90×10^{-4}	\$/m^4
c_3	1.45×10^{-4}	\$/m^3

side of Equation (2.9) indicate, respectively, the capital costs incurred from installation of pumping wells, the capital cost of extraction pumps, the operation costs for extraction wells, and the operation cost for gravity-fed injection wells.

Decision variables are constrained by limitations on pumping rates at each well:

$$Q_{ex}^{max} \leq Q_i \leq Q_{in}^{max} \;;\quad i = 1, 2, .., n_w = n_{ext} + n_{inj} \tag{2.10}$$

$$Q_T = \sum_{i=1}^{n_w} Q_i \leq Q_{dem} \tag{2.11}$$

In (2.10), n_w is the total number of installed wells (n_w=n_{ext}+n_{inj}), and Q_{ex}^{max} and Q_{in}^{max} are the maximum extraction and injection rates at any well, equal to -6.4$\times$10^{-3} m^3/s ($\sim$-550 m^3/day) and 6.4$\times$10^{-3} m^3/s ($\sim$550 m^3/day), respectively. In (2.11), Q_T is the total extraction rate, which must satisfy a groundwater supply demand $Q_{dem} = -3.2\times10^{-2}$ m^3/s ($\sim$-2,750 m^3/day) [39]. In this work, no injection wells are considered (n_{inj}=0; n_w=n_{ext}), thus Q_{in}^{max} is set to zero. In addition, the extraction rates at the potential well locations are assumed to be constant during the considered groundwater supply operation time interval, (t_{in}, t_{fin}), whose length is equal to 10 years.

In [39], constraints on well locations, (x_i, y_i), are also prescribed in order to limit the quantity of water withdrawn from the aquifer constant-head boundaries (Figure 1):

$$x_{min} \leq x_i \leq x_{max} \;;\; y_{min} \leq y_i \leq y_{max} \;\;;\; i = 1, 2, .., n_w \tag{2.12}$$

where x_{min}=y_{min}=0 m, and x_{max}=y_{max}=800 m. Hydraulic heads at pumping wells are constrained within minimum and maximum bounds:

$$h_{min} \leq h_i \leq h_{max} \;;\quad i = 1, 2, .., n_w \tag{2.13}$$

where $h_{min} = 40$ m and $h_{max}=z_{gs}=60$ m.

In this work, constraints on pumping rates (inequalities (2.10-2.11)) are strictly enforced by setting lower and upper bounds to the values of the decision variables between which the optimum is sought. Constraints on well locations (inequalities (2.12)) are automatically met by fixing the locations of n=64 candidate wells uniformly distributed within a portion of the domain that already comply with these constraints (Figure 1). Instead, the constraints allowed for violation are those corresponding to inequalities (2.13). Accordingly, for any given pumping strategy $\mathbf{Q}$, P_{fail} is calculated using Equation (2.4), which requires determining the number of realizations of the hydraulic conductivity field where constraints (2.13) are not met. On the other hand, $Violation$ is obtained using Equation (2.6), where, in each hydraulic conductivity realization, the violation of constraints (2.13) is calculated as:

$$\max\{0, \| \boldsymbol{\chi}(\mathbf{Q}, \mathbf{s}_k) - \boldsymbol{\chi}_c \|\} = \sum_{i=1}^{n} \max\left\{0, h_{min} - h_i^{(k)}, h_i^{(k)} - h_{max}\right\} \tag{2.14}$$

In (2.14), $h_i^{(k)}$ denotes the hydraulic head in well i for the realization $\mathbf{K}_k$ under the pumping scheme $\mathbf{Q}$. Note that the sum is extended over the n=64 candidate wells rather than the n_w wells that are actually activated ($n \geq n_w$). Since the candidate wells are uniformly distributed (Figure 1), Equation (2.14) provides a measure of the "volume of violation", that is, the volume where the hydraulic head surface resides outside the bounds $h_{min} = 40$ m and $h_{max} = 60$ m prescribed by constraints (2.13).

2.2 Response Matrix Approach

The computational cost required to solve the stochastic MO problems (2.5) and (2.7) may be greatly reduced by taking advantage of the characteristics of linearity of the investigated groundwater management problem. Indeed, groundwater flow in the confined aquifer is governed by the classic diffusion linear equation [9], subject to Dirichlet and Neumann boundary conditions (Figure 1) that are time-invariant and homogeneous (equal to zero) with respect to the aquifer drawdown. In this situation, there exists a linear relationship between the piezometric heads in the aquifer and the pumping rate at well locations, and the superposition of the effects of multiple pumping wells may be applied.

In the considered management problem, the estimation of hydraulic head h_i's based on pumping rates Q_i's is a necessary step to calculate the groundwater supply cost (2.9) and the constraint inequalities (2.13), upon which the objective functions (2.3), (2.4), and (2.6) depend. For each realizations of the hydraulic conductivity field, $\mathbf{K}_k(k = 1, 2, .., N_{MC})$, this calculation may be carried out using the following equation [1]:

$$\mathbf{h}^{(k)} = \mathbf{h}_0^{(k)} + \mathbf{R}^{(k)} \cdot \mathbf{Q} \tag{2.15}$$

where $\mathbf{h}^{(k)}$ and $\mathbf{h}_0^{(k)}$ are the vectors of hydraulic heads at well locations at a generic time t and initially (before pumping starts), respectively. The vector $\mathbf{Q}$ of pumping rates at the n candidate pumping wells is here assumed to remain constant during the withdrawal operations. $\mathbf{R}^{(k)}$ is the "response matrix" [1, 27], of dimensions $n \times n$, whose generic component, $r_{i,j}^{(k)}$, represents the sensitivity of the drawdown $s_i^{(k)} = h_{0,i}^{(k)} - h_i^{(k)}$ observed in well i to pumping from well j. In general, the coefficients of the response matrix depend upon the aquifer parameters (hydraulic conductivity and elastic storage spatial distributions), boundary conditions, pumping schedule and observation time.

In this work, groundwater flow is assumed to be at steady state, so that the response matrix is time-invariant. For each of the generated realizations of the hydraulic conductivity field, $\mathbf{K}_k(k = 1, 2, .., N_{MC})$, the response-matrix coefficients $r_{i,j}^{(k)}$ are obtained using the three-dimensional finite-element flow model SAT3D [23, 24]. This model solves the classic groundwater flow equation [9] and is used to calculate the hydraulic head change at any well location i due to a single well activated at location j with a unit pumping rate.

2.3 Multi-objective Optimization Algorithm

In this study, the solution to the MO problems (2.5) and (2.7) is tackled by combining the stochastic response-matrix simulator (2.15) with a MO evolutionary algorithm stemming from the NPGA developed by [34] and later improved and applied by [17] to the design of pump-and-treat systems for the cleanup of contaminated aquifers.

The NPGA constitutes an extension of the traditional genetic algorithm (GA) developed by [26] to unconstrained MO optimization problems. With the GA, mechanisms of natural evolution are simulated with two fundamental operators: selection and reproduction [26, 45, 40, 35]. The NPGA involves two additional operators: Pareto domination ranking and niching or fitness sharing [17].

In this work, following a typical formulation for evolutionary methods (e.g. [8, 17]), each alternative pumping scheme is represented as a "chromosome", *i.e* a string of binary (0 or 1) variables. A chromosome consists of a sequence of as many substrings as the number n of candidate pumping wells. Each substring indicates a well pumping rate in the form of a n_r-digit long binary number, which is used to discretize the interval $(Q_{ex}^{max}, 0)$ (see constraints (2.10) with $Q_{in}^{max} = 0$) into a finite set of n_Q equally spaced flow rates. The so-called "resolution number", n_Q, is equal to the maximum number of integers enumerable with a n_r-digit long binary variable, *i.e* $n_Q = 2^{n_r}$. The pumping rates at well i may thus take on the discrete values:

$$Q_{i,j} = \frac{j-1}{n_Q - 1} \cdot Q_{ex}^{max} \ ; \ j = 1, 2, ..., n_Q = 2^{n_r} \tag{2.16}$$

The total chromosome length is equal to $n \times n_r$. It is worth pointing out that the choice of discrete flow rates considered here is fully justified in the standard practice, since commercial pumps can work only at a finite set of pumping regimes.

Figure 2 describes the NPGA-based procedure devised to address the solution to problems (2.5) and (2.7). In step (a), an initial population of n_{pop} candidate designs, namely chromosomes, is randomly generated. In step (b), the objective functions (2.3) and (2.4) or (2.6), associated with each of these designs are calculated. In this stage, the stochastic response-matrix simulation model is run for each pumping scheme $\mathbf{Q}$ in the population to estimate the hydraulic head ensembles $h_i^{(k)} (i = 1, 2, .., n; k = 1, 2, .., N_{MC})$ at the n candidate wells, which are necessary to calculate the objective function values. These values are then archived in order to avoid redundant simulation calls in the following of the procedure. In step (c), the chromosomes in the population are ordered according to their Pareto rank, *i.e* the number of chromosomes in the population that have a performance that is better in at least one objective, and equal in the other objectives. Chromosomes with a rank equal to zero are called "non-dominated" and form a "Pareto front" in the objective function space.

Step (d) is the primary stage of the selection process that creates the next generation of chromosomes. This is obtained with a number of n_{pop} "tournaments", in each of which n_{tourn} chromosomes are randomly chosen and opposed against one another. A tournament is won by the chromosome with the lowest rank [17].

Tournaments involving at least two equally-ranked chromosomes that dominate all other designs will have no clear winner. This "impasse" is resolved by ranking the deadlocked chromosomes on the basis of their niche count, which quantifies the degree of crowding, *i.e*, the number of chromosomes in the current generation that are located within a specified distanced from the candidate in the objective functions space. In the case of problems (2.5) and (2.7), since the magnitudes of the objective functions are rather different, a scaling to their respective maximum becomes necessary to search a circular region of the scaled objective function space centered around each candidate and having a radius r_N called "niche radius". The winner is ultimately chosen as the chromosome with the lowest niche count, which is the "least similar" to other individuals in the population. This promotes genetic variability, so that the population of winners will tend to have more diverse chromosomes and will eventually form a more disperse Pareto front.

In the NPGA, the selection of chromosomes is thus controlled primarily by n_{tourn} and

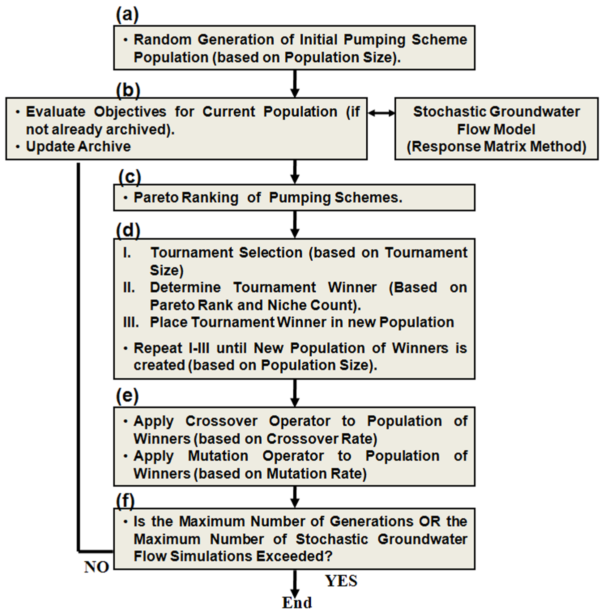

Figure 2: Process flow chart for the NPGA-based multi-objective optimization/simulation framework.

r_N. Note that the same chromosome may be selected and win multiple tournaments, thus entering the next generation more than once.

Step (e) consists of the application of the reproduction operator to the n_{pop} chromosomes obtained after selection. Reproduction occurs through the two fundamental genetic processes of crossover and mutation. With crossover, chromosomes are randomly paired with a probability prescribed by the crossover rate c_r, and their corresponding portions comprised between two randomly selected bit locations are permutated. The goal of the crossover operator is to improve the pumping strategies by combining their positive features in terms of management objectives. The mutation operator aims at reintroducing information that may have been lost during the selection and crossover stages. In the NPGA, mutation is performed with a probability prescribed by the mutation rate m_r and consists of the reassignment of each binary variable of the current set of chromosomes.

After crossover and mutation, the next generation of chromosomes is created. The steps (b)-(e) of the process are then repeated starting from this newly generated population and iterated generation after generation. The NPGA may be set up so that the optimization process stops: (i) when the number of generations reaches a prescribed maximum value n_{gen}; or (ii) the number of calls to the stochastic groundwater flow simulator exceeds a given maximum n_{sc}. It can be shown that the stopping criterion (ii) is irrelevant if n_{sc} is greater than $n_{pop} \cdot n_{gen}$. The stopping check is performed in step (f) of the procedure depicted in Figure 2.

3 Results and Discussion

In this section, results from the application of the NPGA-based framework to the management problems described in Section 2.1 are presented and discussed. Figure 1 shows the locations of 64 potential extraction wells chosen to identify the optimal groundwater supply strategies. These locations are uniformly distributed in the portion of the domain defined by constraints (2.12), which are thereby automatically met. Constraints (2.10) on decision variables are implicitly enforced by considering discrete flow rates as in Equation (2.16). The water demand constraint (2.11) is imposed by setting the objective functions to their respective maximum for those pumping schemes under which these constraints are not met. Hydraulic head constraints (2.13) are the only ones allowed for violation.

In our study, the size of the ensemble of hydraulic conductivity realizations is chosen after running a series of stochastic simulations with increasing value of N_{MC}. These preliminary tests show that, for the considered problem, a number of N_{MC}= 100 realizations is normally sufficient for the objective function values (Equations (2.3), (2.4), and (2.6)) to reach convergence. The hydraulic conductivity ensemble is generated using the sequential Gauss simulation algorithm developed by [7] with the geostatistical parameters given in Table 1.

It must be observed that the hydraulic conductivity field fits to an unconditional, second-order, stationary random process [15]. In practice, the joint probability distribution of K is spatially invariant, so that the hydraulic conductivity field can be considered statistically homogeneous. Given this assumption, and since the configuration of the aquifer boundary conditions and the selected candidate well locations (Figure 1a) are symmetric with respect the axis S-S shown in Figure 1, the optimization problem is solved by considering only pumping schemes that retain the symmetry to S-S. This assumption allows for sampling pumping schemes from 8 candidate well locations on the symmetry axis and 28 symmetric couples of candidate wells off the symmetry axis. In practice, the condition of symmetry produces a reduction of the size of the decision variable space from n=64 to n=36.

The optimization problems (2.5) and (2.7) are here solved by assigning n_r=2, which yields a chromosome length equal to $n \times n_r$=36×2=72. With n_r=2, a resolution number n_Q=2^{n_r}=4 is prescribed. Since $Q_{ex}^{max} \cong -550$ m^3/day, the possible extractions rates at each candidate well are equal to 0, -183.3, -366.7 and -550 m^3/day (Equation (2.16)). In any given pumping scheme, the n_w activated wells with a non-zero extraction rate are the only ones counted in the calculation of the total cost (Equation (2.9)).

$\boxed{3.0.1}$ Trade-off Analysis

The application of the NPGA-based framework requires intensive preliminary analyses to determine NPGA parameters that ensure the identification of the Pareto-optimal sets at the least computational cost[17]. Based on the results of these preliminary tests (not shown here), a population size n_{pop}=5000, a maximum number of generations n_{gens}=200, a crossover rate c_r=0.9, a mutation rate m_r=0.01, and a niche radius r_N=0.01 are selected. As for the tournament size, values n_{tourn} equal to 2, 5 and 10 are considered. The adopted population size and number of generations are large enough to guarantee the convergence of the NPGA to trade-off sets that are optimal or close-to-optimal in a Pareto sense. However, when using evolutionary algorithms in problems characterized by a decision variable space of large size, there is no absolute certainty that the Pareto-optimal set is completely identified.

The results of these NPGA runs are shown in Figure 3a for problem (2.5) and Figure 3b for problem (2.7). The numbers displayed between parentheses in the legend of each figure indicate the total number of "calls" to the response-matrix simulation model made in each simulation-optimization run, which has a prevailing impact on the computational cost of the procedure.

Figures 3a and 3b display a minimal difference between the optimal trade-off sets obtained using the three considered tournament size values. However, a significant advantage is achieved, in terms of computational cost, by using a larger tournament size. In particular, the total number of response-matrix simulations is reduced of about five and eight times by increasing n_{tourn} from two to five and 10, respectively. This happens because tournament competition controls the evolutionary process by promoting genetic pressure. The use of larger values of n_{tourn} typically enhances selection pressure and increases the chance of the fittest chromosomes in the population to enter following generations, thus promoting the convergence of the evolutionary process. However, the tournament size should not be deliberately increased as it can produce convergence to local optima, particularly when small populations are considered.

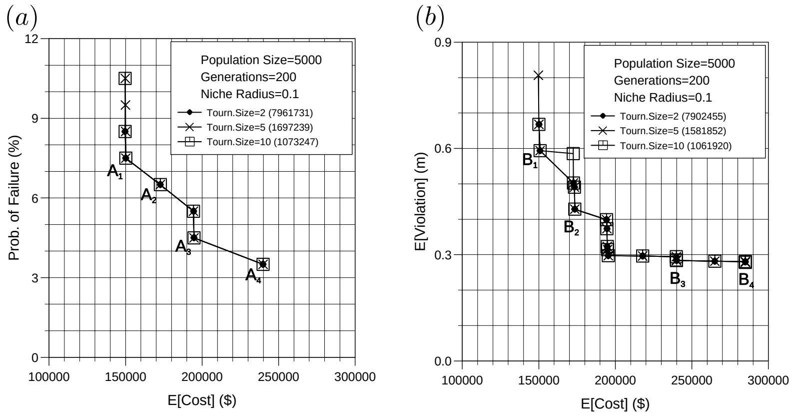

Figure 3: Trade-off fronts for (a) $Cost$ vs. P_{fail} and (b) $Cost$ vs. $Violation$ obtained for n_{pop}=5000, n_{gens}=200, r_N=0.1, and n_{tourn} values of 2, 5, and 10. Displayed between parentheses in the legend is the total numbers of "calls" to the response-matrix simulation model made in each simulation-optimization run. The decision alternatives A_1, A_2, A_3, and A_4 in subpanel (a) represent the most reliable strategies identified by installing 5, 6, 7, and 9 pumping wells, respectively. The decision alternatives B_1, B_2, B_3, and B_4 in subpanel (b) can be regarded as the lowest-violation strategies attainable with the activation of 5, 6, 9, and 11 pumping wells, respectively.

The comparison between the $Cost$-vs.-P_{fail} (Figure 3a) and the $Cost$-vs.-$Violation$ (Figure 3b) trade-off sets reveals that the latter approach offers a much larger set of pumping schemes than the former. Indeed, while with P_{fail} attention is focused on the frequency of violation of constraints (2.13) over the set of realizations considered in the stochastic simulations, with $Violation$ not only the frequency but also the intensity of violation is accounted for. Therefore, while the probability of failure (Equation (2.4)) may take on only a discrete set of N_{MC} values, the expected value of violation (Equation (2.6)) is likely to be different for each alternative pumping strategy. As a consequence, framework (2.7) produces a trade-off front that results more dispersed than that obtained with framework (2.5). This may be seen as an advantage of using $Violation$, as opposed to P_{fail}, to quantify the reliability of pumping strategies.

From the perspective of the decision maker, the framework (2.7) may thus be more convenient than framework (2.5) as the expected value of the violation intrinsically retains more complete information on the reliability of any given pumping scheme, and also provides a larger number of decision alternatives.

In Figures 3a and 3b, the trade-off sets form stair-shaped profiles characterized by Pareto-optimal clusters of pumping schemes having approximately the same expected cost and different values of either the probability of failure (Figure 3a) or the expected violation (Figure 3b).

The analysis of the pumping schemes in a cluster reveals that these have the same number n_w of activated wells. Since in the groundwater supply problem formulated by [39] the total cost (Equation (2.9)) is mainly affected by its capital component, the difference in total cost depends merely on how these wells are distributed, which affects the hydraulic head distribution and thus the operating cost. Accordingly, it may be shown that two consecutive clusters have a difference in cost of about $22,800, which is the capital value of one additional pumping well. Given that the pumping schemes in a cluster have similar expected costs, the most convenient solution for each cluster is that with a lower value of P_{fail} in Figure 3a or $Violation$ in Figure 3b.

3.0.2 Analysis of Pumping Strategies

Figure 4 represents the characteristics of the four pumping schemes associated with the points A_1, A_2, A_3, and A_4 on the *Cost* vs. P_{fail} trade-off front graphed in Figure 3a. The subfigures show well locations and extraction rates for each pumping scheme, along with the contour representation of the expected distribution of the piezometric surface. The four pumping schemes A_1, A_2, A_3, and A_4 represent the lowest-cost and most reliable pumping strategies identified by installing 5, 6, 7, and 9 pumping wells, respectively.

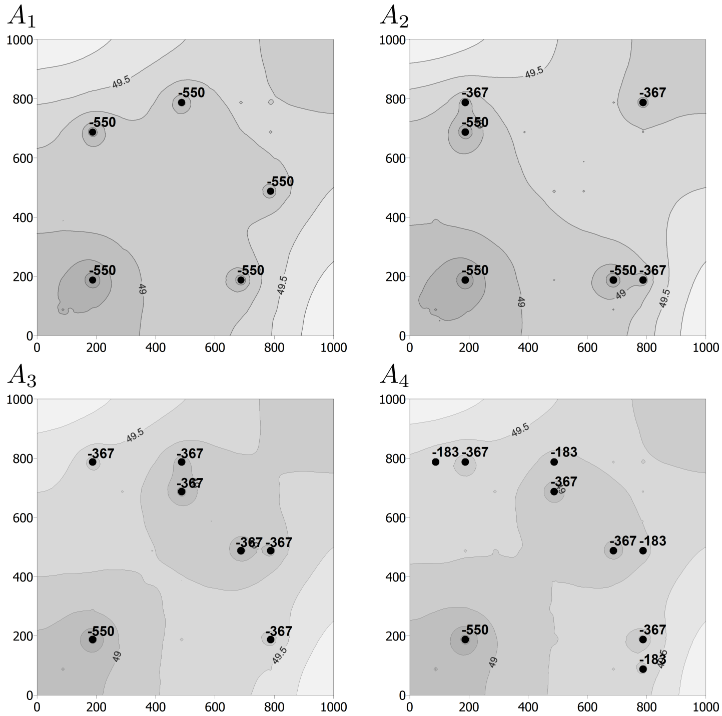

Figure 4: Characteristics of the pumping schemes associated with the points A_1, A_2, A_3, and A_4 on the trade-off fronts indicated in Figure 3a.

Figure 5 displays four pumping schemes corresponding to the points B_1, B_2, B_3, and B_4 on the *Cost* vs. $Violation$ trade-off front plotted in Figure 3b. Pumping schemes B_1, B_2, B_3, and B_4 can be regarded as the lowest-cost and lowest-violation pumping strategies attainable with the activation of 5, 6, 9, and 11 pumping wells, respectively.

In both Figures 4 and 5, it may be observed that all pumping schemes strictly meet the groundwater demand constraint (2.11). For the *Cost* vs. P_{fail} problem, all four alternatives presented in Figure 4 have one well in common located in proximity of the lower-left corner of the domain and pumping at the maximum allowed extraction rate, while the other pumping wells are generically located along the constant-head boundaries of the domain (Figure 4). These results reveal that, in order to minimize P_{fail}, one needs to position one large-capacity well in the lower left corner of the aquifer, where the ambient hydraulic head is higher, due to the combined effect of vertical recharge no-flow boundary conditions, and a number of wells with smaller capacity along the upper and the right boundaries, where the aquifer is subject to fixed-head conditions, which smooth out the effects of well interference.

On the other hand, for the *Cost* vs. $Violation$ problem, a close analysis of the pumping patterns in Figure 5 indicates that an effective reduction of the average intensity of violation of constraints (2.13) is achieved –however a larger total cost– by installing a larger number

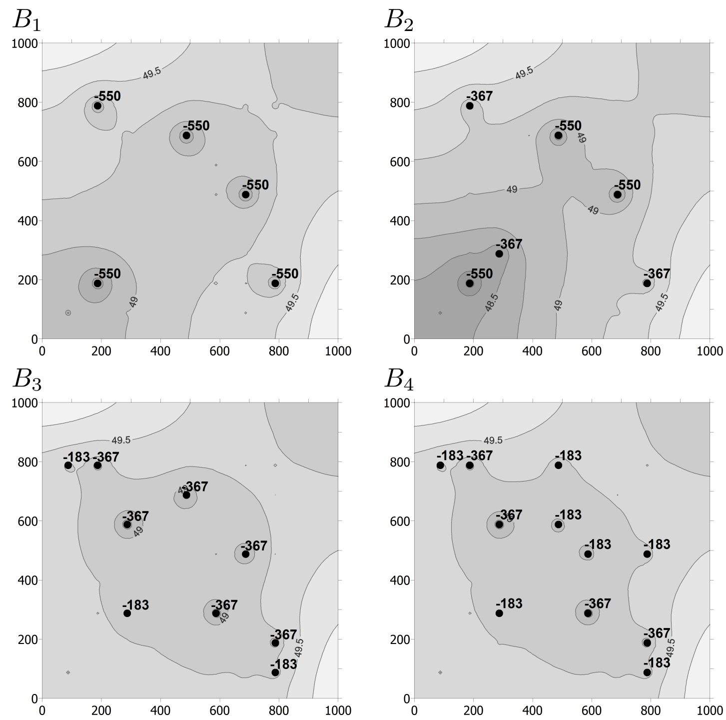

Figure 5: Characteristics of the pumping schemes associated with the points B_1, B_2, B_3, and B_4 on the trade-off fronts indicated in Figure 3b.

of wells in centralized locations along the upper/left-lower/right diagonal of the domain, and possibly reducing the extraction rates below the maximum pumping capacity. This is shown to create hydraulic head regimes that, while having a sub optimal (larger) probability of failure, that is, violate the hydraulic head constraints with higher frequency, are on average characterized by a minimum intensity of violation smaller than those displayed in Figure 4. Indeed, wells are positioned in areas of the aquifer where effects of well interference are more important, but the ambient hydraulic head is also higher, than they are along the fixed-head boundaries.

$\boxed{3.1}$ Computational Performance

All processes performed in this work are run on a computer equipped with four dual-core AMD-Opteron 885 processors, each operating at 2,600 MHz, with a total 32 Gb Ram memory. The computational cost associated with the solution to the MO optimization problems (2.5) and (2.7) may be quantified by the sum of the central processing unit (CPU) times required to: a) calculate the response matrix coefficients; and b) identify the Pareto-optimal set using the response-matrix/NPGA simulation-optimization approach.

The calculation of the response matrices $\mathbf{R}^{(k)}$ requires as many stochastic SAT3D simulations as the number n of candidate wells. An additional simulation run is required to calculate the initial hydraulic heads $\mathbf{h}_0^{(k)}$ at potential well locations. The CPU time required by each of these simulations is about 2,300 CPU seconds.

The computational cost associated with each NPGA-based optimization run is substantially related to the number of calls to the stochastic response-matrix simulation model. The computational time associated with each run varies slightly depending upon the assumed NPGA parameters, and is, on average, equal to about 1320 simulation calls per CPU minute

(4.5×10^{-2} seconds each). For example, the NPGA process whose trade-off set is shown in Figure 3a, obtained with 10 random seed trials, n_{pop}=5000, n_{gens}=200, n_{tourn}=5, and r_N=0.1, involves a number of 1,697,239 response-matrix simulation calls, which require about 21 hours and 26 minutes CPU time to be completed.

The overall computational cost is thus significant, but still viable with the available computer capabilities. It is worth pointing out that the feasibility of these processes is made possible only by substituting the stochastic groundwater flow simulation model with the response-matrix model. Since the average CPU time of one stochastic flow simulation is about 2,300 seconds, while the average stochastic response-matrix simulation takes about 4.5×10^{-2} seconds, one can easily estimate that, if the stochastic flow model was directly embedded in the NPGA, the identification of trade-off fronts such as those shown in Figures 3a and 3b would require a CPU time ($2{,}300/4.5\times10^{-2}=$) 5×10^{4} times larger than that spent using the response matrix simulator. In practice, this would drastically limit the capability of the simulation-optimization framework to problems characterized by a very low number of candidate well locations.

4 Conclusions

In this study, we have presented a stochastic optimization framework to support the design and the management of groundwater supply systems in confined aquifers under uncertain hydraulic conductivity distribution. The framework stems from the combination of a stochastic flow simulation model with an evolutionary algorithm. The stochastic flow model relies on a Monte Carlo method, where an ensemble of hydraulic conductivity scenarios is used to simulate the piezometric distribution in the aquifer needed to calculate both the total cost of the pumping system and the management constraints.

The computational efficiency of the framework is drastically improved by adopting a response-matrix approach, which is made possible by the linear relationship existing between pumping stress and piezometric head in confined aquifers. The response matrix coefficients are calculated outside the optimization loop using a stochastic flow simulation model, so that the evolutionary algorithm can be linked to a stochastic response-matrix simulator, instead of the computationally "expensive" stochastic flow model.

The framework is structured into a MO optimization problem, whose goal is to identify sets of alternative pumping designs that –because of the uncertain response of the aquifer to pumping stress– necessarily trade off cost optimality against the risk of not complying with the management constraints. The risk is defined according to two alternative formulations: the probability of failure, that is, the frequency of violation of management constraints, or the expected intensity of constraint violation.

This methodology is applied to one of the benchmark management problems formulated by [39]. The computational efficiency of the framework is such that the investigated problem may be addressed using as many as 64 candidate well locations with four potential extraction rates each, with a computational cost that, although significant, can be sustained with the available computational capabilities.

The analysis shows that, from the perspective of the decision maker, the $Cost$-vs.-$Violation$ formulation may be more convenient than the $Cost$-vs.-P_{fail} approach. Indeed, while P_{fail} accounts only for the frequency of violation, $Violation$ accounts also for the the intensity of violation, thus providing more complete information on the reliability of any given pumping scheme. In addition, the solution to the $Cost$-vs.-$Violation$ trade-off problem yields a larger set of pumping schemes, and thus wider range of decision alternatives, than that obtained for the $Cost$-vs.-P_{fail} trade-off problem.

For the considered groundwater management problem [39], both $Cost$-vs.-P_{fail} and $Cost$-vs.-$Violation$ trade-off fronts form stair-shaped profiles characterized by clusters of points having approximately the same expected cost and different values of either the probability of failure or the expected violation. Since the total groundwater supply cost is mainly affected by its capital component, which is directly proportional to the number of installed wells, the pumping schemes in a cluster are characterized by the same number of activated wells. The location of these wells affect significantly both P_{fail} and $Violation$. Given that $Cost$ is about the same, the most convenient pumping scheme in a cluster appears to be be that with either the lower frequency or the lower intensity of constraint violation.

The extraction rates in each trade-off pumping scheme are such that an imposed constraint on the minimum groundwater supply demand is strictly met. The more expensive pumping schemes, with more wells installed, are thus characterized by generally lower extraction rates and are less prone to violation of hydraulic head constraints.

A future extension of this work will include the analysis of effects of transient flow assumptions, which require modifying the response matrix approach in order to account for the possible variations of pumping rates over time. Since this is expected to produce a significant increase in the computational cost of the procedure, it will be important to resort to parallel programming techniques allowing for the simultaneous distribution of simulation model calls to multiple processing units. Another extension will explore the option of using injection wells as a measure for reducing the risk of aquifer depletion and simulate the potential benefits of aquifer storage and recovery techniques in terms of cost and sustainability.

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