METHODOLOGY FOR THE OPTIMIZATION OF GROUNDWATER QUALITY MONITORING NETWORKS ORIENTED TO SATISFY A SPECIFIC SPATIAL COVERAGE

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Abstract. Through the optimal design of groundwater monitoring networks, it is possible to obtain the maximum level of information for certain variables (water level, some quality indicator parameters, and/or the presence of some contaminant) at minimum cost; the methodologies for this kind of designs follow a procedure to discard wells that provide redundant information. The information collected by monitoring networks is fundamental for supporting decision making that aims for a sustainable management of groundwater. In this paper, an existing methodology for the design of optimal groundwater quality monitoring networks is modified to include a new algorithm that allows to obtain alternative spatial distributions of the wells that provide the highest level of information, expressed in terms of the estimated uncertainty over an estimation grid. Additionally, different weights can be assigned to each monitoring site and to the analyzed variable(s) within the objective function in order to accomplish specific objectives without a significant loss of information. The final result represents a significant improvement to the original methodology by adjusting the spatial coverage of the optimal monitoring network to satisfy specific objectives.

Keywords: geostatistics, Kalman filter, estimation grid, water management, sustainable

Introduction

Groundwater is a vital resource for human beings; it provides 50% of the total water used worldwide (WWAP, 2016). This data shows the dependence of people on groundwater, mainly in regions with extensive cropping areas for food production and industrial activities (Li et al., 2015).

Considering the importance of groundwater, it is necessary to know, in detail, the spatial distribution of the groundwater flow systems and its physical-chemical characteristics to improve its management (Esquivel et al., 2015; Kim et al., 2007). It is relevant to assure sustainable levels of groundwater quality when it is used for water supply (Yang et al., 2018). The implementation of groundwater quality monitoring programs is of paramount importance; for instance, it was detected that in almost 15% of the monitoring stations in Europe, the standard for nitrates in drinking water established by the World Health Organization (WHO) was exceeded (WWAP, 2018). It is possible to characterize the groundwater quality in some areas of interest (AOI) by measuring some physical-chemical parameters of water extracted by wells and

estimating the spatial distribution of their concentrations; however, the costs and time involved in visiting and sampling all the existing wells are often not economically viable; specially in low income countries.

The optimal design of groundwater monitoring networks is an alternative to reduce time and costs associated to the acquisition of data to accomplish specific objectives (Júnez-Ferreira et al., 2016a); in addition the development of a sustainable strategy for groundwater extraction management is required.

The methodologies for the optimal design of groundwater monitoring networks can be subdivided in three main groups: 1) those based on elements of hydrogeological conceptual models, 2) those that execute data analysis with statistical techniques, and 3) those that use groundwater flow numerical models (Júnez-Ferreira et al., 2016a; Loaiciga et al., 1992; Herrera and Pinder, 2005; Zhang et al., 2005). The latter can be considered as the most robust framework, since it does not only consider hydrogeological aspects (as group one) but also takes into consideration groundwater levels evolution (in space and time). It is important to note that some methodologies combine aspects of two or the three groups.

The hydrogeological framework usually uses a Geographic Information System (GIS) in order to incorporate as much areal information as possible of the hydrogeological factors that control the groundwater functioning such as geology, recharge and discharge zones, rainfall data, groundwater levels, land use/land cover images derived from satellites, among others (Singh and Katpatal, 2017; Zhou et al., 2013). The statistical-based methodologies usually employ a variance-based objective function evaluated by an optimization method, they are commonly based on spatial and/or spatiotemporal geostatistical techniques, entropy theory, harmonic series models and principal component analysis (Mirzaie-Nodoushan et al., 2017; Júnez-Ferreira et al., 2016b; Andricevic, 1990; Kim et al., 2007; Júnez-Ferreira and Herrera, 2013), some of them are multicriteria (Hosseini and Kerachian, 2017a, b). The combination of hydrogeological criteria through the use of GIS and statistical techniques has been used in (Baalousha, 2010; Uddameri and Andruss, 2014; Sizirici and Tansel, 2015; Júnez-Ferreira et al., 2016a; Alizadeh and Mahjouri, 2017). The methodologies based on a numerical flow model include optimization methods and are always combined with a GIS (Kim, 2015) or with statistical estimation methods such as the Kalman Filter (KF), Monte Carlo simulations (Herrera and Pinder, 2005; Zhang et al., 2005; Kollat et al., 2011; Luo et al., 2016; Jiang et al., 2018), or can have characteristics of the three groups of methodologies for the optimal design of groundwater monitoring networks (Nobre et al., 2007).

Most of these methodologies require a large amount of information about the study site that includes a comprehensive database of sampling campaigns, geological data, and an advanced understanding of flow systems.

In those areas with scarce data, it is necessary to implement methodologies to start with the data generation. In the literature, the KF or different types of kriging have been widely used as estimation methods for the design of optimal monitoring networks oriented to the reduction of the estimate error variance in areas with few hydrogeological data (Júnez-Ferreira et al., 2016a; Júnez-Ferreira and Herrera, 2013); however, the spatial distribution of the wells with higher priority selected by these methodologies preferably covers the central area of a pre-defined estimation grid, frequently assigning a lower priority to those wells located at the periphery of the study area. This is considered as a deficiency because a poor spatial coverage of the

monitoring network may lead to the undesirable extrapolation of the monitored variable(s) at those areas. In addition, a resilient monitoring network in regard to sampling station distribution, in practice could be easier to implement and to explain to stakeholders. The design of an optimal monitoring network results in an academic exercise not feasible to real-world limitations (data availability, budget), hence the implementation of alternative methodologies is advisable (Bode et al., 2018).

In Mexico there are 653 administrative aquifers, 105 of them have been classified with intensive abstraction resulting in negative environmental effects such as the ongoing deterioration of water quality (Esteller et al., 2011), sea water intrusion problems, presence of brackish water (CONAGUA, 2017), and high fluoride and arsenic concentrations in groundwater (Banning et al., 2012; Cardona et al., 2018). However, the natural evolution of the groundwater quality has not received the required attention as a tool for management planning.

Mexico and a number of countries around the world are involved in the Sustainable Development Goals (SDG) to address global challenges such as environmental (water) degradation. Specifically, goal 6: Clean Water and Sanitation, indicator 6.3.2: Proportion of water bodies with good water quality requires the implementation of groundwater monitoring networks to compile data for some core parameters at existing sampling stations (UN WATER).

The lack of properly designed wells for groundwater quality monitoring purposes makes necessary employing the available long screened production wells. The spatial distribution of these production wells depends on factors such as the location of irrigation lands and populated areas. Therefore, it is relevant for water management institutions to consider methodologies that contribute to the design of optimal groundwater monitoring networks, with water quality data obtained from production wells. This is an important issue for making decisions regarding groundwater sustainable development, not only in Mexico, but in several other countries around the world.

This paper proposes a methodology for the design of multivariable groundwater monitoring networks. The approach includes 1) irregular shape estimation grid according with the spatial sampling station distribution 2) a ponderation grid map based on sampling station density per unit area 3) the definition of an objective function that considers simultaneously, the ponderation grid map, priority determination for any water quality parameters included in the monitoring network and/or for sampling stations and a KF for the reduction of the estimate uncertainty for each variable provided by the selected sampling stations. The methodology allows obtaining alternative spatial distributions of the wells that provide the highest level of information, expressed in terms of the estimated uncertainty over an estimation grid.

Materials and methods

The methodology presented in this paper is based on that proposed in Júnez-Ferreira et al. (2016a); the original methodology selects the optimal monitoring positions by using spatial correlations expressed as covariance matrices derived from semivariogram models obtained through geostatistical analyses to data of groundwater quality parameters. The optimization of the monitoring network is carried out by successive inclusions employing the KF as the estimation method, minimizing a function called the joint total (JT) normalized variance of the estimation error (Júnez-Ferreira et al., 2016a).

This methodology requires of a spatial estimation grid where the objective function is evaluated. During the optimization process, the addition of weights to the groundwater quality parameters, or different densities in the estimation grid have been useful to satisfy specific objectives, like assigning a higher priority to contaminated sites or to highly dangerous parameters (Júnez-Ferreira et al., 2016a; Esquivel et al., 2015).

For the proposed methodology, the objective function incorporates the spatial coverage of the available sampling stations (by means of a supplementary function, SF) besides a modified version of the joint total (JT) normalized variance of the estimation error. The modified JT, besides having a weight for each groundwater quality parameter includes a weight for each sampling station, this new algorithm is now called the weighted joint total normal variance of the estimation error (WJT). Both, the WJT and the SF are weighted in order to define different alternatives of the spatial coverage for the selected monitoring networks without a significant loss of information.

The objective function (OF) (Eq. 1) for the proposed methodology is:

$$OF = V \times WJT + W \times SF \tag{Eq.1}$$

where V and W are the weighting factors for the WJT and the SF, respectively; V + W = 1. Based in Júnez-Ferreira et al. (2016a) to obtain WJT, the KF is implemented through the use of \hat{q}^0 and P^0 that represent an initial state vector and the initial error covariance matrix, respectively. The KF process employs the following equations (*Eqs. 2, 3* and 4):

$$\hat{q}^{n+1} = \hat{q}^n + K_{n+1}(z_{n+1} - H_{n+1}\hat{q}^n)$$
 (Eq.2)

$$P^{n+1} = P^n - K_{n+1} H_{n+1} P^n$$
 (Eq.3)

$$\mathbf{K}_{n+1} = \mathbf{P}^{n} \mathbf{H}_{n+1}^{T} (\mathbf{H}_{n+1} \mathbf{P}^{n} \mathbf{H}_{n+1}^{T} + \mathbf{r}_{n+1})$$
(Eq.4)

where K_{n+1} is the Kalman gain, H_{n+1} is the sampling matrix, z_{n+1} is the measurement vector, and r_{n+1} is the measurement error covariance. Superscripts refer to the number of measurements employed in the estimation; subscripts are used to indicate the transition when a new measurement is going to be used in the process.

The spatial covariance matrix for each parameter is calculated as follows (Eq. 5):

$$C(h) = C(0) - \gamma(h)$$
(Eq.5)

where C(h) represent the covariance matrix, C(0) is the variance for each analyzed parameter, and $\gamma(h)$ is the variogram model function.

The WJT value is calculated with (*Eq. 6*):

WJT =
$$\sum_{p=1}^{np} \sigma_{w,p}^2 \times \alpha_w \times \alpha_p$$
 (Eq.6)

where $\sigma_{w,p}^2$ represents the normalized estimate error variance (located at the principal diagonal of the corresponding updated covariance matrix) at each estimation position

for the **p** parameter, when the **w** well has been sampled, α_w represents the **w** well weight, α_n represents the **p** parameter weight, and *n***p** is the number of parameters.

The main advantages of this proposal are: a) it considers the possibility of obtaining alternative monitoring networks designs oriented to a desired spatial coverage b) it allows the assignation of different weights to a particular sampling point, which gives the opportunity to take into account specific hydrogeological conditions such as contaminated areas without affecting, within the optimization procedure, those wells located around this specific sampling point.

Custom estimation grid

As part of the proposed methodology, it has been developed an algorithm for the generation of a custom estimation grid (CEG). The KF estimates will be obtained and the OF evaluated at the CEG; it offers advantages when compared to a regular grid as implemented in commercial software such as XTools Pro 18 (XTools Pro), create fishnet (ArcGIS) and sampling design tool (Buja, 2012) because it avoids extrapolation areas since it is an adjusted envelope of the sampling points.

The definition of the CEG starts with the calculation of the distance between the extreme coordinates of the wells (maximum distance), followed by the calculation of the grid density with half the maximum distance divided by ten; this density (separation between the grid nodes) is selected to draw a rectangular grid that covers all the area where the wells with available data are located, an initial value of 0 is set to all these nodes. The CEG will be composed by values different than 0, the following procedure is carried out from the top (North) to the bottom (South) row of the original rectangular grid to the assignation of these values:

- 1. Values of 1 are assigned to the nodes that are next to the wells.
- 2. For each row it is given a value of 2 to the nodes that are between those with a value of 1.
- 3. A value of 3 is assigned to the nodes in empty rows to connect the nodes with values different to 0.
- 4. Values of 4 will be assigned to the nodes with an original value of 0 in such a manner that each row of the CEG cannot be longer one node to the West and one node to the East than the next row at the south.

The flowchart and pseudocode for this process are shown in *Figure 1*.

The colours in *Figure 2* are directly related to the value that indicates in which part of the algorithm the node for the CEG was selected.

Supplementary function

For the case study, the SF is proposed trying to establish a higher priority to those wells that have influence over the highest number of nodes of the estimation grid, and at the same time, with small influence of the other wells on their estimates (i.e., there is a poor spatial coverage of wells at that area). For that purpose, it is necessary to define a Custom Smooth Grid (CSG) based on the CEG and the maximum range used in the semivariogram models. For each node of the CEG, it is calculated the sum of wells located at a distance less than the model range, obtaining the values of the CSG (*Fig. 3*).

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Figure 1. CEG generation flowchart and pseudocode



Figure 2. Custom estimation Grid (CEG)

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Figure 3. Custom Smooth Grid (CSG)

The SF is defined as follows:

The lower values in the CSG represent zones with a poor spatial coverage of wells. The formulas for the values of the CSG are (Eq. 7):

$$ie_{w,p} = \sum_{n=1}^{nn} node_n \tag{Eq.7}$$

where $ie_{w,p}$ represents the influence of the well w over the nodes of the CEG, corresponding to the p parameter, $node_n$ is 1 when the node is inside a circumference with center on the w well and radius equal to the range of the semivariogram model in the p parameter; $node_n$ is 0 when the node is outside the circumference, nn is the total number of nodes in the CEG (*Eq. 8*);

$$iw_{n,p} = \sum_{w=1}^{nw} well_w$$
(Eq.8)

where $iw_{n,p}$ represents the influence of the sampling wells over the node n, corresponding to the p parameter, $well_w$ is 1 when the well is inside a circumference with center on the n node and radius equal to the range of the semivariogram model in

the *p* parameter, $well_w$ is 0 when the well is outside that circumference, nw is the total number of sampling wells (*Eq. 9*);

$$inw_{w,p} = \sum_{n=1}^{nn} (iw_{n,p} \times r_{n,p})$$
(Eq.9)

where $inw_{w,p}$ represents the influence of the sampling wells over circular zones of the CEG, $r_{n,p}$ is 1 when the node is inside a circumference with center on the w well and radius equal to the range of the semivariogram model in the p parameter, $r_{n,p}$ is 0 when the node is outside the circumference (*Eq. 10*);

$$f_{w,p} = \frac{\alpha_w}{ie_{w,p} \times inw_{w,p}}$$
(Eq.10)

where $f_{w,p}$ represents the w well factor for the p parameter (Eq. 11);

$$ff_w = \sum_{p=1}^{np} f_{w,p} \alpha_p \tag{Eq.11}$$

where ff_w represents the *w* well final factor, *np* represents the total number of parameters considered in the network design.

In the case study, it is proposed that $SF = ff_w$.

Results

Case study: hydrogeological setting

In order to evaluate the performance of the proposed methodology, it was applied for the design of a monitoring network in the "El Bajío" Region of Central Mexico (Fig. 4). The Bajío Region, specifically the Irapuato-Valle aquifer has become recently a focus of attention due to the intensive water extraction regime for agricultural, population, and industrial use. Groundwater extraction (about $600 \times 10^6 \text{ m}^3/\text{year}$) through more than 2900 production wells in the area supports the water supply for more than 900,000 inhabitants in urban and rural areas, the irrigation of approximately 60,000 hectares and the water consumption for a refinery, a power production plant and several industrial parks (Comisión Nacional del Agua, 2015; Esteller et al., 2011; Gómez and Sandoval, 2004). The rock units in the study area include a sequence of Mesozoic plutonic and vulcano-sedimentary rocks affected by several metamorphism stages and Tertiary intrusive rocks outcropping in the Sierra de Guanajuato located at the North of the study area that constitutes the hydrogeological basement. The Tertiary sequence include volcanic (ignimbrites, lava flow and tuffs) and continental sedimentary rocks (conglomerates and basin fill sediments). The Oligocene volcanic sequence is comprised of andesite and rhyolite; the overlying Miocene and Pliocene volcanic rocks are mainly andesite and basalt associated with the Mexican Neo-volcanic Belt (Nietosamaniego et al., 2012). From the Oligocene, the Sierra de Guanajuato underwent a rapid uplift, the main geologic structures are NW-SE trending normal faults, displacing

more than 500 m the Oligocene volcanic sequence (Gómez et al., 1989; Nietosamaniego, 1990). During this stage of deformation, several faults were reactivated, the N-S (Taxco-San Miguel de Allende fault) and NE-SW trending directions, together with the "El Bajío" Fault with NW-SE trend, formed half grabens, leading the formation of the "El Bajío" region (Botero-santa et al., 2015). At the same time, the erosion from the mountains led to transfer clastic material to the graben structure. The deposition of basin fill sediments in the graben structure produced a granular permeable regionally unconfined aquifer with a maximum thickness of 350 -400 m. Basin fill sediments are inter-bedded poorly consolidated fluvio-lacustrine sediments, including sands, interbedded sandy-clay and silts. From pumping test data, typical hydraulic conductivity values for that aquifer are 1 to 10 m/day (Júnez-Ferreira et al., 2016a). The Tertiary volcanic rocks are cut by a set of NW-SE and N-S normal faults, creating the possibility of a fractured heterogeneous aquifer (200-300 m thickness). The basaltic Pliocene rocks outcropping in the southern portion of the study area are in contact with the basin fill sediments, they confirm an unconfined aquifer with hydraulic conductivity values from 6 to 18 m/day (Júnez-Ferreira et al., 2016a). The Oligocene and Miocene volcanic rocks below the basin-fill sediments can also constitute a deep aquifer, fractured conditions along the NW-SE trending structures have been identified in deep wells (600-700 m deep) producing thermal groundwater (well-head temperature 35-45 °C).



Figure 4. Location map of the study area. (Sources: Simplified El Bajío Region map modified Suárez-mota and Villase, 2015; Irapuato-Valle Aquifer from National Water Information System, 2019; countries boundaries from Tapiquén, 2019)

A sampling campaign for groundwater quality determination was carried out in December 2003 for laboratory measurement of 20 physicochemical parameters and in situ measurements of six field parameters (Júnez-Ferreira et al., 2016a), a total of 140 water samples were taken in production wells from the study area. A map displaying the sampled wells is presented in *Figure 2* (UTM coordinates datum WGS84, Zone 14N). Wells ranging from 46 to 700 m deep (mean 180 m, standard deviation 115 m), most of

them screened along the saturated length of the well, promoting intra-well artificial mixing. This implies that sampled water represents a mixture of several water-bearing layers. It was identified that water in recharge areas is HCO₃-Ca dominant type (650 mg/L of total dissolved solids in average). Along the groundwater flow, water chemistry evolves to dominant HCO₃-Mix and HCO₃-Na. Groundwater quality analysis indicates the contribution of geogenic and anthropogenic contamination sources. The volcanic rocks, especially those of rhyolitic composition and the basin fill sediments derived from them, are potential trace element sources specifically for Arsenic. The water samples were analyzed for arsenic composition (mean 0.011 mg/L, max. 0.083 mg/L), 35% of the samples exhibit concentrations in excess of the WHO guideline value (0.010 mg/L) (Fig. 5a). Dissolved arsenic is usually found as arsenic (III) in reducing environments, which usually develops at some depth within aquifers, while near the water table oxic condition prevails (Appelo and Postma, 2005). There is a lack of vertical water quality profiles information in wells, for this reason it is not possible to demonstrate the existence of any vertical transition between oxic and anoxic conditions in the tapped aquifer. However, aerobic and oxic conditions (dissolved oxygen above 1 mg/L. Eh values above 100 mV) were detected in all the groundwater samples, suggesting that oxic conditions should prevail in most of the water bearing geologic formations tapped by the production wells. Considering that the sample depth could be assigned to mid-well screen depth, no correlation between sample depth and arsenic values was identified ($R^2 = 0.07$), indicating that dissolved arsenic is not explained by desorption from Fe-(hydr)oxide minerals in reducing conditions (Fig. 5b). Most of the high arsenic water samples are associated with HCO₃-Na dominant type, indicating that leaching from volcanic rocks with rhyolitic composition is a major control. Evidence from north-central Mexico suggests that dissolution of volcanic glass of felsic composition seems to be the dominant process for arsenic release into groundwater (Banning et al., 2012); the concentration in the central and northwest region of the study area seem to be derived from this source. The basin fill sediment constitutes an additional source; arsenic values above the WHO drinking water standard in the southwest region of the study area are probably derived from the basin fill sediments. Decarbonatization of basin-fill sediments could constitute an additional process for arsenic mobilization (Banning et al., 2012). The identification of groundwater impacted from anthropogenic sources, considered water types such as Cl-Mg, Mixed-Ca, Mixed-Na, and SO₄-Mixed; they exemplify impacted groundwater by diffuse contamination. Impact of diffuse contamination produced by irrigation can be evaluated with a combination of indicators, such as chloride, sulphate, nitrate, phosphate among others (Cardona et al., 2008). Chloride is a conservative solute; it is useful to detect the infiltration of diffuse contamination from agricultural activities. In addition, electrical conductivity is a function of the total concentration and charge of the ions; the relationship between them is approximately linear in most of the cases. The relation between chloride and electrical conductivity for water samples from the study area is shown in Figure 6. The characteristics of the local surface water and wastewater are presented as an additional reference. Despite the scatter, there is an evident general trend for most of the samples, suggesting that infiltration of wastewater modify to some extent groundwater composition. A few samples are not following the general trend, especially high electrical conductivity values with low chloride values; for these samples high alkalinity values (> 500 mg/L CaCO₃) linked with low nitrate

concentration (about 4-5 mg/L N-NO₃), suggest a limited influence of irrigation return flow or wastewater infiltration.

From the above considerations, the methodology proposed in this paper was applied for the design of an optimal groundwater quality monitoring network oriented to characterize the spatial distribution within the study area of only three parameters of the database presented in Júnez-Ferreira et al. (2016a): arsenic, chloride and electrical conductivity. Six cases were analyzed: 1) $\mathbf{V} = 1$ and $\mathbf{W} = 0$ within the OF ("100 – 0"), 2) $\mathbf{V} = 99.999$ and $\mathbf{W} = 0.001$ ("99.999 – 0.001"), 3) $\mathbf{V} = 99.995$ and $\mathbf{W} = 0.005$ ("99.995 – 0.005"), 4) $\mathbf{V} = 99.99$ and $\mathbf{W} = 0.01$ ("99.999 – 0.01"), 5) $\mathbf{V} = 0.5$ and $\mathbf{W} = 0.5$ ("50 – 50") and 6) $\mathbf{V} = 0$ and $\mathbf{W} = 1$, but in this case the optimization procedure is applied in such a manner that the highest priority in wells is assigned to the highest estimate error variance ("Worst" case). For the six cases $\boldsymbol{a}_{\mathbf{w}} = \boldsymbol{a}_{\mathbf{p}} = \mathbf{1}$.



Figure 5. Arsenic analysis in a) the number of samples for groups and the reference of the WHO, in b) the correlation between concentration and well depth



Figure 6. Correlation between chloride and electrical conductivity

Geostatistical analyses

As a result of the geostatistical analyses carried out to the selected groundwater quality parameters, semivariogram models for each parameter were obtained (*Table 1*). With these models, covariance matrices were derived and normalized for each parameter and used in the optimization process, using the CEG and the CSG values.

Table 1. Semivariogram models used for the generation of the groundwater monitoring network

Parameter	Model	Nugget (u ²)*	Sill (u ²)*	Range (m)
Electrical conductivity	Spherical	0	125097	6792
Arsenic	Spherical	6.5x10 ⁻⁵	0.000142	4685
Chloride	Spherical	60.98	1490	6515

*u in (mg/L) for arsenic and chloride, in (µmhos/cm) for electrical conductivity

Discussion

The methodology proposed by Júnez-Ferreira et al. (2016a) considered the selection of sampling points by choosing the well positions that minimize the estimate error variance of the selected indicator parameters with the option to include priority zones according to the groundwater quality data. The optimization process is supported by a Kalman filter to calculate WJT. The comparison between Júnez-Ferreira et al. (2016a) and the methodology proposed in this paper was carried out for various weighted values of the Kalman filter and the ponderation map proposed also in this new methodology. For the first case (100 - 0), the 100 indicates the percentage used for the calculations of the WJT with the Kalman filter and 0 the percentage of the SF; meaning that this is the equivalent of the Júnez-Ferreira et al. (2016a) methodology.

Figure 7 shows the percentage of reduction of the initial WJT that is obtained on the CEG each time a new well is added to the monitoring network for the six analyzed cases. The fastest reduction in the WJT is, as expected, produced for case "100 – 0", on the other hand, the lowest reduction corresponds to what we called the "Worst" case. The introduction of non-zero values to the SF produces a slower reduction in the WJT compared to the "100 – 0", it can be shown that assigning the same weight to both functions of the OF ("50 – 50") results in a reduction of the WJT that is found approximately in the middle of the "100 – 0" and the "Worst" cases. Assigning a very small weight to the SF produces almost the same estimates than in the optimal case in terms of the estimate uncertainty value ("100 – 0"); however, a different set of wells is now selected.

Figure 8a shows that for the "100 - 0" case, the first 10 positions are selected mainly at the central part of the cloud of the sampling stations, when the optimal monitoring network includes 30 positions; it extends to cover a larger area of the cloud of available sampling stations. However, it does not include positions in the periphery. An optimal monitoring network with 50 positions reaches some of the peripheral sampling positions with a high density at the central zone of the cloud.

Even though a priority order was assigned to all the monitoring wells, only those with the highest priority will be monitored in an optimal scheme since they achieve the highest reduction in the estimation grid uncertainty. In order to compare the set of wells selected for cases "100 - 0", "99.999 - 0.001", "99.995 - 0.005", "99.999 - 0.01", and

"50 - 50", an analysis of *Figure 8* was done, where 10, 30 and 50 wells comprise the selected monitoring networks for each case. The resulting monitoring network for the "worst" case is not analyzed further; their WJT values were only used as a reference in *Figure 7*, to visualize how close the different cases are to the best and worst possible estimation scenarios.



Figure 7. Comparison of the WJT (%) vs number of monitoring positions

When analyzing the "99.999 – 0.001" case (*Fig. 8b*), the first 10 positions are slightly biased to the south, including some of the peripheral wells. When 30 positions are selected, the wells are more homogeneously distributed within the cloud of points, but unlike the "100 - 0" case, the peripheral well with a priority value of 27 is included. With 50 positions, the same spatial coverage than the "100 - 0" case is virtually obtained.

For the "99.995 – 0.005" case shown in *Figure 8c*, the first 10 positions are notoriously biased to the extreme Southern part; only the position with a priority value of 9 is located at the Northwest. For 30 positions, the distribution is considerably better, with small areas uncovered at the central part. Finally, with 50 positions, the spatial coverage is better than in cases "100 - 0", "99.999 - 0.001", considering various wells at the Western periphery. The increase in the WJT value when selecting 50 wells for the "99.995 - 0.005" and the "100 - 0" cases is of 0.25%, this means that the loss of information is minimum for this alternative.

In *Figure 8d* it can be shown that for the "99.99 – 0.01" case, the first 10 and 30 selected positions are more biased to the south compared to the previously analyzed cases. When 50 positions are included in the monitoring network, the coverage is very similar to *Figure 8c*; however, the WJT value has increased in 0.40% with respect to the "100 - 0" case.

The "50 - 50" case (*Fig. 8e*), is clearly biased to the selection of wells along the Southern periphery when 10 positions are included in the monitoring network. The selection of 30 wells now includes the Western periphery and one well is selected at the North. When 50 positions are selected, the monitoring networks is denser at those peripheral zones, leaving the central part of the cloud uncovered.



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Figure 8. Groundwater monitoring networks and priority order for cases: a) "0-100", b) "0.001-99.999", c) "0.005-99.995", d) "0.01-99.99" and e) "50-50"

Conclusions

Various methodologies for the design of optimal groundwater monitoring networks are based on the reduction of the estimated error variance of the variable(s) involved in the design; these estimates are obtained over an estimation grid. In most cases, the shape of the estimation grid is square or rectangular; therefore, at poorly sampled peripheral areas, the estimates are extrapolations. On the other hand, these methodologies are biased to assign a higher priority to those wells that have more influence over a larger number of nodes of the estimation grid, thus assigning a low priority to those wells closer to the periphery of the estimation grid (Júnez-Ferreira et al., 2016a).

When the design is oriented to reduce the estimated error variance only, without assigning specific weights to the nodes of the estimation grid, the monitoring network could fail in covering some pre-defined priority zones or wells with valuable information. Therefore, it is necessary to evaluate alternative designs to consider those areas or sites of interest, minimizing the loss of information when estimating with the selected optimal monitoring network.

The proposed methodology includes a new algorithm for the definition of the estimation grid that takes into account the shape of the cloud of available sampling positions, trying to avoid extrapolation. The inclusion of a supplementary function in the optimization procedure allows the monitoring design to achieve a better spatial coverage, especially at the periphery of the estimation grid, without having a significant loss of information. The objective function considers also the assignment of weights to the wells; this aspect is important when some of them have been previously identified as relevant.

Through this methodology, it is possible to analyze alternative designs in which the spatial coverage of the monitoring networks changes, but its estimates are close to the optimal in terms of the estimate error variances.

Geochemistry evolution, along with groundwater flow in thick heterogeneous aquifers can be interpreted by specific methodologies; hydrogeochemistry is useful to solve questions of origin and attenuation of geogenic and anthropogenic contaminants. The proposed methodology considers statistical techniques to analyze the spatial distribution of specific water quality parameters as a result of sampling campaigns. In this regard, the understanding of groundwater chemical evolution and/or impacts of

diffuse contamination with the monitoring network is beyond of the scope of the proposed methodology. This methodology is useful for the selection of the most convenient set of sampling stations in selected areas from a number of alternatives, it was specifically oriented for the implementation of drinking water monitoring networks. Once the monitoring network is designed, the collected data will include information from the whole selected area, data redundancy will be avoided and WTJ customized accordingly for example with financial resources and/or available time. The implementation of this methodology should facilitate to decision makers the classification of water quality in aquifers.

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APPENDIX

Sam	ples
Sum	pics

UTM X	UTM Y	Electrical conductivity (µmhos/cm)	Arsenic (mg/l)	Chloride (mg/l)
255942	2293883	721	0.02835	38.85
258294	2294106	865	0.032	29.1
264225	2294358	563	0.0232	13.8
266037	2293737	698	0.0153	10.8
249273	2284968	248	0.0034	29.75
250397	2283463	739	0.0056	19.2
247341	2280044	581	0.0097	10
241239	2281506	674	0.0101	14.9
260375	2292217	1113	0.0107	50.22
264528	2288593	502	0.0069	6.84
269331	2289364	787	0.0066	25.43
254750	2279539	839	0.0057	26.9
256120	2281124	802	0.0059	26.7
256090	2282764	821	0.0051	13.7
258212	2285624	857	0.0053	25.43
266723	2282010	594	0.0061	8.56
268873	2283108	876	0.0068	21.77
274098	2279465	666	0.0085	13.45
270904	2279933	749	0.0101	12.96
261117	2281813	500	0.0038	11.25
265579	2279966	678	0.0047	20.3
261324	2272237	1471	0.0046	166.98
259981	2276218	748	0.0036	24.7
261502	2283669	482	0.0074	17.86
271738	2270976	1474	0.0102	58.96
272305	2265668	916	0.0146	29.1
272657	2271001	977	0.0165	27.64
264019	2265292	2410	0.0383	293.52
261750	2269664	1105	0.01285	85.48
278536	2287752	626	0.0042	7.09
275567	2287348	590	0.0068	6.06
276558	2284583	750	0.0047	8.31
272818	2285517	647	0.0171	8.56
273267	2282492	828	0.0232	13.45
261399	2282976	413	0.0041	65.43
257767	2287796	655	0.0263	15.9
256467	2285587	572	0.0136	11.49
255569	2285435	1378	0.00345	50.17
255547	2287556	1000	0.002	58.21
254566	2288936	663	0.0141	22.74
267229	2274569	1034	0.0085	53.81

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270070 2266911 867 0.0206 27.39 265991 703 0.0056 14.75 2257299 264823 2256684 681 0.0082 16.38 277246 2281242 570 0.0102 10.27 278314 2278407 727 0.0205 26.58 22.01 282529 2278425 690 0.0176 7.09 551 0.006 258815 2286160 2290276 11.69 255955 485 0.008 254101 2290424 610 0.0114 19.56 252790 2286848 628 0.0042 32.28 249309 2288653 590 0.004 16.38 255582 2286945 933 0.0044 44.51 0.0059 265851 2258103 673 10.51 263772 2258257 746 0.0088 17.12 260077 2259299 703 0.0045 21.03 261545 2263341 1067 0.0297 42.395 8.055 257189 2257498 446 0.00365 285064 2268748 1299 0.0103 39.62 39.13 282307 2271012 1182 0.006 282371 2274499 686 0.01695 18.91 278506 2273692 925 0.0131 31.55 279172 2275540 943 0.0081 24.21 270591 2276591 748 0.0219 21.77 269822 2275460 1119 0.0046 55.28 2274092 945 0.083 38.4 269893 270976 2274737 56.75 823 0.054 270973 2274224 1076 0.0107 50.39 269655 2272381 1149 0.0096 32.29 8.875 262022 2252546 406 0.002 257694 2255060 782 0.004 10.27 254349 2256718 507 0.0034 8.8 254400 2261222 887 0.0035 14.84 257494 2265699 1779 0.01635 54.84 284469 2265951 1166 0.0047 16.63 283214 2258544 1117 0.0033 74.36 276376 2258892 520 0.0066 15.65 272009 2254911 1533 0.0029 100.77 276613 2253958 615 0.0057 40.11 271331 2278492 620 0.0218 14.43 272962 2278788 679 0.0206 15.41 274982 2278628 726 0.0114 19.81 268410 2275364 874 0.0057 35.96 270001 2277455 827 0.0205 19.57 272675 2276129 621 0.0168 13.94 270933 2275990 1430 0.0067 146.76 261448 2278096 775 0.0049 15.9

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289764	2260054	1149	0.0023	35.9
273830	2274505	872	0.033	104.9
275319	2272939	684	0.0066	39.3
276204	2272290	909	0.0242	53.4
274578	2274772	657	0.0333	47.6
274275	2276426	743	0.0376	25
274206	2276950	650	0.0328	16.3