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# Implications of heterogeneity on transport simulations at large scale: the Morroa aquifer case

# Implicaciones de la heterogeneidad en simulaciones de transporte de contaminantes a escala de cuencas: el caso del acuífero Morroa

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## Abstract

The Morroa aquifer located in Sucre state (northern Colombia) represents the exclusive source of water supply for nearly 500.000 people, including the capital of the state Sincelejo. Although multiple studies have been performed in this area, and a considerable amount of data including piezometric levels, stratigraphy at wells, and pumping tests has been collected; this information is in general fuzzy, heterogeneous and incomplete. The uncertainty in this information affects any quantification of the response of the aquifer. Therefore a methodology able to account for all of the available data and integrate it in a comprehensive conceptual model represents the starting point of our investigation. The uncertainty is accounted for by generating multiple realizations of the aquifer, so that these realizations honor statistical properties of the data. To generate the realizations, two different methods were employed: (1) the well-known Sequential Indicator method (SISIM) which is a semi-variogram based geostatistic method; and (2) the multiple-point geostatistics algorithm SNESIM, based on the concept of training images that represents the database of geological patterns, from which multiple-point statistics are borrowed. Results of the geostatistics simulations show the great ability of MPS to reproduce complex curve heterogeneities.


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Flow and transport simulations are performed using two different conceptual models of the Morroa aquifer considering heterogeneities. Steady-state flow and conservative contaminant were assumed. Results show a considerable influence of heterogeneity and the geostatistic method used to generate the conceptual model, i.e. two-points or multiple-point geostatistics. In particular, large differences on the aquifer response distribution were observed that may have an important effect on the design of mid- and large term water management policies regarding both quantity and quality at the Morroa aquifer, as well as on the design of remediation techniques.

----------*Keywords:* heterogeneity, multiple-point geostatistics, transport simulations, Morroa aquifer

## Resumen

El acuífero Morroa, localizado en el departamento de Sucre (Colombia), representa la única fuente de suministro de agua potable de cerca de 500.000 habitantes que incluyen la totalidad de los habitantes de la capital del departamento Sincelejo. Aunque se han desarrollado muchos estudios en esta zona que incluyen la recolección de gran cantidad de información relacionada con niveles piezométricos, información estratigráfica, pruebas de bombeo, esta información es difusa, heterogénea y fraccionada. La incertidumbre asociada a esta información afecta cualquier intento de cuantificar la respuesta del acuífero, por esta razón el punto de partida de esta investigación es el desarrollo de una metodología capaz de integrar todas las variables en un modelo conceptual. Para considerar la incertidumbre se generaron múltiples realizaciones del acuífero de tal manera que todas respetan las propiedades estadísticas de la información disponible. Para generar estas realizaciones se utilizaron dos metodologías: (1) SISIM, que es un método basado en estadísticas de dos puntos (semivariograma), y (2) SNESIM, que es un algoritmo basado en el concepto de imágenes de entrenamiento (estadística de puntos múltiples). Resultados de las simulaciones muestran la gran capacidad de este último para reproducir geometrías curvilíneas complejas.

En una segunda fase, se desarrollaron simulaciones de flujo y transporte de contaminantes de una manera integrada usando los dos modelos conceptuales obtenidos a través de las dos aproximaciones geoestadísticas. Condiciones de flujo estacionario y un contaminante conservativo fueron asumidos para todas las simulaciones. Los resultados obtenidos muestran una influencia notable de la heterogeneidad en general, así como una gran sensibilidad al método geoestadístico usado para generar la heterogeneidad. Las diferencias observadas tendrían un gran efecto en el diseño de políticas de manejo integral del recurso hídrico a medio y largo plazo, así como en el diseño de medidas de remediación.

----------*Palabras clave:* heterogeneidad, geostadística de puntos múltiples, simulaciones de transporte de contaminante, acuífero Morroa

## Introduction

In Colombia, the definition of the availability and quality of groundwater resources has a large degree of uncertainty due to the complexity of geological conditions and lack or reliable information, making very difficult the definition of conceptual models of aquifers. This situation is particularly problematic in areas where the groundwater represents the only source of water supply. One of these areas is the Morroa Aquifer located mainly within the Sucre state at the northern coast in Colombia. This aquifer serves as the water supply system of about 500.000 inhabitants, including the two major towns of the state: Sincelejo and Corozal. For many decades, these people have suffered from water scarcity and more recently water quality problems have been detected, in particular increases in electrical conductivity at some areas have been measured (Carsucre, internal reports). The water scarcity problems in this area tend to increase in a near future as a possible side effect of the climate change, where the tropical regions are especially vulnerable.

Many studies have been developed at the Morroa aquifer. However most of them have been mainly focused on either the study of the recharge area (e.g. [1]), or the estimation of global hydraulic parameters (e.g. [2]). Studies in the recharge area included piezometric wells located up to 500 m depth. Another important study included the analysis and interpretation of seismic lines that comprises a large area within the aquifer [3]. These lines allowed defining the real limits of the aquifer and the hydrostratigraphic units [4]. However, problems of geophysical techniques to characterize the first 500 m of the subsurface are well known.

From this perspective, it is difficult to develop a reliable conceptual model, because the available information is scarce, fuzzy and segmented. Furthermore, the hydrostratigraphic complexity associated to the Morroa aquifer makes the challenge even harder. Semivariogram-based geostatistics has become the most used methodology to simulate subsurface heterogeneity in geoscience. Most popular algorithms include Sequential Gaussian Simulation (SGSIM) [5] and Sequential Indicator Simulation (SISIM). Although both SISIM and SGSIM are very popular among modelers, these methods are deemed to have many limitations, i.e. [6-10]. For the purpose of this study, the most worrying limitation is that this kind of methodologies fail to define specific patterns related to structured geological connectivity, i.e. SGSIM is unable to reproduce channeled structures.

Due to the limitations of the semivariogram-based geostatistics (the so-called two-points geostatistics) to simulate complex curve heterogeneities, various alternatives have been proposed. Among the various existing methods, multiple-point statistics (i.e. [11-13]) results appealing because it provides a simple mean to integrate a conceptual geological model in a stochastic simulation framework. The conceptual model is provided as a training image (TI) representing the heterogeneity patterns that the user expects at a given site [14]. For example, the TI can represent channels if the user knows that the geological environment is supposed to be characterized by channeled structures. TI may also come from different sources as geological sketches, interpreted outcrop photography or from an object-oriented algorithm (Boolean methods). In the first two cases, original data must be preprocessed to be converted into digitalized and extended 2D or 3D images (commonly using CAD software). As an alternative to represent large variability within the study area, many training images may be used, each of them representing a different kind of heterogeneities at different scales.

In this work, we used a two-fold methodology. First, we tested the ability of two different aproaches to reproduce the complexity of the Morroa aquifer: (i) of semivariogram-based SISIM, and (ii) the multiple-points statistics algorithm SNESIM (Single Normal Equation Simulation) [7, 15]. The ζ Model was used to integrate soft and hard data into the conceptual model of the Morroa aquifer. The starting point of this stage was the work presented in [4]. Once consistent conceptual models, that take heterogeneity into account, were developed, we performed flow and transport simulations in order to study the implications of heterogeneity on transport at the Morroa Aquifer, which represents a large-scale aquifer.

This article differs from the presented by [4] mainly because we performed a more comprehensive analysis of subsurface heterogeneity at the Morroa aquifer that includes a comparison on the ability of the methods to reproduce channeled structures, and we investigate the effect of subsurface heterogeneity on concentration distribution using a physics-based modeling framework and hydraulic conductivity values taken from a field survey.

## The Morroa aquifer

### *Location*

The Morroa aquifer (Area= 4200 km2, Depth= 4800 m), located in northern Colombia, represents the only source of water supply for a half a million inhabitants, mainly located in the Sucre state. For some decades, these people have suffered from water scarcity and recently from water pollution. The problem has become even worse in recent years due to a significant water quality problems associated to an increase in salinity measured close to towns and local landfills, and to dramatic drawdowns of the aquifer. This situation has led to increase efforts to study flow and transport dynamics associated to this aquifer.

### *Climate and hydrography*

The climate of the Morroa aquifer region may be classified as Tropical Savanna Climate in most of the area, characterized by moderate rainfall (P = 1000-1200 mm), high potential evapotranspiration (ETp = 1200 mm) and alternative wet and dry seasons, being the driest months from December to March and the rainiest from May to October. Average temperature is 28 °C. Main streams at the area are the *Arroyo Grande de Corozal* and the *Arroyo Morroa,* both run over the Morroa aquifer recharge area but only during the rainy season.

### *Geology*

The Morroa aquifer is geologically characterized by sandstones and conglomerates with low consolidation, intercalated with claystones whose genesis is associated to detritus sedimentation in an alluvial fan environment and alluvial channels [16]. Many studies from different authors (i.e. [17-20]) have mentioned ten different formations within the Morroa aquifer area:

1. *San Jacinto (Pgsi):* it consists of alternating sandstones and calcareous claystones over a lithic conglomerate [18]. San Jacinto formation underlies the Carmen and Sincelejo formations in paraconformity (nondepositional unconformity).
2. *Ciénaga de Oro (Pgc):* it consists of sandstones alternated with plain parallel bioturbated siltstones. This formation overlies in angular unconformity the San Cayetano formation and in conformity the Carmen formation. Spatial changes observed in this formation from south to north may indicate changes in the depositional environment. In particular, at the southern part the deposition is associated to deltaic environment while in the northern part to shallow transgressive environment.
3. *Carmen*: It consists of claystones with very thin intercalations of siltstones and sandstones. Carmen formation overlies in paraconformity the Toluviejo formation and in apparent conformity the Ciénaga de Oro formation.
4. *San Cayetano*: It consists of sandstones alternated with mudstones. Three facies can be noticed: (i) the lower-most facie made of lithic sandstones in medium size layers, intercalated with gray mudstones, (ii) the intermediate facie is predominantly

made of brown mudstones alternated with lithic sandstones, (ii) the upper-most facie is characterized by fine and white quartz-arenites in very thin layers.

5. *Toluviejo*: It consists of four facie: (i) bioclastic limestones, (ii) calcareous arenites, (iii) calcareous mudstones y (iv) massive mudstones. At the western, the formation overlies in angular unconformity the San Cayetano formation and in paraconformity the Maco formation.

6. *Cerrito (Ngc)*: It consists of calcareous bioclastic arenites and conglomerates in the lower layers that varies in the upper layers into fine-grained arenites, siltstones and claystones. The Cerrito formation overlies in paraconformity the Carmen formation and underlies in angular unconformity the Sincelejo formation. Its thickness varies from 0 to 600m.

7. *Sincelejo (NgQs)*: It consists of conglomeratic sandstones with low cementation, with local variations of mudstones. Sincelejo formation overlies in unconformity the Carmen formation and underlies in paraconformity the Betulia formation. The thickness of Sincelejo formation is estimated between 350 and 400 m. [17] subdivided the Sincelejo formation in inferior and superior members. The inferior is associated to more clayey facies while the superior to sandy facies.

8. *Morroa (NgQs)*: It consist of poorly cemented sandstones intercalated with conglomerates made of small pebbles of quartz, lutites, sandstones and very thin layers of clay. Morroa formation overlies the Sincelejo formation in conformity. [3] proposed that the Morroa formation may be considered as a third member of the Sincelejo formation.

9. *Betulia (Qpb):* in the past this formation has been associated to an inferior member characterized by clayey facies, overlying a sandy member. However direct observations and geophysics studies developed by INGEOMINAS suggest that at some areas within the Morroa aquifer the inferior member is predominantly sandy, while the superior member seems to be a clayey facie. These findings may indicate an important variation of facies within Betulia formation that may modify their hydrogeological properties. More recent studies [3] suggested that only a member should be associated to Betulia formations as the changes of facies obey to typical characteristic in a fluvio-lacustrine environment that can occur randomly in space and time.

10. *Recent deposits (Qcal-Qli):* this formation is associated to coastal plain and colluvial deposits. Among these formations, a first group (mainly Qcal) are alluvial and lacustrian deposits with marine influence made of sand, silt and clay. A second group of formatios (mainly *Qli*) are associated to recent fluvial sedimentation and colluviums related to streams and foothills made of sands, graves, silt and clay.

The complex stratigraphy associated to the Morroa aquifer and the poor knowledge of the thickness and age of the main formations (i.e. Betulia, Morroa and Sincelejo) makes the construction of a reliable conceptual model a real challenge.

### Hydrogeology

Within the study area, about 60 monitoring wells are available. However, there is not reliable information in most of them. Hence, a selection and analysis process was carried out that provide a set of 15 wells with reliable data. Hydraulic conductivity and storage coefficient values estimated at these wells in previous studies (e.g. [2]) are shown in table 1. From this table, it can be observed that the equivalent hydraulic conductivity (averaged value in depth) varies over two orders of magnitude while the equivalent storage coefficient appears to be constant.

**Table 1** Hydraulic properties of the Morroa Aquifer (Adapted from [2])

| *Pozo* | *Coordenadas X* | *Coordenadas Y* | *K [m/d]* | *S [-]* |
|---|---|---|---|---|
| 44-IV-C-PP-08 | 864330 | 1520560 | 1.7 | 1.05e-4 |
| 44-IV-C-PP-11 | 862270 | 1522180 | 0.4 | 1.10e-4 |
| 44-IV-D-PP-16 | 866410 | 1523510 | 7.3 | 1.10e-4 |
| 44-IV-D-PP-18 | 86700 | 1524100 | 12.3 | 1,10e-4 |
| 44-IV-D-PP-19 | 867600 | 1524700 | 0.5 | 1.68e-4 |
| 44-IV-D-PP-24 | 867670 | 1522400 | 3.0 | 1.40e-4 |
| 44-IV-D-PP-30 | 866690 | 1525800 | 0.7 | 1.50e-4 |
| 44-IV-D-PP-34 | 866640 | 1521160 | 2.8 | 1.81e-4 |
| 44-IV-D-PP-36 | 868120 | 1524880 | 2.9 | 1.35e-4 |
| 44-IV-D-PP-39 | 865525 | 1524800 | 0.9 | 6.73e-4 |
| 52-II-A-PP-01 | 857060 | 1512470 | 4.6 | 1.50e-4 |
| 52-II-A-PP-08 | 862660 | 1519400 | 2.0 | 4.78e-4 |
| 52-II-A-PP-09 | 864700 | 1515720 | 4.3 | 1.50e-4 |
| 52-II-A-PP-13 | 861270 | 1514390 | 1.1 | 1.50e-4 |
| 52-II-A-PP-15 | 863880 | 1519150 | 0.9 | 1.10e-4 |
| 52-II-A-PP-19 | 861740 | 1517210 | 0.5 | 1.5e-4 |

## Geostatistic simulations

In this study, a 3-D grid of 1.200.000 cells is used to represent the Morroa Aquifer. Boundaries of the aquifer were defined based on the seismic lines as presented in [4]. To account for the uncertainty associated to the definition of the conceptual model, we generate 1000 geostatistics realizations using the sequential indicator method SISIM, and the multiple-point geostatistics algorithm SNESIM. In order to obtain the best conceptual model possible, all available well and seismic information was used to condition the realizations.

Training images were built from the combination of geological interpretations and interpreted outcrop photography of the area, converted into digitalized 3D images. In figure 1, the schematic geological interpretation developed by the regional environmental authority (CARSUCRE, 2009) is presented.

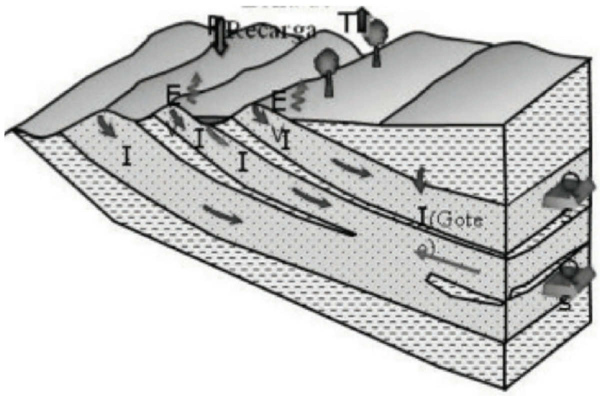



**Figure 1** Schematic conceptual model of the Morroa aquifer (Source: Carsucre, scheme not scaled)

Seismic lines covering the whole study area were used as soft data, while lithology coming from deep wells was assumed as hard data. Seismic lines not covering the whole length were used to generate *seismic wells* assumed as soft data. In figure 2 shows the digitalization process of seismic lines. Probabilities of occurrence of sand were assigned to each cell of the digitized seismic line according to the proportions of sand and clay: the proportion of sand is assumed as the probability of occurrence. These values were estimated from lithology data and seismic amplitude at 4 calibration wells.

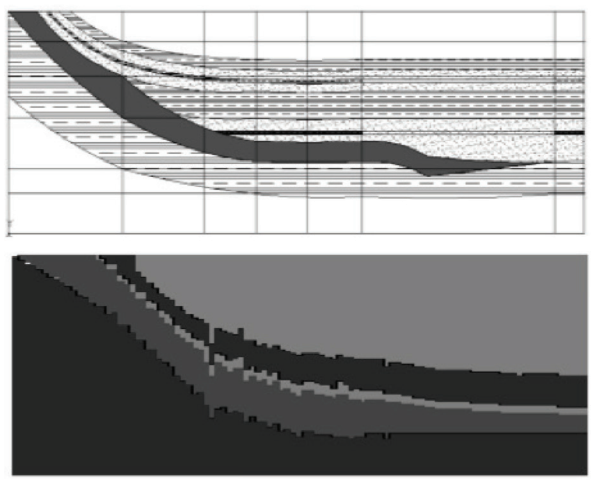
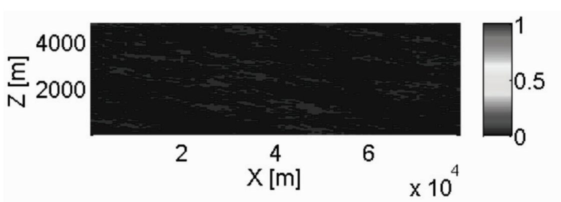


**Figure 2** Digitized seismic line (dark gray: high-conductivity facies, gray: intercalation of low and high conductivity facies and bright gray: low-conductivity facies, scheme not scaled)

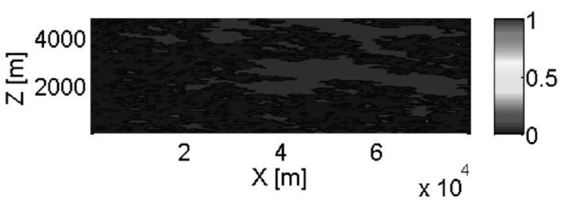
Eighteen (18) *seismic wells* were generated from the *incomplete* seismic lines together with information coming from shallow wells (less than 200 m depth).

Results obtained from SISIM and SNESIM were processed using the algorithm POSTSIM available from the GSLIB library, to estimate the most probable lithology at each node [5] so that conceptual models that accounts for heterogeneity and incorporate hard and soft conditioning are achieved.

To investigate the ability of the methods used to reproduce the heterogeneity associated to the Morroa aquifer, we transform the results obtained into two categories (high-conductivity: 1 and low-conductivity: 0), high-conductivity was assumed between 0.1 y 15 m/d and low-conductivity between 0.001 y 0.1 m/d. At the SISIM simulations, we can identify areas with higher conductivity; however, the method appears to fail to reproduce the channeled structure observed in the interpretation of seismic lines and the schematic conceptual model (Figure 3a). Conversely, continuos curvilinear facies can be observed in the SNESIM simulations, which may indicate that the method is capable of reproducing the channeled structures, at least at the Morroa aquifer (Figure 3b).




a) SISIM simulation

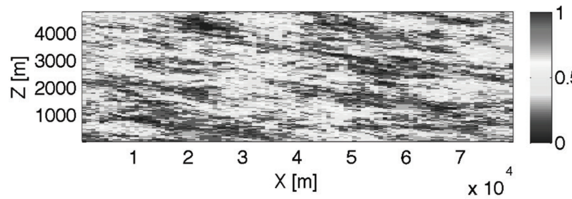



b) SNESIM simulation

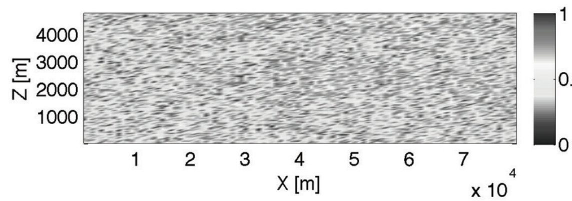
**Figure 3** 2D-slices Comparison between (a) SISIM simulation and (b) SNESIM simulation

## Transport simulations

To investigate the implications of using two- or multiple-points statistics on flow and transport dynamics at the Morroa aquifer, we extracted two X-Z slices from the conceptual model obtained for SISIM and SNESIM methods, respectively (figure 4). The slices shown in figures 4 were used. Hydraulic conductivity of reference used for this work varies over 3 orders of magnitude from 0.1 to 12 m/d, according to the results presented by [2] listed in table 1.




a) SISIM




b) SNESIM

**Figure 4** X-Z slice for a) SISIM and b) SNESIM method

Flow velocities and concentrations were calculated in an integrated manner using the numerical model *Hydrogeosphere* (e.g. [22-24]). A hydraulic gradient along the horizontal direction is assumed, and a conservative contaminant is advected into the system at the left boundary. The system was simulated for 4320 hrs. Results from transport simulations at different time-steps for SISIM and SNESIM are shown in figure 5. To better visualize the effect of heterogeneity, results are compared to a homogeneous case where an equivalent hydraulic conductivity is assumed.

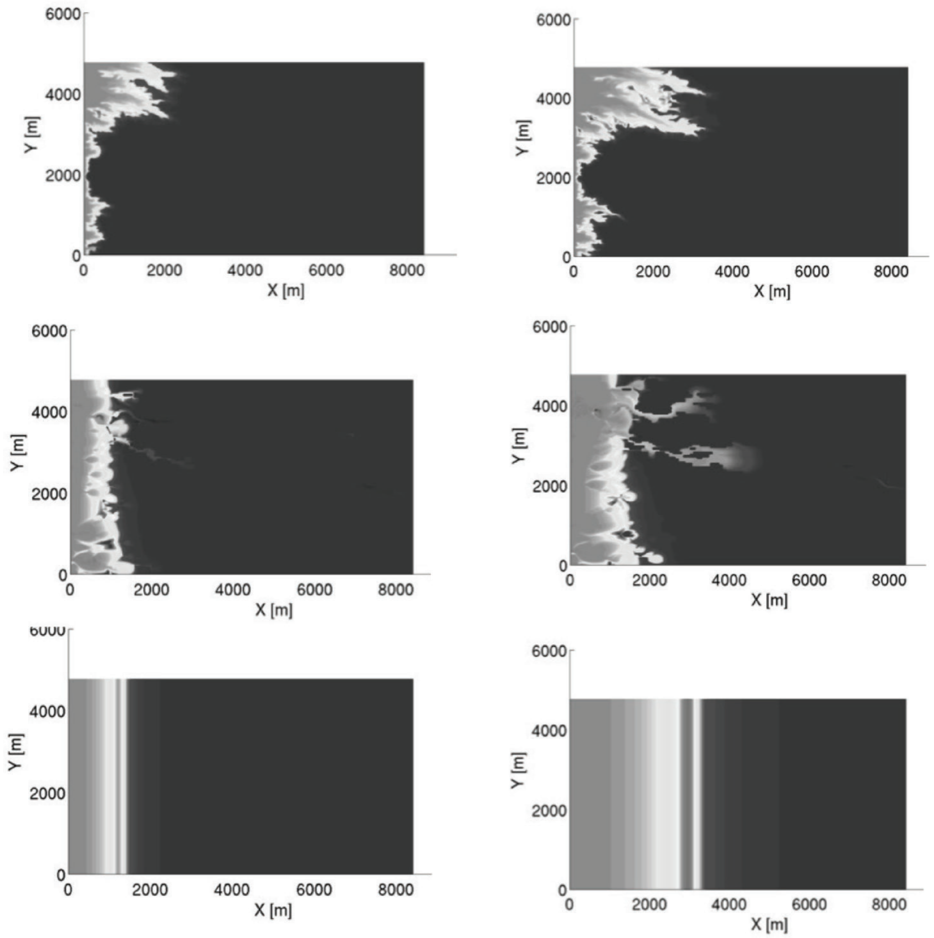



**Figure 5** The relative concentration after 2160 h (left column) and 4320 h (right column) for the SISIM case (above), SNESIM case (middle) and homogeneous case (below)

The concentration distribution for the simulations using two-point statistics (SISIM) allows to identify two preferential paths associated to high-conductivity facies located between less permeable formations. This observation may strengthen the theory of the existence of a relatively shallow Morroa aquifer located up to 800 m depth, and a deeper aquifer located up to 2000 m depth. Higher concentrations regions observed at the borders of the preferential paths indicate the limit between high- and low-conductivity facies. In this case, despite the inability to reproduce important features of the channeled structure, the sequential indicator simulation (SISIM) method can reproduce important features of the concentration distribution, even the features associated to the shallow and deep aquifers previously reported by [25].

For the case of the simulations performed using the conceptual model produced by using multiple-point geostatistics (SNESIM), again two preferential path are clearly observed. In this case, the contaminant flow paths are highlighted as the method is able to reproduce channeled structures. In the figure, it can be observed that contaminant moves faster along the main flow paths depicted by high-conductivity channels reproduced by SNESIM simulations, while accumulates in spots associated to low-conductivity areas. The latter illustrates the main advantage of multiple-point statistics: using MPS we are able to reproduce complex flow dynamics associated to curvilinear structures.

## Discussion and conclusions

From the results, it can be said that multiple-point statistics have a greater ability to reproduce curvilinear structures when compared to variogram-based statistics. However, generating training images for both soft and hard data represents a challenge in very complex problems as additional uncertainties may be introduced by the use of interpolation methods.

Comparing heterogeneous cases with the homogeneous case, significant differences associated to the contaminant concentration distribution can be observed. It is clear from the concentrations distribution that the idealization of the flow field derived from the homogenous case produces a much simpler distribution that the one obtained using all the heterogeneous complexity. The latter implies that eventual mitigation actions may widely differ depending on which conceptual model is used to understand the system at the Morroa aquifer. Furthermore, also it can be stated that the design of water exploitation systems may also be affected by the type models used, as it has been previously suggested by [4].

The results of the simulations for three different conceptual models suggest that it is impossible to design water management strategies regarding both quantity and quality in complex systems like the Morroa aquifer without considering implications of subsurface heterogeneity

This investigation represents the first step towards the construction of a Decision Support System at the region associated to the Morroa aquifer. For this purpose, a more realistic approach using collected data on soil hydraulic properties, recharge estimation and well extraction values will be developed. In this work, calibration and validation processes will take place so that the model can be used for the regional authorities. The model may be used also to investigate implications of heterogeneity at a large scale on reactive transport. For this purpose, simulations of nitrate transport associated to agricultural practices in the region will be also performed.

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