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Issues in characterizing heterogeneity and connectivity in non-multiGaussian media

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Abstract

The performances of kriging, stochastic simulations and sequential self-calibration inversion are assessed when characterizing a non-multiGaussian synthetic 2D braided channel aquifer. The comparison is based on a series of criteria such as the reproduction of the original reference transmissivity or head fields, but also in terms of accuracy of flow and transport (capture zone) forecasts when the flow conditions are modified. We observe that the errors remain large even for a dense data network. In addition some unexpected behaviours are observed when large transmissivity datasets are used. In particular, we observe an increase of the bias with the number of transmissivity data and an increasing uncertainty with the number of head data. This is interpreted as a consequence of the use of an inadequate multiGaussian stochastic model that is not able to reproduce the connectivity of the original field.

Keywords: Aquifer characterization; Inverse; Kriging; Stochastic simulations; Uncertainty; Well-capture zones; Connectivity; Multiple-point statistics

1. Introduction

Groundwater flow and transport are controlled by physical properties that are characterized by a high degree of heterogeneity and by scales of variation that span several orders of magnitude. A major difficulty is that this heterogeneity, whose knowledge is fundamental for modelling relevant environmental problems (e.g. protection zone design, contaminant migration prediction, aquifer remediation, seawater intrusion), has to be inferred on the basis of sparse measurements. In the past decades, a large number of techniques has been developed with the aim of characterizing the spatial variability of aquifer parameters and their uncertainty [11,26,31]. Generally speaking, the characterization of the heterogeneity can be addressed based on direct observations of the *physical parameters* (direct methods) or on observations of the *state variables* of the system (inverse methods).

Direct methods infer the distribution of the physical parameters (transmissivity, porosity, etc.) from the local information about the parameters themselves. Note, however, that this information is often obtained by solving an inverse problem involving the state variables (e.g. pumping tests) but their interpretation is local and provides parameter values that become the input of the characterization methods. Additional direct information about the characteristics and the position of geological facies can be provided by geophysical observations. Among the most widely employed direct interpolation techniques are kriging and stochastic multiGaussian simulations. They both are two-point geostatistical methods that proved efficient in a wide variety of applications in hydrogeology but also in other fields such as mining, or petroleum engineering [4,13,25].

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In practice, however, direct methods are seldom used alone because they do not account for the global information on state variables (e.g. hydraulic head or concentration) and lead to groundwater models that do not reproduce the observed values of those state variables. Instead, this information is taken into account by inverse methods, which characterize the physical parameters from measurements of the state variables. Inverse modelling has been a topic of intense research and developments [1,5,12,19,21]. As argued in a recent review by Carrera et al. [9], most methods do not differ from each other in essence, but they may differ with respect to the computational details. Among the inverse techniques, the Monte-Carlo approach, in which multiple equally likely realisations of aquifer properties are conditioned to hydraulic head and concentration data, allows estimating uncertainty. Inverse methods have been applied successfully in a wide range of problems [7,27,28,41].

Since both direct and inverse methods rely on measurements acquired at few discrete locations, some hypotheses have to be made on the parameter statistics in order to infer the continuum distribution. Most two-point geostatistical techniques illustrated in the previous sections are based on the assumption that the physical parameters follow a multiGaussian distribution, which is analytically simple and fully characterized by a mean and covariance function. Numerical testing is usually performed by applying the characterization techniques to synthetic fields that also feature multiGaussian statistics. The results demonstrate the accuracy and the consistency of the methods. While remaining in the multiGaussian framework, few studies have shown how uncertainty can be reduced by increasing the number of transmissivity, head or concentration data [19,40].

MultiGaussian fields maximise entropy (disorder), and in return, minimize the spatial continuity of the extreme values, thus, a loss of connectivity [24]. This feature has a high impact on flow and transport as shown by a number of numerical investigations [17,33,39,42]. While these studies were limited to the context of direct techniques, they all showed that the selection of a multiGaussian model might be consequential on flow and transport simulations. Both direct and inverse techniques are available to handle non-multiGaussian media. Examples of direct techniques include the sequential indicator simulation method [16], truncated pluriGaussian simulations [2], or multiple-point statistics [36]. Examples of inverse methods that are able to handle non-multiGaussian media are the conditional probabilities method [8], a combination of truncated pluriGaussian simulation and the gradual deformation approach [21], the inverse modelling of multimodal hydraulic conductivity distributions with the representer method [22], or the probability perturbation method combined with multiple-point statistics [6] among others.

Although it is known already now for more than a decade that multiGaussian models have severe limitations, and although alternative methods exists, most groundwater hydrology studies adopt a multiGaussian model, often also because data are not available to infer a non-multiGaussian model. Therefore, this study explores what happens if a multiGaussian model is adopted for a non-multiGaussian medium, a situation that is most probably very common in practice. In particular, we do not only investigate the implications of a wrong random function model in direct studies, but also in inverse problems.

In summary, the goal of the present study is to investigate and compare the reliability of direct and inverse multiGaussian techniques when applied to characterize fields that are not multiGaussian and exhibit preferential flow paths. A main question of interest in this study was to what extend hydraulic head data, used in inverse modelling, are able to correct the consequences of the wrong assumption of a multiGaussian random function model. Two situations may occur: either the inverse conditioning is able to detect non-multiGaussian structures and would alleviate the problems associated with a wrong random function (multiGaussian), or the discrepancy between the model and the reality would still lead to inaccurate predictions. In the latter case, checking the multiGaussianity assumption for a particular case study would be extremely important; moreover, the groundwater community would be encouraged to further develop and adopt methods based on different statistics.

After creating a synthetic reality, our methodology mimics the procedure that would be followed during a practical case study. We start constructing a synthetic transmissivity field such that it possibly represents a real aquifer characterized by long-correlation structures such as channels and lenses (Section 2.1). A reference head field, which mimics natural flow conditions, is obtained by simulating the flow on this transmissivity field (Section 2.2). The transmissivity and the head fields are sampled in order to obtain a series of datasets with an increasing number of data points, which represent synthetic experimental data to be used as input for the aquifer characterization (Section 3.1). At this point, we first analyse the datasets in order to infer the statistics required for the characterization step and compute histograms and variograms (Section 3.2). Then, for each dataset, we reconstruct three transmissivity fields by applying three multiGaussian characterization techniques, i.e. kriging, stochastic direct simulations and self-calibrated sequential simulations (Sections 3.3 and 3.4). The performance of the characterization techniques is evaluated both in terms of reproduction of the real transmissivity field and reproduction of the initial flow situation (Section 4.1). Most important, the inferred transmissivity fields are used to make predictions on different flow scenarios. In particular, we consider the response of the aquifer to the construction of a well. Forecasts in terms of total fluxes through the domain, head in the pumping well, and protection-zone extension around the pumping well are considered (Sections 4.2 and 4.3). The reliability of the techniques is estimated as a function of the number of transmissivity and head data used to condition the transmissivity fields.