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# Impact of two geostatistical hydro-facies simulation strategies on head statistics under non-uniform groundwater flow

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SUMMARY

We present a numerical study keyed to the analysis of the impact on hydraulic head statistics of two selected methodologies for the stochastic simulation of hydro-facies spatial arrangement. We analyze the distribution of hydraulic heads in a confined aquifer under steady-state convergent three-dimensional flow to a fully penetrating well, superimposed to a mean uniform regional gradient. The heterogeneous structure of the system is modeled on the basis of available field information comprising detailed lithological data collected within an aquifer system located in northern Italy. These data are grouped into five litho-type categories and the aquifer system is modeled as a random composite medium. Monte Carlo realizations of the three-dimensional geo-material distributions are generated through the Sequential Indicator and the Truncated Plurigaussian Simulation methods. The latter enables one to integrate geological conceptual information in the simulation procedure, while the former relies mainly on a variogram-based analysis. Point and vertically averaged hydraulic heads, corresponding to typical observations collected within screened boreholes, are analyzed by evaluating the dependence of their sample probability distributions on (i) the hydro-facies generation scheme, (ii) the extent of the vertical averaging interval and (iii) the relative distance between the location of observation boreholes, hydrological boundaries and the source term. Theoretical probability density function models are fitted against numerically simulated distributions within a maximum likelihood context. Our results indicate that hydraulic heads associated with the Truncated Plurigaussian Simulation method exhibit increased variability when compared to their counterparts evaluated upon relying on a Sequential Indicator based modeling strategy of the system heterogeneity. Covariance matrices and probability distributions of point and vertically averaged hydraulic heads display similar key representative features and patterns. This suggests that typical measurements collected in screened boreholes can be used to infer qualitative information about the correlation structure and the statistical properties of heads.



## 1. Introduction

The present work is focused on the assessment of the impact on hydraulic head statistics of two geostatistically-based methodologies for the stochastic simulation of the spatial arrangement of hydro-facies in field scale aquifer systems. The relevance of an appropriate characterization of the probability distribution of hydraulic heads is critical in the context of Probabilistic Risk Assessment (PRA) procedures which are nowadays considered as viable procedures to estimate the risk associated with catastrophic events in environmental problems (Tartakovsky, 2013 and references therein). Application of PRA to actual settings typically requires the estimate of the probability density function (pdf) of a target environmental performance metric (EPM, a terminology introduced by De Barros et al., 2012). In the groundwater literature, the functional format of probability distributions of solute travel/residence times, trajectories and concentrations has been extensively analyzed during the last years (Fiorotto and Caroni, 2002; Bellin and Tonina, 2007; Riva et al., 2008, 2010; Schwede et al., 2008; Enzenhoefer et al., 2012 amongst others). On the other hand, less attention has been devoted to study the probability distribution of hydraulic head, *h*, in complex groundwater systems and under non-uniform (in the mean) flow conditions. These settings are crucial for the analysis of the (negative) consequences arising from events associated with the occurrence of *h* dropping below or rising above a given threshold. These basic events are critical for various goal oriented risk assessment practices, including, e.g., the

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protection of natural springs or ponds or the prevention of damages to underground infrastructures, and constitute core requirements in the planning of groundwater abstraction procedures or during the design of protection barriers. In this context, estimates of first and second (conditional or unconditional) statistical moments of $h$ have been largely analyzed by means of analytical (e.g., Guadagnini et al., 2003; Riva and Guadagnini, 2009 and references therein) or numerical (e.g., Guadagnini and Neuman, 1999b; Hernandez et al., 2006) methods for bounded randomly heterogeneous aquifers under the action of pumping. Low-order (statistical) moments (i.e., mean and variance–covariance) of hydraulic heads in unbounded and bounded domains under uniform (in the mean flow) conditions have been investigated, amongst others, by Dagan (1985, 1989), Rubin and Dagan (1988, 1989), Ababou et al. (1989), Osnes (1995), Guadagnini and Neuman (1999a,b). Even as these low-order moments have a considerable theoretical and practical interest, they are not directly suitable to PRA protocols where the behavior of the tails of the target variable distribution needs to be identified. This behavior can differ from the one dictated by the classically assumed Gaussian or lognormal distributions and can be influenced by the type of system heterogeneity, hydraulic boundaries and source/sink terms, as we discuss in this work.

Jones (1990) observed the non-Gaussian shape of heads pdf close to pumping wells in a two-dimensional confined aquifer where the transmissivity is lognormally distributed and spatially correlated according to an exponential covariance model. Kunstmann and Kastens (2006) modeled an aquifer in Gambach (Germany) under general non-uniform flow conditions as a two-dimensional, block-heterogeneous system, where transmissivity is homogeneous within each of five considered distinct zones. These authors noted that groundwater velocities could be well approximated by lognormal distributions while heads could be best described by long-tailed pdfs (such as the Weibull or the Gamma distributions). Nowak et al. (2008) presented a detailed numerical study centered on the analysis of statistical moments and pdf of heads and velocity components. Their work involved three-dimensional flow through realizations of randomly heterogeneous conductivity fields subject to uniform mean flow conditions. The authors noted that the shape of heads pdf is similar to a Gaussian or a Beta distribution at locations which were respectively far or close to the Dirichlet boundaries. The longitudinal discharge components appeared to be well interpreted by a lognormal distribution while their transverse counterparts displayed long tails. Additional studies which are concerned with key statistics of groundwater fluxes under uniform (in the mean) flow conditions include the works of Englert et al. (2006) and Zarlenga et al. (2012).

The selection of a model through which one can describe the natural heterogeneity of a system is a key point in the analysis of the distribution of groundwater flow (and possibly transport) variables. The model choice strongly depends on the scale of investigation. At the large field scale, geological heterogeneity of sedimentary bodies can be represented and modeled from information on depositional facies distributions. Statistical grid-based sedimentary facies reconstruction and modeling (FRM) methods can be employed to provide consistent representations of facies distribution and are amenable to include conditioning to hard and/or soft data. Falivene et al. (2007) provide an overview of the most widely used deterministic and stochastic FRM methods, including pixel-based methods termed as Sequential Indicator (SISIM), transition probability schemes (e.g., T-PROGS; Carle, 1999), multiple point simulation (Strebelle, 2002; Zhang et al., 2006; Wu et al., 2008), truncated Gaussian (TGS) and plurigaussian (TPS) simulation.

Sequential Indicator algorithms are widespread geostatistical simulation techniques that rely on indicator (co-)kriging. These have been applied to diverse datasets to study the influence of the random distribution of aquifer sedimentological facies on target environmental variables. In this context, Riva et al. (2006) present a synthetic numerical Monte Carlo study aimed at analyzing the relative importance of uncertain facies architecture and hydraulic attributes (hydraulic conductivity and porosity) on the probabilistic distribution of three-dimensional well catchments and time-related capture zones. The authors base their comparative study on a rich data-base comprising sedimentological and hydrogeological information collected within a shallow alluvial aquifer system. Riva et al. (2008, 2010) adopt the same methodology to interpret the results of a field tracer test performed in the same setting. These authors consider diverse conceptual models to describe the system heterogeneity, including scenarios where the facies distribution is random and modeled through a SISIM-based technique and the hydraulic properties of each material are either random or deterministically prescribed. Comparisons between the ability of diverse geostatistical methods to reproduce key features of field-scale aquifer systems have been published in the literature (e.g., Casar-González, 2001; Falivene et al., 2006; Scheibe and Murray, 1998; Dell'Arciprete et al., 2012). Lee et al. (2007) performed a set of Monte Carlo simulations to mimic a pumping test in an alluvial fan aquifer using the sequential Gaussian simulation method and the transition probability indicator simulation. Emery (2004) highlights limitations of SISIM upon examining the conditions under which a set of realizations is consistent with the input parameters.

Truncated Gaussian simulation enables one to condition simulations on prior information stemming from various sources while guaranteeing consistency between variogram and cross-variogram of the variables considered. The possibility of using a multiplicity of Gaussian functions to codify hydro-facies extends the potential of TGS and is the cornerstone of TPS (Galli et al., 1994). TPS allows taking into account complex transitions between material types and simulating anisotropic distributions of litho-types, whereas TGS explicitly considers only sequentially ranked categories. The application of TPS usually aims at (a) assessing the uncertainty associated with the location of the internal boundaries demarcating geo-materials within the domain, and (b) improving the geological constraints in the characterization of quantitative attributes, such as mineral ore grades. TPS is typically employed to simulate geological domains in diverse contexts, including petroleum reservoirs and mineral deposits, spatial arrangement of hydro-facies in aquifers, or soil types at a catchment scale (e.g., Betzhold and Roth, 2000; Dowd et al., 2007; Mariethoz et al., 2009).

The study of the relative impact of diverse conceptualization and simulation techniques to represent random hydro-facies spatial arrangement on the probabilistic distribution of hydraulic heads in three-dimensional aquifer systems under non-uniform mean flow conditions of the kind that is associated with large scale field settings is still lacking. As highlighted above, this analysis is tied to Probabilistic Risk Assessment procedures and constitutes one of the steps which can be adopted in modern PRA applications based on the idea of decomposing the full problem (that might comprise several uncertainty sources, including those associated with hydro-stratigraphic structure, aquifer recharge, boundary conditions, location and/or pumping/injection rate of wells) into sets of basic events (e.g., Bolster et al., 2009; Jurado et al., 2012; Tartakovsky, 2013 and references therein).

Here, we perform a numerical Monte Carlo study based on a geological system whose heterogeneous structure mimics the one associated with an alluvial aquifer system located in northern Italy where abundant lithological and geological information are available. Our analysis considers a non-uniform flow scenario due to the superimposition of a base uniform (in the mean) flow and the action of a pumping well. Field-scale available lithological