Reducing uncertainty of hydrogeological parameters by co-conditional stochastic simulation: lessons from practical applications in aquifers and in low permeability layers

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Abstract Stochastic simulation of aquifer heterogeneity is now often performed to provide a confidence interval of the modelled results for flow and solute transport problems. In practice, due to the few available measurements of the hydraulic conductivity (hard data), it is useful to integrate several other properties of the medium as indirect data (soft data). The additional conditioning obtained from the use of these secondary data allows reduction of the variance of the distribution and consequently decrease of the uncertainty of the results. This practice can also be extended to low permeability clay layers. For example, stochastic sequential simulation can be performed involving hydraulic conductivity values as hard data, and grain size measurements, electrical resistivity log, gamma ray log and a description of the lithology variation as soft data. However, other important properties can also be considered. The possible fracturing of clay strongly influences the flow and solute transport. On the other hand, in very low permeability media, diffusion can be considered as the dominant transport mechanism, so that heterogeneity in terms of the effective diffusion coefficient becomes important. Examples of application are summarized considering aquifers and low permeability clay layers. It clearly shows the great advantage of collecting multiple data sets of inter-correlated data on the same geological medium to be modelled. In high conductivity aquifers as well as in low permeability layers, this kind of additional conditioning obtained from various data is always useful when considering applications such as, among many others, well capture zones delineation, impact studies and geological confinement of wastes.

Keywords aquifer; clay layers; conditioning; secondary data; solute transport modelling; stochastic simulation

INTRODUCTION

In aquifers, most of the solute spreading is governed by the hydraulic conductivity (K) spatial variability, which is generally considered to be the main uncertain parameter. Developments integrating conditioning procedures on hydraulic conductivity values (van Leeuwen *et al.*, 2000), on head observations (Gómez-Hernández *et al.*, 1997; Vassolo *et al.*, 1998; Feyen *et al.*, 2001) and on additional soft data (Nunes & Ribeiro, 1999) allow decrease of the prior uncertainty of hydraulic conductivity and therefore reduction of the uncertainty of the well protection zone. Here, a stochastic approach integrating hydraulic conductivity measurements (hard data), head observations and shallow electrical resistivity tomography (soft data) is presented. The ensemble of capture zones obtained was then treated statistically to infer the capture zone probability distribution (CaPD).

In low permeability layers, the same kind of approach can also be applied. For simulating the 1-D vertical output solute transport fluxes at the boundaries of a clay layer (the Boom Clay in Belgium), from a given contamination source located within the layer, direct sequential simulation of the hydraulic conductivity was carried out using measurements of hydraulic conductivity and four types of "soft data" or secondary variables: resistivity logs, gamma ray logs, grain size measurements, and descriptions of the lithology. The possible fracturing of a clay layer can influence the heterogeneity of the vertical hydraulic conductivity. Moreover, as the diffusion is often the dominant transport mechanism, simulation of the spatial variability of the effective diffusion coefficient and the diffusion accessible porosity is probably required.

APPLICATION IN AQUIFERS

In practice, due to the few available hydraulic conductivity measurements (hard data), it is useful to integrate other information (soft data) like piezometric heads or geophysical data, into the conditional stochastic generation of hydraulic conductivity fields. Application of these techniques is considered for delineating well capture zones.

Stochastic simulations of equiprobable hydraulic conductivity fields are generated and subsequently conditioned on the hydraulic conductivity measurements by a kriging technique. Geophysical data can directly be integrated in the generation process by conditioning the stochastic simulation on both hydraulic conductivity measurements and electrical resistivity values by a co-kriging technique. Another additional conditioning can also be obtained by calibrating the groundwater flow on head measurements (inverse modelling) for each simulated medium generated previously. For this last step, resolution of the inverse problem requires one to carry out a parameterization: reducing the number of adjustable parameters. Therefore a zonation is performed that consists, based on specified threshold values (S_i), in dividing the hydraulic conductivity variation interval into classes (C_i) of uniform value (K_{Ci}), representing the adjustable parameters (Fig. 1). The threshold values were defined by determining the best hydraulic conductivity data combination that minimizes the variability within each class (Rentier & Dassargues, 2002). Then, the inverse procedure was applied to optimize the value of hydraulic conductivity in each class. Rentier (2003) has shown that provided the rejection of the realizations does not respect the prior relative order $K_{Ci} < K_{C(i+1)}$, the spatial structure of the optimized remaining equiprobable media is not drastically disturbed by these parameterization and inverse procedures. For each remaining realization, the capture zone is determined using a particle tracking process. The capture zone probability distribution (CaPD) gives the spatial distribution of the probability that a conservative tracer particle released at a particular location is captured by the well within a specified time span (van Leeuwen *et al.*, 2000). Example results for the well capture zones corresponding to 24 hours and 50 days are given in Fig. 2, for a practical case study located in the alluvial plain of the River Meuse (Belgium). The location of isoline $\Gamma_{(0.5)}$ for which 50% probability of capture is

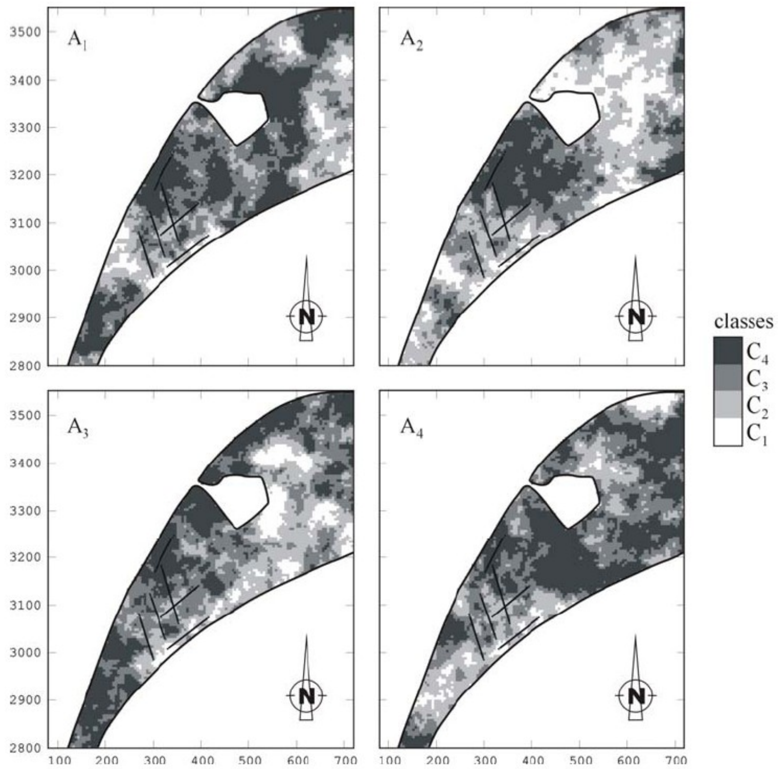

Fig. 1 Four generated equiprobable media for a practical case study. Hydraulic conductivity values are zoned in four classes to facilitate the inverse modelling procedure.

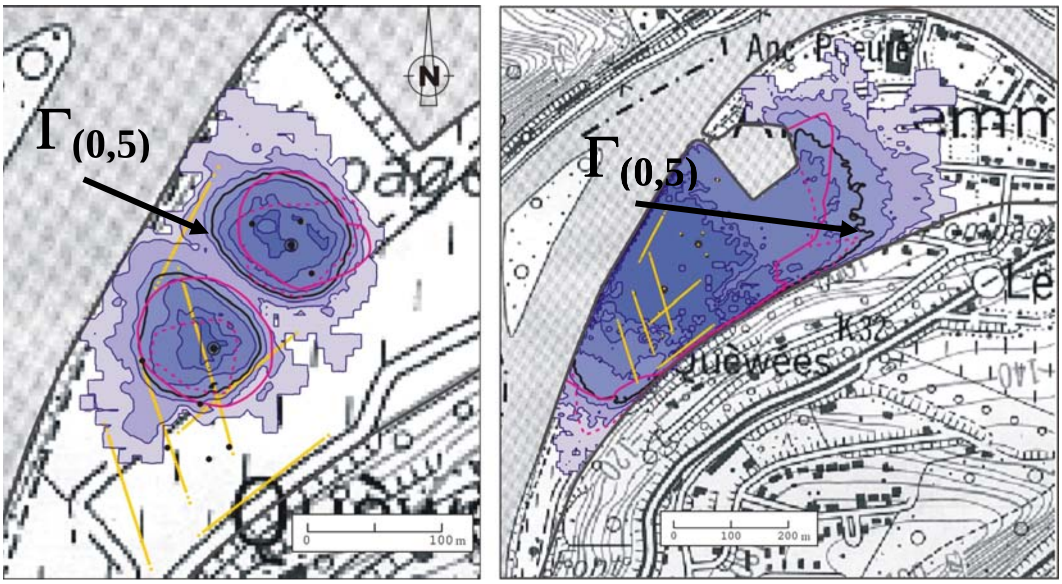

Fig. 2 Spatial distribution of well capture zones at 24 h (on the left) and 50 days (on the right). Isoline (0.5) is compared to other contours from previous deterministic studies. CaPD values are given by the grey ranges from 95% (dark grey) to 5% (light grey).

obtained, can easily be compared to results from previous deterministic studies. In this case study (Figs 1 and 2), electrical resistivity measurements were performed in a part of the alluvial plain providing 293 measurements along six profiles.

Introduction of additional available data decreases the prior uncertainty of the parameters and, in consequence, reduces the uncertainty of the well capture zone probability distribution (CaPD). Since geophysical data and head observations are easier to collect in the field than hydraulic conductivity measurements, they are generally more abundant. The methodology can now be used in real applications to quantify the uncertainty in the location and extent of well capture zones when little or no information about the hydraulic properties is available, through the conditioning on geophysical data and/or head observations.

APPLICATION IN LOW PERMEABILITY LAYERS

Co-conditional stochastic simulations can also be used in low permeability sediments, for taking into account the effect of geological heterogeneities on groundwater flow and solute transport. Development of such a methodology was initiated by Huysmans *et al.* (2003) in a research study applied on the Boom Clay in Belgium. In this 100 m thick formation, the spatial structure of the hydraulic conductivity (K_v) data in the vertical direction is studied by determining the variogram of the K_v-values in each of three horizontally delimited zones. The next step consists in collecting and analysing secondary variables along this vertical direction. The measured variables available in this study are electrical resistivity, gamma ray, grain size and lithology. The electrical resistivity shows a clear correlation with the hydraulic conductivity. Between the gamma ray measurements and the hydraulic conductivity values, a lower correlation is observed caused by the presence of organic matter and glauconite. The grain size is well correlated with the hydraulic conductivity. The lithostratigraphic column, determined on the basis of a Formation Micro Imager log (Mertens & Wouters, 2003), also shows a relationship with the hydraulic conductivity values. This last secondary variable has a qualitative nature. It is coded to obtain numerical data, which can more easily be included in a geostatistical approach: clay = 1, sandy clay = 2, clayey sand = 3 and sand = 4. The spatial structure of the secondary variables in every zone is also investigated. The variogram of each secondary variable is calculated and a model is fitted. For every combination of two variables, the experimental cross-variogram is calculated and a model is fitted.

All the spatial information is then used to perform co-kriging and co-simulation. The method is based on direct sequential simulation with histogram reproduction (DSSIM-HR; Oz *et al.*, 2003) but, here, the algorithm is adapted to replace the simple kriging by a co-kriging. Figure 3 shows one result of 100 equiprobable direct sequential simulation realizations of the vertical hydraulic conductivity of the Boom Clay using hydraulic conductivity (hard data) and electrical resistivity, gamma ray, grain size and lithology (soft data). Each of the equiprobable hydraulic conductivity fields is introduced as input for a simple 1-D vertical groundwater flow and transport model (the Boom Clay is here assumed to be horizontally layered and the flow is assumed to be in the vertical direction only). It enables the predictive distribution for the advective travel times and for solute fluxes to be obtained. In the case of a contamination source assumed to be in the middle of the clay layer, an increase of the mean advective travel time (7.5%) and of the standard deviation (51%) was computed when including the influence of the secondary data in the stochastic analysis (Huysmans *et al.*, 2003).

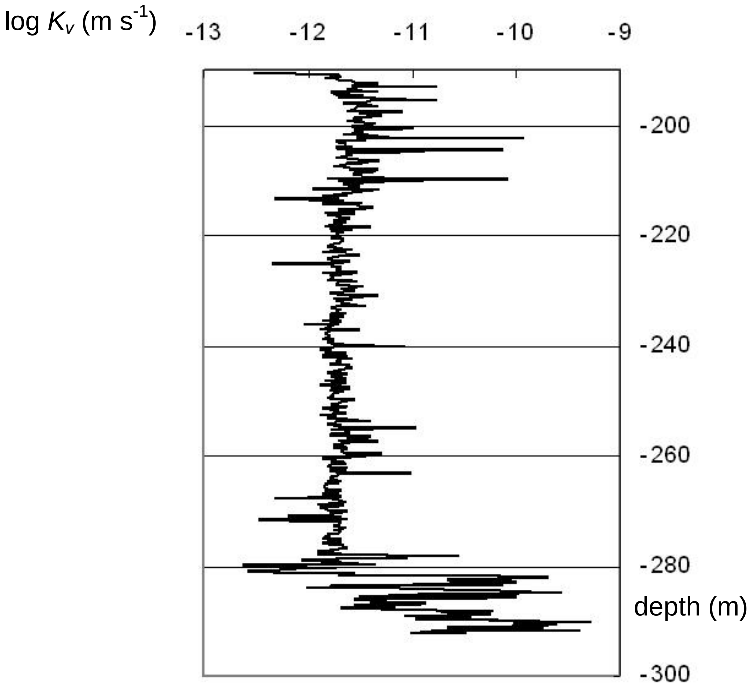

Fig. 3 One realization of the direct sequential simulation of the vertical hydraulic conductivity (K_v) using measurements of hydraulic conductivity, resistivity, gamma-ray, grain size and lithology (after Huysmans *et al.*, 2003).

Péclet number calculations have shown that diffusion is the overall dominant transport mechanism in this clay layer. Advection might become locally important in zones where possible fractures are induced due to excavation. Two main issues are thus being further investigated for their respective possible influence on the computed travel times and contaminant fluxes in low permeability layers: (a) fractures hydraulic properties and distribution; (b) the heterogeneity of the effective diffusion coefficient.

Fractures around the future disposal galleries are modelled as discrete fractures. Their properties (i.e. extent, aperture, spacing, dip and strike) can also be simulated using Monte Carlo simulation. Since these fractures will probably have similar properties to the fractures observed in previously excavated galleries in the clay layer, the input probability distributions of the fracture properties are derived from measurements carried out during recent tunnel excavation. The fracture geometry and properties are simulated by independent sampling from the proposed marginal distributions of fracture extent, aperture, spacing, dip and strike. FRAC3DVS (Therrien & Sudicky, 1996; Therrien *et al.*, 2003) is then used as the flow and transport simulator. The fractures are modelled as discrete planes with a saturated hydraulic conductivity calculated classically on the basis of the aperture and the fluid properties. This model was run for different simulations of hydraulic conductivity and fractures. Details about these simulations and results can be found in Huysmans *et al.* (2004). The total mass fluxes leaving the clay, taking excavation induced fractures and high-conductivity sublayers into account, are not very different from the mass fluxes calculated by a previous simple homogeneous model. This is probably caused by the relatively small importance of transport by advection compared to transport by diffusion in such media (Huysmans *et al.*, 2004).

Then, the diffusion coefficient and the diffusion accessible porosity for iodide were simulated in the Boom Clay with direct sequential simulation with histogram reproduction. The effect of spatial variability of the diffusion parameters (i.e. the effective diffusion coefficient and the diffusion accessible porosity) on the computed travel times and contaminant fluxes, is presented by Huysmans & Dassargues (2005) in a companion paper. It is shown that, although hydraulic conductivity has a much larger relative spatial variability than the diffusion coefficient and the diffusion accessible porosity, the heterogeneity of the diffusion parameters proved to have a much larger effect on the output fluxes than the heterogeneity of hydraulic conductivity.

CONCLUSIONS

From these practical experiments, it is clear that including all available geological/hydrogeological/geophysical data in a conditional stochastic modelling is advantageous for solving practical problems in geological media of high or low permeability.

The co-conditional stochastic simulation methods, described here, assume that the geostatistical properties of each data set are known from calculated (co-)variances and/or (co-)variograms. If these statistics are also unknown or partly unknown, the Bayesian framework (Feyen *et al.*, 2003) can be used.

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