

# Combining stochastic simulations and inverse modelling for delineation of groundwater well capture zones

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**ABSTRACT:** In hydrogeology, protection zones of a spring or a pumping well are often delimited by isochrones that are computed using calibrated groundwater flow and transport models. In heterogeneous formations, all direct and indirect data, respectively called hard and soft data, must be used in an optimal way. Approaches involving in situ pumping and tracer tests, combined with geophysical and/or other geological observations, are developed. In a deterministic framework, the calibrated model is considered as the best representation of the reality at the current investigation stage, but result uncertainty remains unquantified. Using stochastic methods, a range of equally likely isochrones can be produced allowing to quantify the influence of our knowledge of the aquifer parameters on protection zone uncertainty. Furthermore, integration of soft data in a conditioned stochastic generation process, possibly associated with an inverse modeling procedure, can reduce the resulting uncertainty. A stochastic methodology for protection zone delineation integrating hydraulic conductivity measurements (hard data), head observations and electrical resistivity data (soft data) is proposed.

## 1 INTRODUCTION

Time-related capture zones delimited by isochrones (contour lines of equal travel time to the well) are only parts of the well capture zone. In many regions, protection zones, corresponding to particular isochrones, are foreseen in local regulations providing a time-related protection. For example, in Walloon Region of Belgium, as in other regions, a protection zone corresponding to the 50-day isochrone must be delimited which brings essentially an effective protection against bacterial pollution. Ensuring a delay between an eventual injection of pollutant and its arrival at the pumping well, it allows to decide in each case on a priority intervention scheme. In heterogeneous formations, numerical computational methods are used to obtain a delimitation (Kinzelbach & al., 1992; Dassargues, 1994; Derouane & Dassargues, 1998). If many and various data are available in terms of geological and hydrogeological information in the studied domain, a very detailed geological interpretation is possible with a possibly reasonable but unquantified error. Measured parameters can be extrapolated consistently based on geological interpretation to condition model calibration. In a deterministic frame, even if the model is calibrated accurately on many data, these computed protection zones cannot be known exactly due to the limited knowledge of the aquifer parameters.

To assess the uncertainty in the delineation of time-related capture zones due to imperfect knowledge of hydraulic conductivity, different stochastic methodologies using a Monte Carlo simulation approach have been developed (Bair & al., 1991; Varljen & Shafer, 1991; Vassolo & al., 1998; Evers & Lerner, 1998; Levy & Ludy, 2000; Kunstmann & Kinzelbach, 2000). The influence of the variance and correlation length of hydraulic conductivity on the location and extent of the resulting stochastic capture zone uncertainty have been studied (van Leeuwen & al., 1998; Guadagnini & Franzetti, 1999). Further developments integrating conditioning procedures on hydraulic conductivity values (Varljen & Shafer, 1991; van Leeuwen & al., 2000), on head

observations (Gomez-Hernandez & al., 1997; Vassolo & al., 1998; Feyen & al., 2001) and on additional soft data (Kupersberger & Bloschl, 1995; Mc Kenna & Poeter, 1995; Anderson, 1997; Nunes & Ribeiro, 2000; Rentier & al., 2002) allow to decrease prior uncertainty of hydraulic conductivity and therefore to reduce the uncertainty of the well protection zone.

## 2 STOCHASTIC METHODOLOGY

Even if the question of whether a stochastic approach which treats aquifer heterogeneity as a random space function is applicable to real aquifers under field conditions has not been definitively answered (Anderson, 1997), more and more use is made of stochastic description of aquifer heterogeneity. In porous aquifers, most of the solute spreading is governed by the hydraulic conductivity ( $K$ ) spatial variability, which is generally considered as the uncertain parameter. In practice, due to the few available hydraulic conductivity measurements (hard data), it can be useful to integrate soft data, like piezometric heads or geophysical data, in the conditional stochastic generation of hydraulic conductivity fields. This conditioning allows to reduce the variance of the distribution and consequently decrease the uncertainty of the results.

In order to characterize the uncertainty of well capture zones due to aquifer heterogeneity and to show how additional soft data might be used to constrain this uncertainty, a stochastic approach integrating different sorts of data is presented. For the purpose of the demonstration, a synthetic but realistic case was designed involving three data sets: hydraulic conductivity measurements, head observations and electrical resistivity data.

### 2.1 Set-up of a synthetic aquifer

A hypothetical groundwater flow domain was constructed using geological and hydrogeological conditions similar to actual alluvial sites. The domain was chosen large enough to avoid boundary effects. Two layers were distinguished: an upper fine sand and clay layer and a lower coarse sand and gravel layer. A "true" hydraulic conductivity field representing the "reality" was created: a uniform hydraulic conductivity value of  $10^{-5} \text{ m s}^{-1}$  was applied to the upper layer whereas for the lower layer a non-conditional simulation was generated using the Turning Band algorithm (Mantoglou & Wilson, 1982) with an isotropic, exponential correlation structure identical to the one found for the alluvial sediments of the Meuse River valley downwards to Liège (Belgium). From a dense grid of more than 10000 cells, 15 hydraulic conductivity values were selected, representing pumping test results in virtual piezometers and providing the hard data set. A regular pattern of sampling locations was rejected for the purpose of keeping consistent with a probable real-world situation.

A single pumping well (pumping rate of  $60 \text{ m}^3 \text{ h}^{-1}$ ) located in the heterogeneous sand and gravel unconfined aquifer was used for the simulation. Pure deterministic groundwater flow conditions were then computed, providing the synthetic "measured" heads at the 15 virtual piezometers (first set of soft data).

The resistivity data set (second set of soft data) was created based on the observed correlation ( $r = 0.9$ ) existing between electrical resistivity ( $\rho$ ) and hydraulic conductivity ( $K$ ) in the alluvial sediments of the Meuse River. Considering  $N(0,1)$  as a random draw within a standard normal distribution and  $\hat{\sigma}$ , the standard deviation of the regression residual, 300 resistivity values, distributed on 12 tomographic profiles were generated by the following equation:

$$\ln \rho = 6.836 + 0.345 \ln K + \hat{\sigma} N(0,1) \quad (1)$$

Considering advective transport time to the well, the "true" 20-day isochrone line (associated with the concerned pumping rate) resulting from the "true" hydraulic conductivity field was also computed and used as reference for further comparisons.

### 2.2 Monte Carlo stochastic conditional simulations

The stochastic methodology developed by Varljen & Shafer (1991) is applied in order to determine and quantify the uncertainty in the location and extent of the 20-day capture zone due to imperfect knowledge of the hydraulic conductivity field. According to a Monte-Carlo analysis, four hundred stochastic simulations of equally likely hydraulic conductivity fields for the lower

layer were generated using the Turning Bands method. Each of them were subsequently conditioned on hydraulic conductivity measurements by a kriging technique. Groundwater flow and a particle tracking process were computed for each realization. The ensemble of obtained capture zones was then treated statistically to infer the capture zone probability distribution (CaPD). This 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, 2000), in this particular case 20 days. Figure 1a compares the CaPD with the "real" isochrone and show how the stochastic approach reveals the uncertainty about the location of the protection zone. In order to quantify and evaluate the performance of additional conditioning, two measures among several others have been selected (van Leeuwen & al., 2000).  $Wa$  is a measure of uncertainty based on the extent of the uncertainty zone for which the probability  $P$  of capture is  $0 < P < 1$ .  $Wb$  compares the location of the reference isochrone with the location of isoline  $\Gamma(0.5)$  for which 50% probability of capture is obtained. Units of both measures are expressed in number of 5 m x 5 m cells.

### 2.3 Additional conditioning by head measurements (first set of soft data)

This additional conditioning was performed by calibrating the groundwater flow on head measurements for each stochastic conditional simulation generated previously by inverse modelling (PEST code, Doherty, 1994). Resolution of the inverse problem required to carry out a parameterisation reducing the number of adjustable parameters. Therefore a zonation was applied that consist, based on four specified threshold values ( $S_i$ ), in dividing the hydraulic conductivity variation interval in five classes ( $C_i$ ) of uniform value ( $KC_i$ ), representing the adjustable parameters. The threshold values were defined by determining the best hydraulic conductivity data combination that minimize the variability within each class, by minimizing the following equation:

$$f = \sum_{i=1}^{N_c} \sum_{j=1}^{N_{d_i}} (\ln K_{ij} - \overline{\ln K_i})^2 \quad \text{with} \quad \overline{\ln K_i} = \frac{1}{N_{d_i}} \sum_{j=1}^{N_{d_i}} \ln K_{ij} \quad i = 1, N_c \quad (2)$$

where  $N_c$  is the number of classes,  $N_{d_i}$  is the number of data in each class (varying from one combination to an other) and  $\sum N_{d_i} = N_D$ , the total number of  $K$  data.

The inverse procedure was applied to optimize the uniform hydraulic conductivity values for each parameter. However, for some realizations, these optimized hydraulic conductivity values did not respect the relative order  $KC_i < KC_{(i+1)}$  defined by the thresholding. Considering these realizations as geologically erroneous, they were rejected. For each remaining realization, the 20-day capture zone was determined and consequently the CaPD for the ensemble of possible capture zones was estimated. Results show how the use of head conditioning by inverse modelling combined with the use of a selection criterion reduce the uncertainty of the probability distribution (decrease in  $Wa$ ).

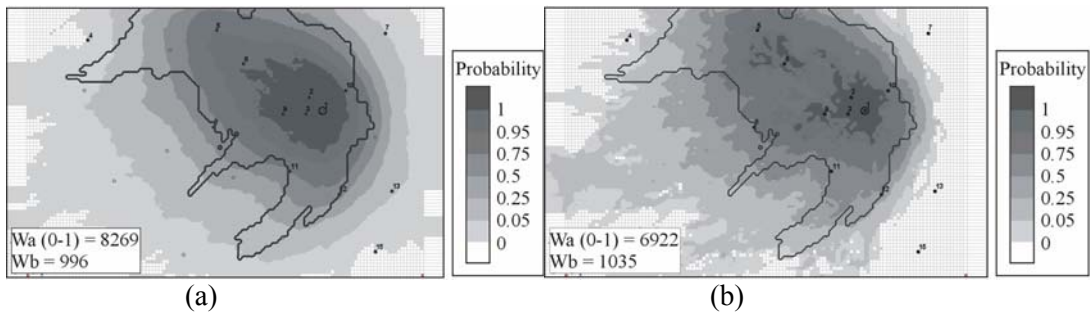


Figure 1. a) Comparison of the CaPD determined by stochastic realizations conditioned on 15 hydraulic conductivity values, and the reference 20-day isochrone (black line) b) Comparison of the CaPD determined by stochastic realizations conditioned on 15 hydraulic conductivity values and inverse modelling using 15 piezometric heads and the reference 20-day isochrone (black line).

## 2.4 Additional conditioning by geoelectrical resistivity data (second set of soft data)

The geophysical data set, as additional useful information, was directly integrated in the generation process by conditioning each stochastic simulation on both hydraulic conductivity measurements and resistivity values by a cokriging technique. Four hundred stochastic "co-conditional" simulations were then generated based on a linear model of coregionalisation that was adjusted on experimental simple and cross-covariances. Following the same procedure as described in the previous paragraph (parameterization and inverse modeling), an advective 20-day isochrone was computed for each remaining realization and the resulting CaPD was calculated (Fig. 2). The use of additional available data decrease the prior uncertainty of the parameters and, in consequence, reduce the uncertainty of the well CaPD (decrease in  $Wa$ ). It can also be observed that the  $\Gamma(0.5)$  isoline tends to approach the reference isochrone (decrease in  $Wb$ ). Comparing results of figure 2 to those of figure 1, a clear improvement is observed in the description of the medium heterogeneity leading to more realistic isochrones with regards to the reference one.

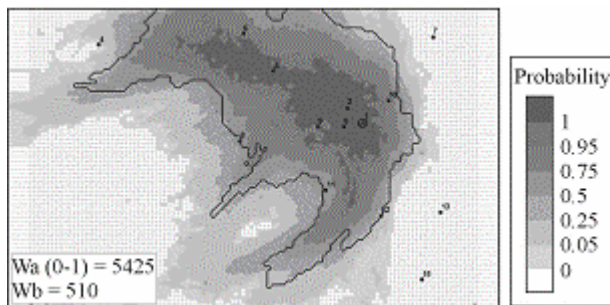


Figure 2. Comparison of the CaPD determined by realizations conditioned on 15 hydraulic conductivity values, 15 piezometric heads and 300 resistivity values and the reference 20-day isochrone (black line).

## 3 CONCLUSION

Advances in the delimitation of protection zones are made by the use of stochastic methodologies. Moreover 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 on the field than hydraulic conductivity measurements, they are generally more abundant. The methodology presented can be used in real applications to quantify the uncertainty in the location and extent of well capture zones when little or no information is available about the hydraulic properties, through the conditioning on geophysical data and/or head observations.

The different stochastic approaches listed previously considers purely advective transport (particle tracking procedure). They do not take the concept of macrodispersivity into account. A topic for further research will be the assimilation of information from solute concentrations (i.e. tracer tests) to further reduce uncertainty in capture zone delineation. Further applied research is needed to design optimal strategies of soft data acquisition like, for example, selection of locations for conditioning measurements.

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