A composite medium approach for probabilistic modelling of contaminant travel time distribution to a pumping well in a heterogeneous aquifer

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Abstract We analyse the probabilistic nature of the time of travel of conservative solutes to a pumping well operating within a heterogeneous aquifer. The latter is modelled as a three-dimensional, doubly stochastic composite medium, where distributions of geological materials and hydraulic properties are uncertain. The problem is tackled within a numerical Monte Carlo framework. We study the importance of uncertain facies geometry and uncertain hydraulic conductivity and porosity on predictions of solute time of travel to the pumping well by focusing on two special cases in which: (1) the facies distribution is random, but the hydraulic properties of each material are fixed, and (2) both facies geometry and material properties vary.

Keywords capture zones; composite media; heterogeneity; uncertainty estimation; well fields

INTRODUCTION

Much of the existing literature on stochastic hydrogeology deals with mildly heterogeneous formations. While this assumption is crucial for closing moment differential equations or for making numerical Monte Carlo simulations manageable, it clearly limits the applicability of most such analyses. In addition to this, a variety of studies suggest the importance of honouring geological features in hydrogeological modelling. A recently proposed method of random domain decomposition (Winter & Tartakovsky, 2002) provides a general framework for modelling flow and transport in highly heterogeneous formations consisting of multiple materials, by quantifying uncertainty in both the spatial arrangement of lithofacies and of hydraulic properties within each facies. Previous studies aimed at analysing the impact of a composite medium model on flow predictions and dealt with relatively simple material distributions (e.g. Winter *et al.*, 2002). Here we focus on the statistical distribution of capture zones of a single pumping well operating within a heterogeneous aquifer which is modelled as a three-dimensional, doubly stochastic composite medium, where the distributions of geomaterials and hydraulic properties are uncertain. The problem is tackled within a numerical Monte Carlo framework. We analyse the importance of uncertain facies geometry and uncertain hydraulic conductivity and porosity on predictions of conservative solute time of travel to the pumping well by focusing on two cases in which: (1) the facies distribution is random, but the hydraulic properties of each material are fixed, and (2) both the facies geometry and the material properties vary.

DATA ANALYSIS, MODEL SET-UP AND COMPUTATIONAL PROCEDURE

The study focuses on the analysis of the time of residence of non-reactive contaminant particles within the "Lauswiesen" pumping well field, which is located in the Neckar River valley, close to Tübingen in southwestern Germany. Field and laboratory scale experiments for subsurface investigation were designed and performed during a 2-year period (2002–2003). Sieve analyses results emphasized the presence of very heterogeneous (variance of natural logarithm of hydraulic conductivity was 2.91), highly conductive (the average hydraulic conductivity was 8.87×10^{-3} m s^{-1}) alluvial deposits. A stochastic three-dimensional model (size of about 800 × 800 × 8 m) was developed within a sub-domain region located in the northeastern part of an existing deterministic two-dimensional model (Martac & Ptak, 2001). The experimental data are used to describe the spatial variability of hydraulic conductivity, K, and effective porosity, n_e, in the rectangular region highlighted in Fig. 1 (size 250 × 400 × 8 m), while the remaining part of the aquifer is modelled as a homogeneous medium, with uniform K and n_e.

Three types of geomaterials (clusters/facies) were identified to characterize the heterogeneity of the aquifer lithology by means of multivariate cluster analysis. Spatial variability of each lithotype was separately analysed via indicator geostatistics (Riva *et al*., 2004). The results are summarized as follows: *Cluster 1* represents the 53% of the samples and is characterized by moderately sorted gravel with very few fines and around 13% sand; *Cluster 2* represents the 44% of the samples and is constituted by poorly sorted gravel, few fines and around 24% sand; *Cluster 3* represents the 3% of the samples and is defined as well sorted sand with very few fines and 23% gravel. Sample directional three-dimensional spherical variograms of the indicators have been

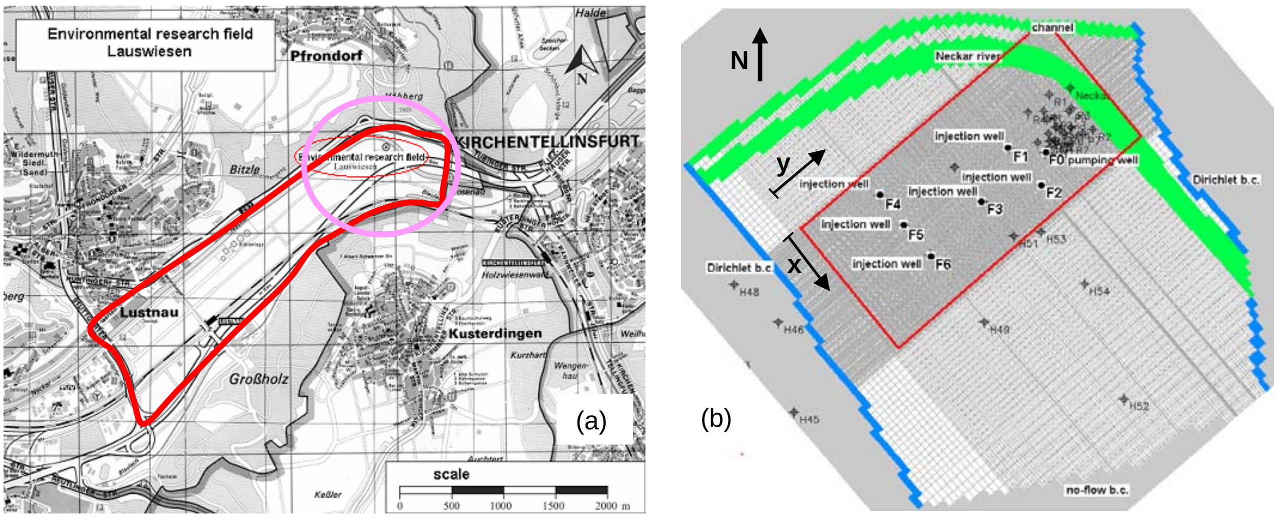

Fig. 1 "Lauswiesen" experimental field site, location of wells, and planar demarcation of the regional two-dimensional (a), and local three-dimensional (b), numerical models.

Table 1 Results of the indicator variography.

	Cluster 1	*Cluster 2*	*Cluster 3*
Maximum continuity angle (deg)	75°	75°	90°
Horizontal maximum correlation length (m)	11	11	35
Minimum continuity angle (deg)	165°	165°	0°
Horizontal minimum correlation length (m)	5.5	5.5	6.0
Vertical correlation length (m)	0.8	0.6	0.4

reconstructed. The results are reported in Table 1 where the maximum and minimum continuity directions are evaluated clockwise starting from the north–south (0°) direction. Values of hydraulic conductivity, K, for each cluster were calculated from the sample grain size distribution curves by means of the empirical relationship of Beyer (1964):

$$K = C_b \times d_{10}^2 \quad [\mathrm{m\ s^{-1}}]$$

where C_b is an empirical value depending on the ratio d_{60}/d_{10}, and d_{10} and d_{60} represent the grain size (in mm) corresponding to the 10th and 60th percentiles of the cumulative grain size distribution curve, respectively. The variability of hydraulic conductivity is then described by means of the first statistical moments ($\overline{K}$ indicates the mean of K): *Cluster 1* – $\overline{K}$ = 15.58 × 10^{-3} m s^{-1} and variance of ln$K$ = 2.41; *Cluster 2* – $\overline{K}$ = 1.49 × 10^{-3} m s^{-1} and variance of ln$K$ = 1.35; *Cluster 3* – $\overline{K}$ = 0.35 × 10^{-3} m s^{-1} and variance of ln K = 0.32.

Geostatistical analysis was then performed separately for hydraulic conductivities of each material. Hydraulic conductivity of *Cluster 3* was taken as constant and equal to its mean due to the limited volumetric fraction of this facies. When analysing the natural logarithms of conductivity data typical of *Cluster 1* and *Cluster 2*, sample horizontal variograms exhibit no clear evidence of directional anisotropy while the vertical range was significantly smaller than its horizontal counterpart. Sample variograms of the log-hydraulic conductivities of both materials were interpreted by a spherical model with a nugget (parameters for log-conductivities of *Cluster 1*: nugget = 0.05, sill = 2.36, horizontal range = 10 m, and vertical range = 0.90 m; parameters for log-conductivities of *Cluster 2*: nugget = 0.05, sill = 1.30, horizontal range = 10 m, and vertical range = 0.80 m). As an example, Fig. 2 depicts the horizontal and vertical sample variograms of log-conductivities derived from samples belonging to *Cluster 1* and the corresponding theoretical models adopted.

The model domain was discretized vertically into 27 layers of 107 520 cells each. Refinement of cell sizes was performed in the proximity of the well (where cells sizes were 0.33 × 0.40 × 0.30 m) with gradual increase of cells sides with distance from the pumping well F0 (Fig. 1(b)), resulting in a total of 2.90 million cells. Boundary conditions are of Cauchy type along Neckar River and either of Dirichlet or Neumann type along the other boundaries (Fig. 1(b)). The Monte Carlo flow and transport simulations were performed according to the following scenarios:

– Test case 1 (TC1): a constant K = 8.87 × 10^{-3} m s^{-1} (average K evaluated on the basis of all samples) and a constant effective porosity, n_e = 9.8%, were adopted. The constant value of n_e was estimated from calibration of simulated breakthrough

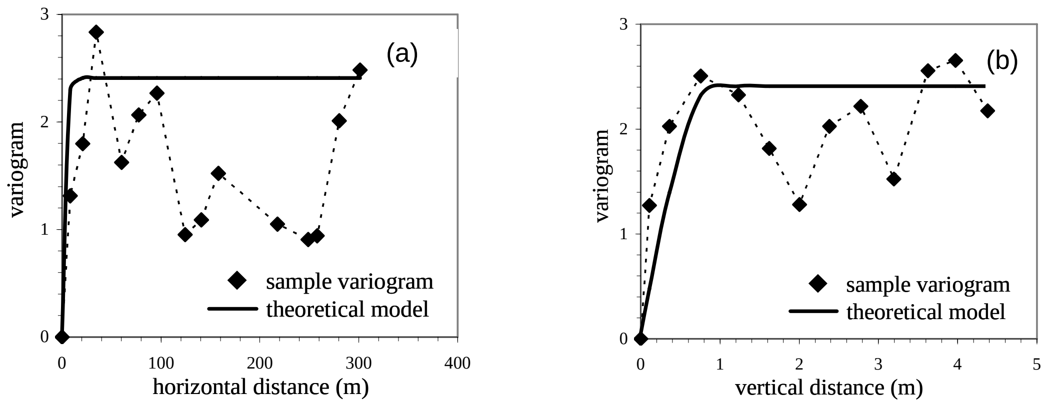

Fig. 2 (a) Horizontal and (b) vertical sample variograms of log-conductivities derived from soil samples belonging to *Cluster 1* together with the theoretical models adopted.

curves to those obtained from field tracer tests. Since K and n_e are two deterministic constants in this scenario, only one realization was performed.

– Test case 2 (TC2): the materials distribution is random and described via the indicator geostatistical analysis; the hydraulic conductivity for each material is set to the corresponding mean value, while a constant n_e = 9.8% is adopted.
– Test Case 3 (TC3): the materials and conductivity distribution are those of TC2; variability of n_e was simulated via the relationship between hydraulic conductivity and effective porosity obtained for the Neckar valley aquifer material samples (Riva *et al.*, 2004). This leads to a different value of n_e to be assigned to each facies: (i) *Cluster 1*, n_e = 10.64%, (ii) *Cluster 2*, n_e = 7.14%, (iii) *Cluster 3*, n_e = 5.00%.
– Test Case 4 (TC4): both the materials distribution and the hydraulic conductivity are random quantities, while the effective porosity is kept constant (n_e = 9.8%).

For each of the test cases, TC2, TC3 and TC4, 200 Monte Carlo iterations were performed. The sequential indicator simulator of categorical variables SISIM (Deutsch & Journel, 1998) was used to obtain multiple 3-D conditional spatial distributions of the three identified facies. The size of the cell blocks employed in the generation procedure (2.0 × 1.0 × 0.3 m) was chosen on the basis of the values of correlation length in Table 1, in order to enable a minimum of two cells per correlation scale. The generated facies blocks were then pasted into the central part of the local 3-D model (Fig. 1), all the neighbouring domains being kept unchanged. The random distribution of materials and hydraulic conductivity considered in TC4 was simulated according to the following steps: (a) three-dimensional unconditional realizations of log-conductivities of *Clusters 1* and *2* were generated on the same grid of TC2 by using the code GCOSIM3D (Gómez-Hernández, 1991), while keeping a constant conductivity for *Cluster 3*; (b) appropriate conductivity values were then assigned to the numerical blocks according to the indicators distribution generated for TC2. When finer discretization is required in the numerical grid, each block is then further divided into smaller elements with the same hydraulic conductivity.

We solved the steady-state flow problem for each realization and delineated the three-dimensional probability distribution of particles travel time to the well F0, where a constant pumping rate was imposed (0.014 $m^3 s^{-1}$). The solute movement in each realization was modelled by particle tracking (Pollock, 1989) upon evenly distributing non-reactive solute particles on the refined computational grid within the central part of the domain (Fig. 1(b)). We then evaluated the distribution of the probabilistic capture zones. Analysis of the convergence of the travel time distributions evidenced that, even though 200 Monte Carlo iterations do not completely lead to statistical stability, the results obtained allow a meaningful understanding of the process.

RESULTS AND COMMENTS

As an example of our results, Fig. 3 contrasts the 5-day capture zone for TC1 to probabilistic 5-day capture zones for TC2 and TC3 along layer 20 (close to the bottom of the aquifer). Along the mean base flow direction, the extent of the capture zone in the homogeneous field (TC1) is larger than that of the 50% probabilistic capture zone. The homogeneous model slightly underestimates the lateral extent of the 50% capture zone. The effect of porosity variations is not relevant for the smallest probability levels considered (Fig. 3(a)). For the largest probabilities, variability of n_e is important for demarcating the extent of the capture zone along the mean base flow direction, while it has practically no effect on the lateral extent of the capture zones. A similar behaviour has been observed within the other layers (not reported here). Increasing the target travel time, the effect of the spatial variability of n_e slightly increases, as reported in Fig. 4, where the depictions of the 7-day capture zones for the scenarios corresponding to Fig. 3 are reported.

The effect of a complete composite medium conceptualization is encapsulated in the results of Figs 5 and 6, reporting depictions of capture zones analogous to those of Fig. 3 and 4 for TC1, TC2 and TC4. For the lowest probabilities (Figs 5(a) and 6(a)), incorporating variability of both facies and hydraulic conductivity distributions (TC4) leads to probabilistic capture zones which are more elongated along the mean base flow direction than those based only on facies variability (TC2); this difference is less

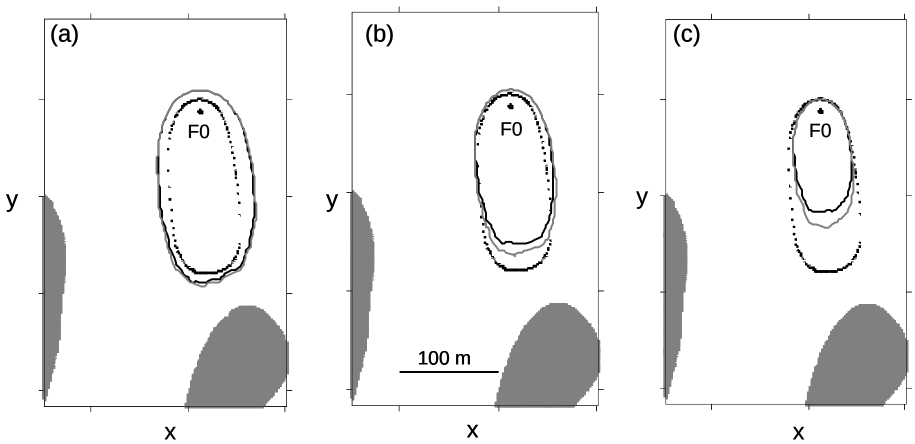

Fig. 3 5-day capture zone for TC1 (dotted curves) and probabilistic 5-day capture zones for TC2 (black solid curves) and TC3 (grey solid curves) corresponding to probability levels: (a) 0.2, (b) 0.5, (c) 0.8. Layer 20 of the model (shaded areas indicate the aquifer bottom).

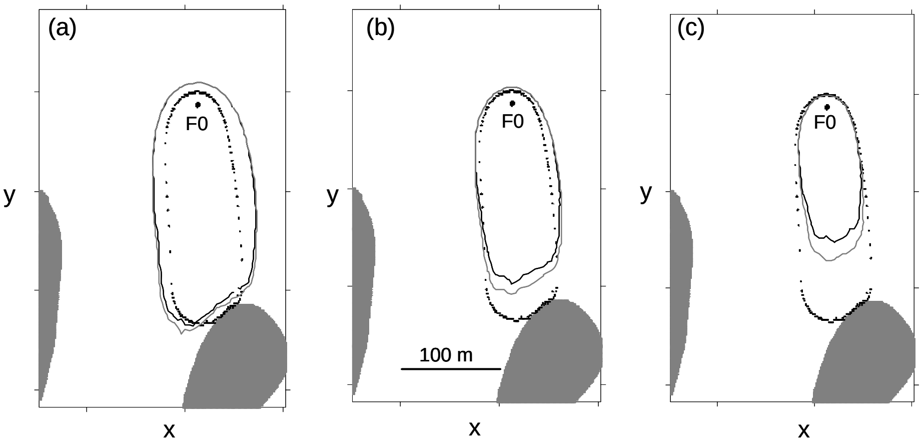

Fig. 4 7-day capture zone for TC1 (dotted curves) and probabilistic 7-day capture zones for TC2 (black solid curves) and TC3 (grey solid curves) corresponding to probability levels (a) 0.2, (b) 0.5, (c) 0.8. Layer 20 of the model (shaded areas indicate the aquifer bottom).

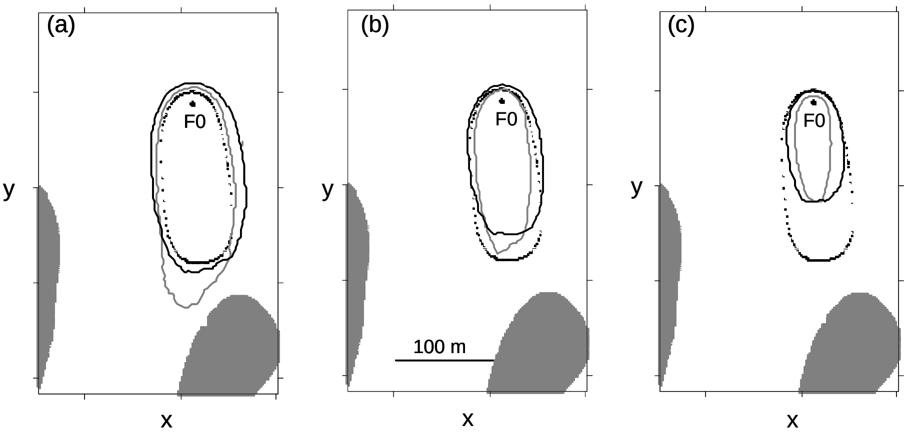

Fig. 5 5-day capture zone for TC1 (dotted curves) and probabilistic 5-day capture zones for TC2 (black solid curves) and TC4 (grey solid curves) corresponding to probability levels (a) 0.2, (b) 0.5, (c) 0.8. Layer 20 of the model (shaded areas indicate the aquifer bottom).

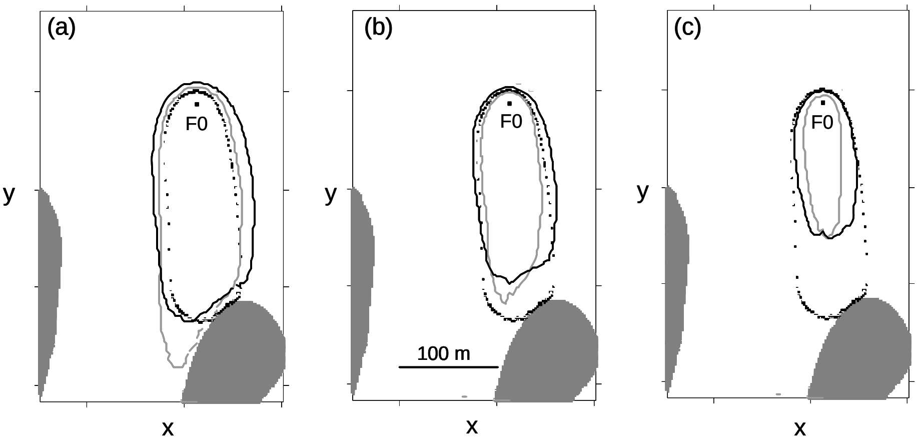

Fig. 6 7-days capture zone for TC1 (dotted curves) and probabilistic 7-days capture zones for TC2 (black solid curves) and TC4 (grey solid curves) corresponding to probability levels (a) 0.2, (b) 0.5, (c) 0.8. Layer 20 of the model (shaded areas indicate the aquifer bottom).

important for the largest probabilities considered. Contrarywise, the transverse extent of probabilistic capture zones is always affected by the adoption of the full composite medium model (TC4).

REFERENCES

Beyer, W. (1964) Zur Beschreibung der Wasserdurchlässigkeit von Kiesen und Sanden (Description of permeability of pebbles and sands). *Zeit. Wasserwirtschaft-Wassertechnik* **14**, 165–168.

Deutsch, C. V. & Journel, A. G. (1998) *GSLIB Geostatistical Software Library and User's Guide*, 2nd edn. Oxford University Press, New York, USA.

Gómez-Hernández, J. J. (1991) A stochastic approach to the simulation of block conductivity fields conditioned upon data measured at a smaller scale. PhD Dissertation, Stanford University, California, USA.

Martac, E. & Ptak, T. (2001) Data set for transport model calibration/validation, parameter upscaling studies and testing of stochastic transport models/theory. *Report D16 of Project "Stochastic Analysis of Well-Head Protection and Risk Assessment – W-SAHaRA", EU Contract EVK1-CT-1999-00041*, Tübingen, Germany.

Pollock, D. W. (1989) Documentation of computer programs to complete and display pathlines using results from the US Geological Survey modular three-dimensional finite-difference ground-water model. *USGS Open File Report 89-381*.

Riva, M., Guadagnini, L., Martac, E. & Ptak, T. (2004) Stochastic modeling of well head protection zones in highly heterogeneous aquifers. In: *Bringing Groundwater Quality Research to the Watershed Scale* (ed. by Neil R. Thompson) (Proc. Int. Conf. GQ'2004, July 2004, Waterloo, Canada), 449–457, IAHS Publ. 297. IAHS Press, Wallingford, UK.

Winter, C. L. & Tartakovsky, D. M. (2002) Groundwater flow in heterogeneous composite aquifers. *Water Resour. Res.* **38**(8), doi:10.1029/2001WR000450.

Winter, C. L., Tartakovsky, D. M. & Guadagnini, A. (2002) Numerical solutions of moment equations for flow in heterogeneous composite aquifers. *Water Resour. Res.* **38**(5), doi: 10.1029/2001WR000222.