Soil structure modelling in a laboratory intermediate-scale experiment.
Application of the iterative cokriging method

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Abstract One-dimensional tracer tests were performed in the laboratory using an intermediate-scale setup (2 m long). Small but non negligible spatial variations in migration velocities were observed and utilized to estimate the spatial pattern of the hydraulic conductivity. The quasi-linear geostatistical method of inversing (Kitanidis, 1995) was used to perform the calculation of the best estimate of the ln(K) field on the basis of 12 mean breakthrough time measurements. The 2D heterogeneous permeability field obtained was then used for the forward modelling of a two-well injection-recovery tracer experiment using Modflow® and MT3D®. A relatively good matching of experimental results could be reached.
Key words laboratory experiment, structure mapping, conditioning

INTRODUCTION

Inverse modelling is key to the correct calibration of any model. It consists in searching values for the model parameters using state variables of the system known at various measurement points (Sun, 1994). However, current numerical models of flow and transport in aquifers are discretized in thousands of elements, each having their own unknown value of hydraulic conductivity K (expressed in ms^{-1}). Moreover, *a priori* information on the system and measurements of dependent state variables are generally very limited. The inverse problem has then so many degrees of freedom to be determined with so few observations that the inverse problem is said to be ill-posed (Sun, 1994). Parametrization aims at reducing the number of parameters of the system to be identified in the inverse approach. Geostatistics provide a parametrization method that eliminates the need for arbitrary and rather inflexible assumptions such as domain subdivision (Kitanidis, 1995), as it is based on a general description of the soil structure through a correlation function.

Incorporating concentration measurements in the inverse modelling of permeabilities has only recently been investigated (Dagan et al., 1996 ; Harvey & Gorelick, 1995 ; Hendricks Franssen et al., 2003). In this paper, it is proposed to apply the iterative cokriging method (Kitanidis, 1995) using migration velocity measurements for the interpretation of laboratory tracer tests. After having briefly recalled the basics of cokriging, the experimental setup will be presented, as well as results of one-dimensional tracer tests. Those results will then be used to determine the spatial pattern of permeability, which will in turn be utilized in a forward modelling approach that will be confronted with experimental results of two-well injection-recovery tracer tests.

BASICS OF COKRIGING

Assuming a lognormal hydraulic conductivity field, so that

$$Y = \ln(K) \tag{1}$$

Y and K are spatially distributed variables that can be discretized on a finite dimension grid. In this case, **Y** and **K** are unknown column vectors of length n_e, n_e being the number of cells in the grid. Assuming moreover that $\mathbf{Z_0}$ is a column vector of n_m measurements of a dependent variable Z, such as the mean breakthrough time, the conditional estimate of Y can be obtained from (Deutsch & Journel, 1998) :

$$\widehat{\mathbf{m}}_{\mathrm{Y}} = \mathbf{m}_{\mathrm{Y}} + \mathbf{C}_{\mathrm{YZ}}\xi \tag{2}$$

where ξ is the solution of the linear system :

$$\mathbf{C}_{\mathrm{ZZ}}\xi = (\mathbf{Z}_0 - \mathbf{m}_{\mathrm{Z}}) \tag{3}$$

in which $\mathbf{m_Y}$ (of size $n_e \times 1$) is the *a priori* mean of the Y field, $\mathbf{m_Z}$ ($n_m \times 1$) is the a priori estimate of Z, $\mathbf{C_{ZZ}}$ ($n_m \times n_m$) its covariance matrix and $\mathbf{C_{YZ}}$ ($n_e \times n_m$) is the cross-covariance matrix of Y and Z. In this paper, an extended version of Eqs. (2) and (3) will be used in order to simultaneously determine the mean of the Y field (details can be found in Cirpka & Kitanidis, 2001). The conditional covariance matrix is :

$$\widehat{\mathbf{C}}_{\mathrm{YY}} = \mathbf{C}_{\mathrm{YY}} - \mathbf{C}_{\mathrm{YZ}}\mathbf{C}_{\mathrm{ZZ}}^{-1}\mathbf{C}_{\mathrm{YZ}}^{T} \tag{4}$$

where $\mathbf{C_{YY}}$ (of size $n_e \times n_e$) is the *a priori* covariance matrix of the Y field and $\mathbf{C_{YZ}}^T$ is the matrix transpose of $\mathbf{C_{YZ}}$. The effect of conditioning is thus to modify the expected value of the variable and to reduce its variance. It must be noted that $\mathbf{m_Y}$ is not required to be constant throughout the domain.

Provided Y is known, it is generally easy to compute the corresponding value of Z (e.g. using a more or less complex transport equation). Obtaining $\mathbf{m_Z}$ from $\mathbf{m_Y}$ is thus straightforward. The main difficulty lies in the computation of $\mathbf{C_{YZ}}$ and $\mathbf{C_{ZZ}}$. In linear cokriging, the way to proceed consists in truncating the series expansion of Z in function of Y to the first order, which can be written in matrix notation as :

$$\mathbf{Z} \approx \mathbf{m}_{\mathrm{Z}} + \mathbf{J}(\mathbf{Y} - \mathbf{m}_{\mathrm{Y}}) \tag{5}$$

where **J** is a matrix of size n_m x n_e and is called *sensitivity*. Cross-covariance and auto-covariance can then be computed according to :

$$\mathbf{C}_{\mathrm{YZ}} = \mathbf{C}_{\mathrm{YY}}\mathbf{J}^{T} \tag{6}$$

$$\mathbf{C}_{\mathrm{ZZ}} = \mathbf{J}\mathbf{C}_{\mathrm{YY}}\mathbf{J}^{T} \tag{7}$$

In case the variance of the Y field is too high (> 1), the linearization in Eq. (4) is not valid anymore. It is then necessary to turn to the quasi-linear method of inversing, also called *iterative cokriging* (Kitanidis, 1995). In this method, linearization is performed about the last estimate $\tilde{\mathbf{m}}_{\mathrm{Z}}$ and a weighted root-mean-square criterion is used to quantify convergence :

$$\varepsilon = \sqrt{\frac{1}{n_m}\sum_{i=1}^{n_m}\frac{\left(\tilde{m}_{Y,i} - \widehat{m}_{Y,i}\right)^2}{\widehat{C}_{YY}(i,i)}} \tag{8}$$

Typically, Cirpka & Kitanidis (2001) require ε to be smaller than 0.1 or 0.25. It must also be noted that Eq. (7) can be adapted to account for measurement errors.

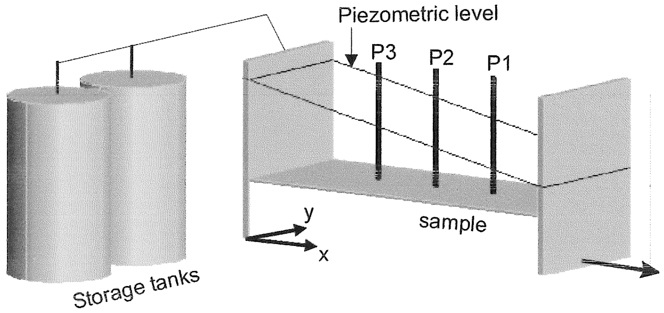

Fig. 1 Schematic view of the laboratory device

EXPERIMENTAL MODELLING

The experimental device, schematically illustrated on Fig. 1, consists of a 2 m long, 80 cm wide and 36 cm thick sand-box, flanked by two water reservoirs used to impose fixed-head upstream and downstream flow conditions (Frippiat et al., 2004a). This device allows one to impose confined flow conditions on intermediate-scale soil samples. Experiments were conducted on Brusselean sand, which is a relatively coarse sand (d_{50} = 315 μm) with a very low clay content. The sample was manually compacted in three layers of about 12 cm each, in order to reach a relatively homogeneous state and a mean total porosity of about 40 %. The tracer was a low concentration saline solution (less than 1 mgl^{-1} of NaCl) and measurements were performed using twelve buried electrical sensors. All of them were placed at a depth of 18 cm and at x and y coordinates listed in Table 1. Three fully penetrating piezometers were also installed (P2 being located at the center while P1 and P3 were placed 40 cm away from P2 on the model longitudinal axis of symmetry).

In a first phase, "one-dimensional" tests were performed under prismatic flow conditions. Upstream and downstream fixed-head conditions were respectively 0.92 m and 0.52 m, yielding a mean hydraulic gradient of 20 %, in order to achieve a relatively short experiment duration. These tests included three step variations of the concentration of the upstream reservoir solution, resulting in three S-shaped breakthrough curves recorded by each sensor. Table 2 shows apparent transport parameters inferred from temporal moment analysis, using the methodology proposed by Yu et al. (1999). Non-negligible discrepancies appear in

Table 1 Sensor position (reference axes shown of Fig. 1)

	C1	C2	C3	C4	C5	C6	C7	C8	C9	C10	C11	C12
x (m)	1.44	1.44	1.27	1.20	1.20	1.13	1.00	1.00	0.87	0.80	0.73	1.00
y (m)	0.36	0.44	0.40	0.30	0.50	0.40	0.30	0.50	0.40	0.50	0.40	0.40

Table 2 One-dimensional tracer test. Results from moment analysis according to Yu et al. (1999).

	C1	C2	C3	C4	C5	C6	C7	C8	C9	C10	C11	C12
v_1 (10^{-5} ms^{-1})	2.95	3.09	2.99	2.71	3.11	3.11	2.74	3.50	3.36	3.42	3.69	3.44
v_2 (10^{-5} ms^{-1})	3.02	3.21	3.05	2.77	3.22	3.13	2.79	3.55	3.35	3.44	3.62	3.33
v_3 (10^{-5} ms^{-1})	2.92	3.16	3.02	2.72	3.16	3.06	2.73	3.46	3.21	3.34	3.36	2.96
$\langle v \rangle$ (10^{-5} ms^{-1})	2.96	3.15	3.02	2.73	3.16	3.10	2.75	3.49	3.31	3.40	3.56	3.24
$\alpha_{L,1}$ (cm)	0.83	0.93	0.51	0.48	0.61	0.53	0.39	0.45	0.32	0.34	0.36	0.88
$\alpha_{L,2}$ (cm)	1.01	0.83	0.47	0.50	0.55	0.47	0.39	0.40	0.30	0.34	0.37	0.81
$\alpha_{L,3}$ (cm)	1.14	0.91	0.90	0.63	0.81	1.03	0.64	0.53	0.82	0.41	1.43	2.10
$\langle \alpha_L \rangle$ (cm)	0.99	0.89	0.63	0.54	0.66	0.68	0.47	0.46	0.48	0.36	0.72	1.23

v_i = migration velocity observed during step n°i of the experiment
$\langle v \rangle$ = averaged migration velocity
$\alpha_{L,i}$ = apparent longitudinal dispersivity observed during step n°i of the experiment
$\langle \alpha_L \rangle$ = averaged longitudinal dispersivity

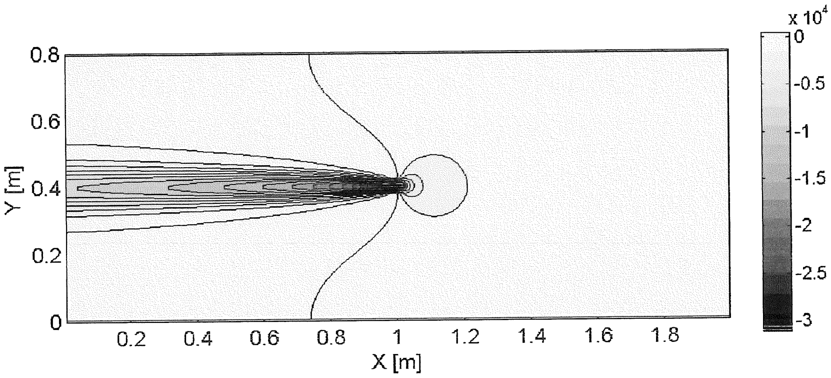

Fig. 2 Sensitivity of first-order temporal moment to Y at the center of the model.

migration velocities, reflecting the heterogeneous nature of the sample. Mean breakthrough time values, that will be used as conditioning data, are obtained by dividing sensor location x by the mean velocities $<v>$. Measurement errors could also be computed but were not included in this analysis.

Then, a two-well injection-recovery experiment was performed from piezometer P1 to piezometer P3, in order to simulate e.g. a pump-and-treat remediation system. First, a steady-state flow was established through the sample by imposing equal injection and pumping rates on P1 and P3 respectively. Concentration of the injected solution was then rapidly changed to a concentration C_0 (corresponding in this case to an electrical conductivity of the flowing solution of 3000 μScm^{-1}) and maintained during 900 s.

INVERSE MODELLING OF PERMEABILITIES

As the sensors were all installed at the same depth in the sample and as vertical transport could be neglected due to flow geometry, a 2D model was adopted to compute permeabilities. The flow domain was discretized into 200 × 80 square cells of 1 cm², leading to 16000 unknown values of the permeability.

Total porosity measurements were previously performed on a similarly compacted sample (Frippiat et al., 2004b). Using the empirical Kozeny-Carman formula, those porosity measurements were converted to (log)permeability values and a geostatistical analysis could be performed. A mean value of -9.48 was found, and an isotropic exponential correlation function with a variance of 0.076 and a correlation length of 15 cm could be fitted on the experimental correlogram. In order to reduce memory requirements and computational times, only the first row of the covariance matrix was explicitly computed and Fourier-transform methods were used to perform matrix products in Eqs. (6) and (7) (Nowak et al., 2003).

Sensitivities of temporal moments to Y were computed using the adjoint-state method proposed by Cirpka & Kitanidis (2001). A finite-element numerical model was developed according to their recommendations in order solve flow and (stationary) transport equations. As an example, Fig. 2 shows the sensitivity of the first-order moment (i.e. the mean breakthrough time) at the center of the domain. It was computed assuming no molecular diffusion, longitudinal and transverse dispersivities equal to the numerical grid, effective porosity n_e equal to 40 % and an homogeneous injection through the inlet boundary. Expectively, the sensitivity is mainly negative, as an increase in permeability leads to shorter mean breakthrough times. It also appears that the mean breakthrough time is mainly influenced by the permeability of a zone upstream of the sensor location, with a shape similar to that of a potential capture zone.

Fig. 3 shows the estimated permeability field assuming an unknown but constant mean Y field. A value of –9.77 for was found for this parameter, which is consistent with the value –9.48 previously obtained. Fig. 4 shows the corresponding variance. A sensitive reduction of

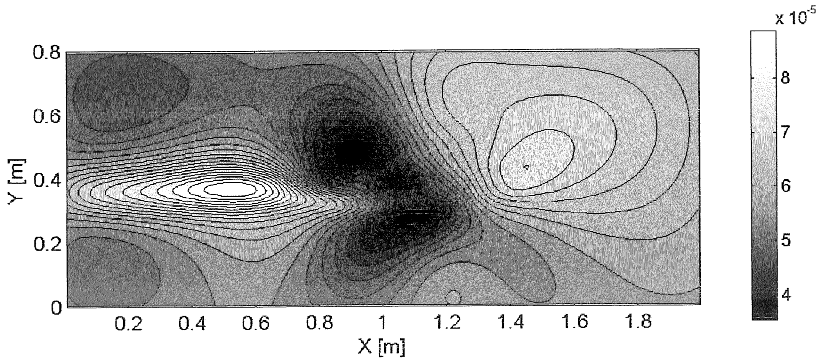

Fig. 3 Estimated permeability field (in ms^{-1}).

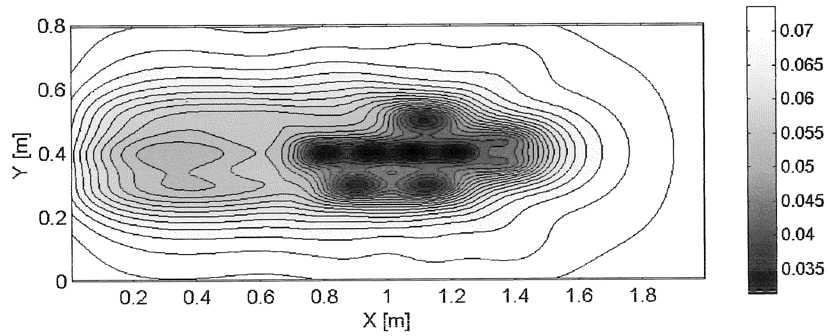

Fig. 4 *Y* variance reduction due to conditioning.

uncertainty in the direct vicinity of the sensors can be observed (up to 60 % of the initial variance), demonstrating the worth of having incorporated conditioning data. Fig. 5 (a) shows the experimental mean breakthrough times versus initial guesses (corresponding to a constant Y field of –9.48) and simulated values (corresponding to the permeability field shown on Fig. 3). While the mean error on velocities was initially about 18 %, the final value was about 4 %. Remaining discrepancies could have been even more reduced if one had incorporated the simultaneous estimation of structure parameters in the inverse modelling process (Kitanidis, 1995).

TWO-WELL INJECTION RECOVERY EXPERIMENT

Modflow® and MT3D® were then used to simulate the two-well injection-recovery experiment in the heterogeneous case. As injection and pumping rates *Q* were difficult to maintain during the experiment, this parameter was adjusted in order to correctly simulate first arrival time at the pumping well. A value of 0.288 $lmin^{-1}$ was found, whereas the mean experimental value was about 0.378 $lmin^{-1}$. Such a relatively high discrepancy could be explained (1) by the experimental errors occurring when monitoring and measuring pumping rates and (2) by the effective porosity, which was not measured and could be higher than 40 %. Apparent longitudinal dispersivity had to be increased to 1.5 cm in order to properly simulate the slope of the breakthrough curve. Fig. 5(b) shows the general agreement between experimental and numerical curves.

CONCLUSION

One-dimensional tests performed on a 2 m long manually compacted sand sample revealed spatial variations in apparent migration velocity. Those measurements were used to determine the spatial pattern of the permeability field. The iterative cokriging method was applied and

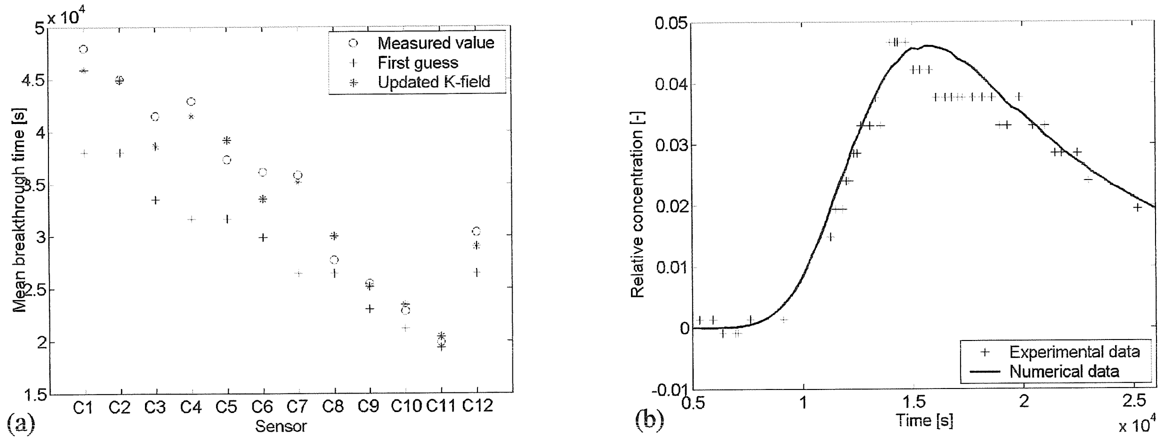

Fig. 5 Modelling of transport experiments (a) one-dimensional test and (b) breakthrough curve at the recovery well during two-well experiment.

yielded an heterogeneous K field that could account for most of the advective transport variations. A two-well injection-recovery experiment was also performed and was confronted to a numerical simulation involving the previously determined heterogeneous K field. Provided that pumping rates and apparent dispersivity were adjusted, a good matching of breakthrough curves could be reached.

Further developments will involve the simultaneous determination of the variance and correlation length in the inverse modelling procedure, and the investigation of the effect of the correlation function. Measurements errors should also be incorporated in the analysis. Finally, Monte Carlo simulations on equiprobable conditional realizations of the permeability field should be performed in order to assess uncertainty on predicted breakthrough curves.

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REFERENCES

Cirpka, O. A. & Kitanidis, P. K. (2001) Sensitivity of temporal moments calculated by the adjoint-state method and joint inversing of head and tracer data. *Advances in Water Resources* **24**, 89-103.

Dagan, G., Butera, I. & Grella, I. (1996) Impact of concentration measurements upon estimation of flow and transport parameters : The Lagrangian approach, *Water Resources Research* **32**(20), 297-306.

Deutsch, C. V. & Journel, A. G. (1998) *GSLIB : Geostatistical software library and user's guide*, 2nd ed., Oxford University Press, New York, 369p.

Frippiat, C., Wauters, B., Feller, V., Conde, P., Talbaoui, M. & Holeyman, A. (2004a) Physical and numerical modelling of 2-well tracer tests at the laboratory scale. In : *Engineering Geology for Infrastructure Planning in Europe*, Lecture Notes in Earth Science 104 (ed. by Hack et al.), Springer-Verlag, Berlin, 285-293.

Frippiat, C., Conde, P., Talbaoui, M. & Holeyman, A. (2004b) Influence de la structure du sous-sol pour l'interprétation d'essais de traçage (Influence of soil structure in the interpretation of tracer tests). In : *Géotechnique et Aménagement : Friches industrielles, côtes et "après-mines"*, JNGG Lille 2004, Lille, France, 131-141.

Harvey, C. F. & Gorelick, S. M. (1995) Mapping hydraulic conductivity : sequential conditioning with measurements of solute arrival time, hydraulic head, and local conductivity. *Water Resources Research* **31**(7), 1615-1626.

Hendricks Franssen, H.-J., Gomez-Hernandez, J. & Sahaquillo, A. (2003) Coupled inverse modelling of groundawater flow and mass transport and the worth of concentration data, *Journal of Hydrology* **281**, 281-295.

Kitanidis, P. K. (1995) Quasi-linear theory for inversing. *Water Resources Research* **32**(10), 2401-2409.

Nowak, W., Tenkleve, S. & Cirpka, O. A. (2003) Efficient computation of linearized cross-covariance and auto-covariance matrices of interdependent quantities. *Mathematical Geology* **35**(1), 53-66.

Sun N.-Z. (1994) *Inverse Problems in Groundwater Modelling*. Kluwer Academic Publishers, the Netherlands, 364 p.

Yu, C., Warrick, A. W. & Conklin, M. H. (1999) A moment method for analysing breakthrough curves of step inputs. *Water Resources Research* **35**(11), 3567-3572.