

# Integrating geophysical and tracer test data for accurate solute transport modelling in heterogeneous porous media

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**Abstract** Aquifer heterogeneity has a critical influence on the motion of water and contaminants in the underground. To optimise remediation techniques or to delineate protection zones, heterogeneity has to be quantified as accurately as possible. Geophysical prospecting and tracer tests can provide useful information to be integrated ideally in transport models. Integration of tomographic geophysical data in a conditioned stochastic generation of hydraulic conductivity fields can yield spatial correlation structure information that is normally not available. Associated with an inverse modelling procedure, it is shown that it has a non negligible impact on computed advective transport results and uncertainty.

Calibration of a transport model on results from tracer tests is often done in a lumped way by considering hypothetical sorption/desorption processes or by an arbitrary reduction of the injection quantity (peak concentration scaling). Improvements in the way of modelling actual injection conditions are proposed. It is shown, on practical cases, how simulating the actual contaminant input function with a better physical consistency can influence considerably the computed transport results.

**Key words** heterogeneity; geophysical prospecting; conditioned stochastic simulation and co-simulation; hydraulic conductivity; tracer test; injection function; transport modelling

## INTRODUCTION

Natural heterogeneity and spatial variability of hydrogeological parameters create much of the problem for optimisation of subsurface remediation. A clear field site characterisation is needed in order to be able to propose efficient remediation and/or protection scheme. For this purpose, an accurate description of the spatial heterogeneity and an accurate evaluation of transport processes (identification and quantification) are needed. In this work, two research topics are presented, aiming to obtain a reliable characterisation of aquifer heterogeneity and quantification of transport parameters using ideally the available data. First, a methodology for integrating information from geophysical tomographic measurements in a stochastic generation process of the hydraulic conductivity field, coupled to an inverse modelling procedure, is described. It is shown that the integration of geoelectrical measured data yields spatial correlation structure information having an impact on computed transport results. Second, starting from the observation that field tracer tests results are often dramatically influenced by injection conditions, improvements in the interpretation are

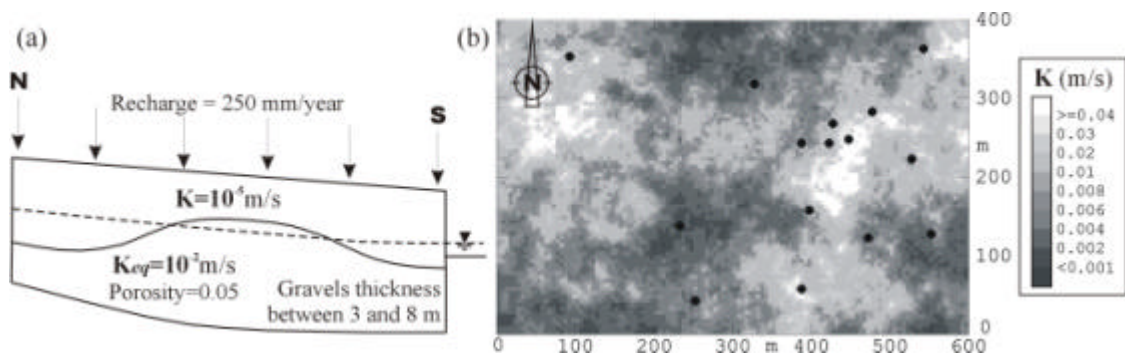
proposed using a accurate modelling of the actual tracer input in the aquifer (Brouyère, 2000). Typical results are shown to illustrate the importance of these improvements for a better assessment of transport processes and parameters through the interpretation of tracer tests.

## INTEGRATING GEOPHYSICAL DATA

### Background and synthetic case

Most of the spreading of solutes in porous aquifers is governed by the spatial variability of hydraulic conductivity ( $K$ ). To account for its irregular variation and for uncertainty of its distribution, stochastic models regard the  $K$ -field as random (Dagan, 1998). In practice however, due to the few available measurements of  $K$ -values (hard data), it can be useful to integrate soft data, like geophysical data, in the conditional stochastic generation of  $K$ -fields in order to improve characterization of the porous medium. In a stochastic framework, this allows reducing the variance of the distribution and consequently decreasing the uncertainty of the results. Some authors like Mc Kenna & Poeter (1995) take soft data into account by defining them as conditional data with an associated degree of uncertainty. This uncertainty is assessed comparing values of hard and soft data at particular points where they are both available. In such a way, Anderson (1997) has integrated seismic tomographic data in groundwater models.

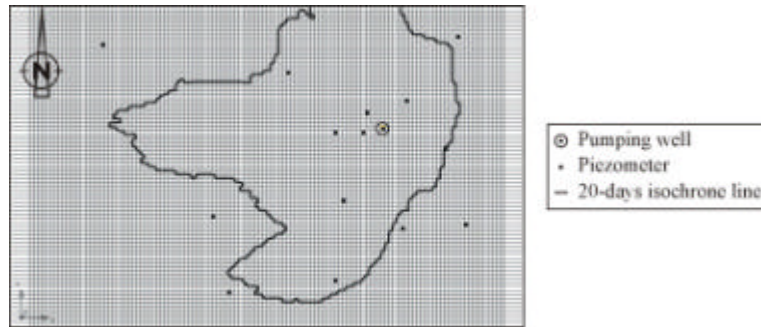
The methodology developed in this work integrate geoelectrical tomographic data, in addition to hard data, to generate directly fully compatible and equiprobable  $K$ -fields. These  $K$ -fields will then be introduced in an inverse modelling procedure in order to optimise the  $K$ -values. To do so, three data sets are needed:  $K$ -measurements (hard data), geoelectrical resistivity values (soft data) and piezometric heads (for the inverse procedure). For the purpose of the demonstration, a synthetic but realistic case has been designed (Fig. 1a) : a synthetic  $K$ -map has been created (Fig. 1b) by generating a non-conditional simulation based on the  $\ln K$  variogram found for the alluvial sediments of the Meuse River valley downwards to Liège (Belgium). 15 virtual piezometers and wells were then located on the map and the  $K$ -value directly read on the non-conditional simulation was attributed to each of them, providing the hard data set.



**Fig. 1** Synthetic case: (a) hydraulic conditions and (b) reference  $K$ -map with the 15 virtual piezometers (black points)

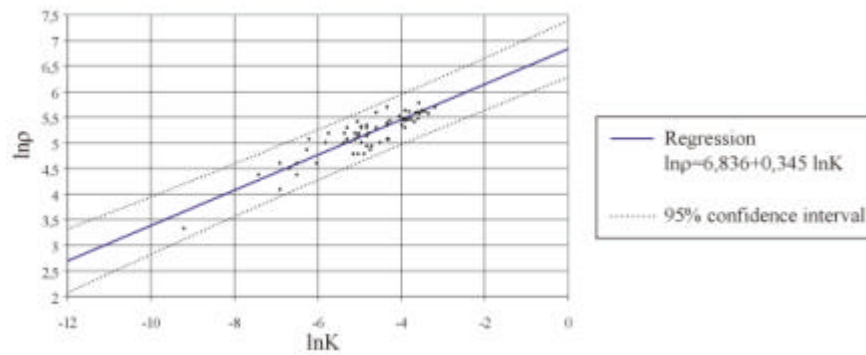
Then a pure deterministic groundwater flow computation, considering a pumping of  $60 \text{ m}^3/\text{h}$  at the well and lateral prescribed piezometric heads (at a distance of 600 m from both eastern and western sides), provided the synthetic ‘measured’ piezometric levels.

Considering only advective transport time to the well, the 20-days isochrone line was also computed (Fig. 2) and used as reference for further comparisons.



**Fig. 2** Synthetic case: computed isochrone for 20 days advective transport time.

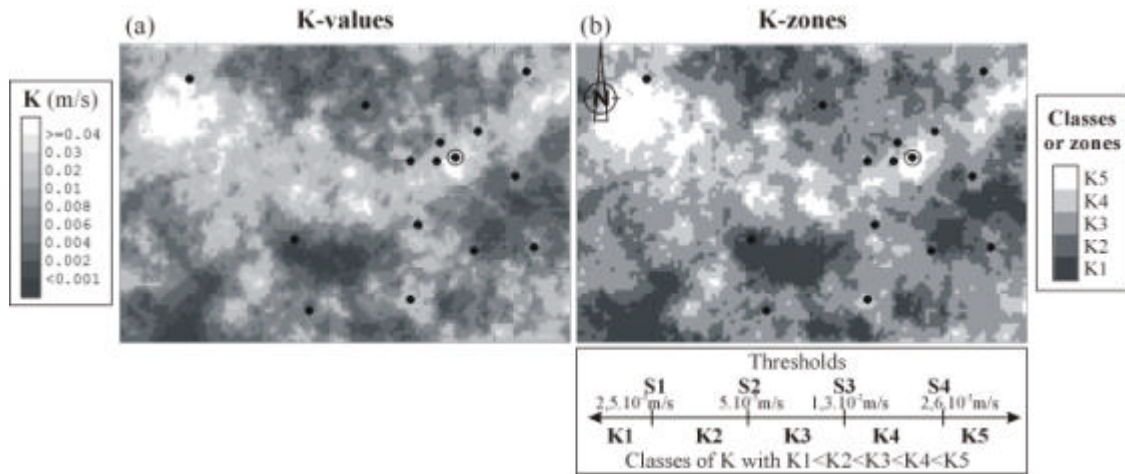
The resistivity data set was created based on the observed correlation between electrical resistivity and  $K$ -values in the alluvial sediments of the Meuse River (Fig. 3). The resistivity values were estimated by choosing random values within the calculated 95% confidence interval.



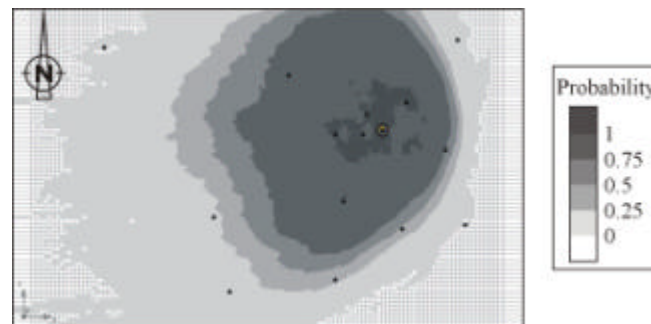
**Fig. 3** Observed correlation between electrical resistivity and  $K$ -values in the alluvial sediments of the Meuse River.

### Stochastic generation of $K$ -fields combined to inverse modelling

According to Monte Carlo analysis, 200 equiprobable realisations of the  $K$ -field conditioned on the 15 measured  $K$ -values were generated stochastically. Figure 4a shows an example of one of these. As well known in the literature, simulations better reproduce spatial variability of the property in an heterogeneous porous medium than kriging. On the basis of chosen threshold values, different classes of uniform  $K$ -values were distinguished (Fig. 4b) by applying a method derived from the Gaussian thresholds method (Matheron et al., 1987; de Marsily et al., 1998; Koltermann & Gorelick, 1996). In order to optimise the  $K$ -value of each class (or zone), these 200  $K$ -fields were then introduced one by one in an inverse modelling procedure (PEST code, Doherty, 1994) using the piezometric head data set. Finally the 200 realisations of optimised  $K$ -values were considered for advective transport computation. For each of them, a 20-days isochrone line was determined using a particle tracking algorithm. The spatial probability distribution of this isochrone line was then calculated for all realisations (Fig. 5) and compared to the ‘reality’ described in figure 2.



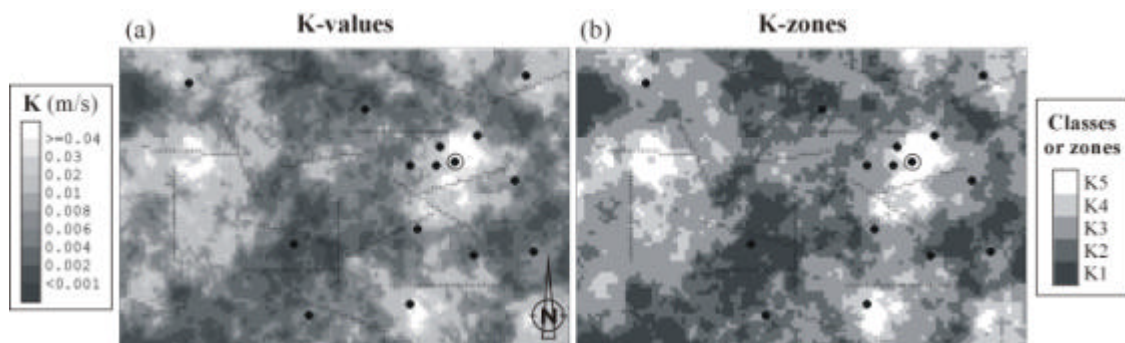
**Fig. 4** Conditional simulations (without soft data): (a) example of a generated  $K$ -field and (b) obtained distribution of the  $K$ -zones with four threshold values of  $K$ :  $2.5 \cdot 10^{-3}$ ;  $5 \cdot 10^{-3}$ ;  $1.3 \cdot 10^{-2}$  and  $2.6 \cdot 10^{-2}$  m/s.



**Fig. 5** Conditional simulations (without soft data): spatial probability distribution of the 20-days isochrone line on the basis of 200 realisations.

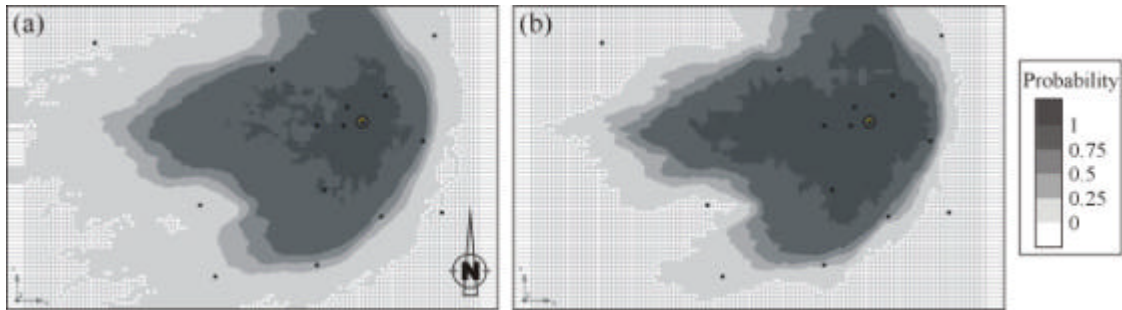
### Additional conditioning by geoelectrical resistivity data

It was suggested by Hubbard *et al.* (1998), that collection and interpretation of tomographic profiles together with limited well-bore data can yield spatial correlation structure information that is traditionally only obtainable by performing extensive and intrusive hydrogeological sampling. In order to generate equiprobable  $K$ -fields integrating directly soft data, a data set of 400 resistivity values, distributed on 16 tomographic profiles, were introduced as additional conditioning data. 200 co-simulations were generated, each of them being conditioned on  $K$ -values (hard data) and resistivity values (soft data) by a cokriging technique. Figure 6a shows an example of one of them. The corresponding  $K$ -zones distribution is given on figure 6b.



**Fig. 6** Conditional co-simulations taking 400 geoelectrical resistivity data into account: (a) example of a generated  $K$ -field and (b) obtained distribution of the  $K$ -zones.

Following the same procedure as described in the previous paragraph, an advective 20-days isochrone line was computed for each of the 200 realisations. The spatial probability distribution based on these 200 isochrone lines was calculated (Fig. 7a). Comparing results of figure 7a to those of figure 5 (which were found without taking soft data into account), a clear improvement is observed in the description of the heterogeneity of the medium leading to more realistic isochrone lines with regards to the reference isochrone shown at figure 2. Figure 7b shows the probability distribution of the 20-days isochrone line found by selecting a restricted number of realisations. 50 realisations were chosen applying the following criteria: (1) a realisation was eliminated if, at the end of the inverse procedure, the relative order of the  $K$ -values of the zones (defined previously  $K_1$  to  $K_5$ ) was not respected; (2) among the remaining realisations, the “best” ones were selected based on the value of a calculated objective function. The use of these criterion reduces the uncertainty of the probability distribution.



**Fig. 7** Conditional co-simulation (with soft data): probability distribution of the 20-days isochrone line (a) on the basis of 200 realisations and (b) on the basis of the 50 “best” realisations (statistically, this spatial probability distribution is not to be compared to those of figures 5 & 7a because it is based on 50 realisations instead of 200)

## MODELLING THE INJECTION OF TRACERS

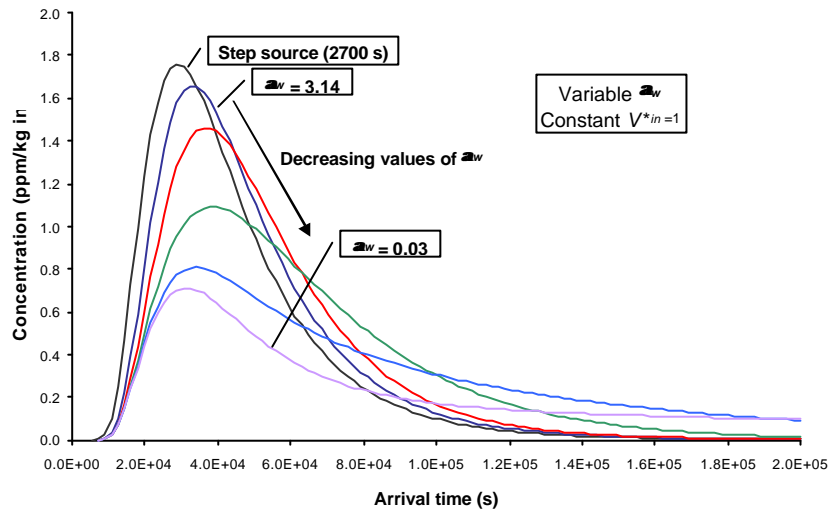
Injection duration and flow rates can play a significant role on tracer test results (Guvanasen & Guvanasen, 1987, Brouyère & Rentier, 1997) but they are usually under control. Besides that, many physical factors mainly related to well aquifer interactions can cause the tracer entry function to depart from theoretical injection profiles, inducing a misleading interpretation. First, a dilution of the tracer occurs in the injection well, resulting in lower recovery peaks at the pumping well (Novakowski, 1992). This effect is usually quantified by a mixing factor expressing the ratio between the volume of injected tracer water  $V_{in}$  and the volume of water initially in the well  $V_w$ :  $V_{in}^* = V_{in}/V_w$ . Second, according to local hydraulic properties (well equipment, aquifer material compaction around the well,...), a local distortion of the flow field can be observed close to the well. This effect is usually considered through a lumping distortion coefficient ( $\alpha_w$ ) expressing the ratio between the actual and theoretical water flow rates crossing the well section orthogonal to the main flow direction. Provided that the hydraulic characteristics of the well and surrounding aquifer are known, the flow distortion coefficient can be evaluated (Drost *et al.*, 1968, Bidaux & Tsang, 1991).

The conceptual model, numerical developments and experimental validation are proposed by Brouyère (2000, 2001). Using this approach, the modelling of a synthetic radially converging tracer test allows to check how injection conditions can influence tracer test results and their



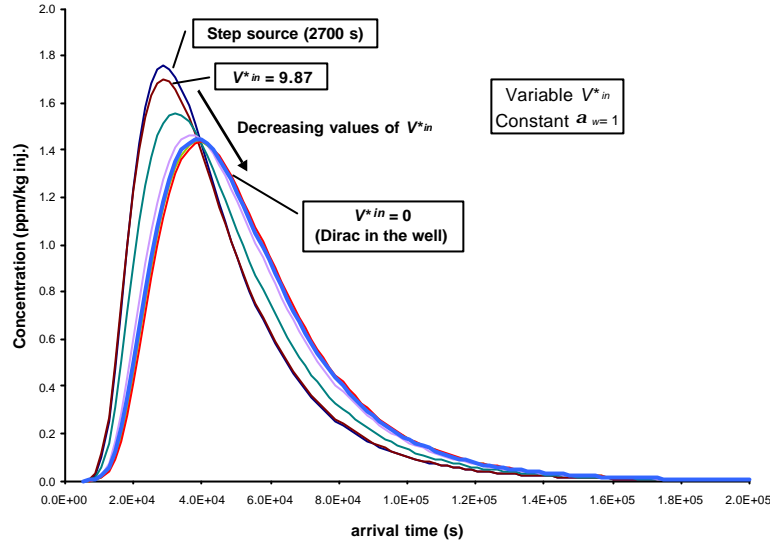
interpretation. A confined aquifer of a thickness of 8 m is characterised by a saturated conductivity of  $5.0 \times 10^{-2} \text{ m.s}^{-1}$ , an effective porosity of 0.05, a longitudinal dispersivity of 2 m and a transverse dispersivity of 0.5 m. The tracer is completely conservative. Initial total heads are uniformly at 10 m. A flow rate of  $50 \text{ m}^3.\text{h}^{-1}$  is pumped out a central well. The injection well is located 20 m away from the pumping well. The injection well and the pumping well radii are respectively of 7.5 and 10 cm. In the injection well, the water column is supposed to be constant (8m).

The tracer injection duration is 2700 s, allowing an accurate visualisation of the concentration evolution (previous tests have shown that this can still be assimilated to a Dirac injection in the aquifer). After the injection, the tracer quantity remaining in the injection well is progressively washed out by the transit flow rate crossing the screens. A series of breakthrough curves were generated by varying both the mixing factor (therefore the tracer water volume) from 0 (Dirac-type tracer input in the injection well) to 10 and the distortion coefficient from 0.01 to 3.14. In figure 8, the breakthrough curves generated with a constant mixing factor  $V_{in}^* = 1$  and a variable distortion coefficient are shown. In figure 9, the distortion coefficient is set to 1 and the mixing factor is varied. These two examples clearly illustrate how important is the influence of injection conditions on tracer test results.



**Fig. 8.** Resulting breakthrough curve for different values of the distortion coefficient ( $\alpha_w$ ) and a constant mixing factor ( $V_{in}^*$ ).

In a second step, assuming that the aquifer hydrodispersive parameters are unknown, a classical transport model (neglecting the influence of injection conditions) was ‘calibrated’ by a trial and error fitting of the breakthrough curves. To do so, the injection is simulated by a classical source step function of 2700 s, fitting the effective porosity and the longitudinal dispersivity values. Additionally, if no satisfactory calibration could be reached, a dual porosity effect was introduced in order to obtain a better fit. This is particularly necessary for breakthrough curves showing strong tailing and concentration peak attenuation. Fitted parameters are summarised in Table 1.



**Fig. 9.** Resulting breakthrough curve for different values of the mixing factor ( $V_{in}^*$ ) and a constant distortion coefficient ( $a_v$ ).

**Table 1.** Hydrodispersive parameters obtained by calibration of a transport model on the breakthrough curves, without taking the actual injection conditions into account.

$a_v$		0.03	0.10	0.32	1.0	3.14	Truth
$V_{in}^* = 1$	$q_n$ (-)	0.067	0.065	0.072	0.061	0.054	0.05
	$a$ (m)	3.0	4.5	2.67	1.88	1.85	2.0
	$q_m$ (-)	0.15	0.035	--	--	--	--
	$a$ (s <sup>-1</sup> )	$1.03 \times 10^{-6}$	$1.0 \times 10^{-6}$	--	--	--	--
$V_{in}^*$		0 (Dirac)	0.1	0.32	1	3.14	9.87
$a_v = 1$	$q_n$ (-)	0.063	0.063	0.063	0.061	0.055	0.05
	$a$ (m)	1.80	1.80	1.80	1.88	2.06	2.15
	$q_m$ (-)	--	--	--	--	0.03	0.04
	$a$ (s <sup>-1</sup> )	--	--	--	--	$3.0 \times 10^{-9}$	$5.0 \times 10^{-9}$

$q_n$  = mobile water porosity or effective porosity  
 $a$  = longitudinal dispersivity

$q_m$  = immobile water porosity  
 $a$  = first order transfer coefficient

It appears clearly that neglecting the influence of the actual injection conditions can lead to two types of errors: (a) the values of the fitted parameters can be far from reality (see the obtained values for the effective porosity and the dispersivity with respect to the actual values); (b) the identification of the main active transport processes can be misled. Indeed, in some cases, the observed long tailing and attenuation could be erroneously attributed to the occurrence of a dual porosity effect or a kinetic sorption process when actually they are the result of a delayed release of the tracer remaining in the well at the end of the injection. In terms of remediation, this can lead to a misleading interpretation of the transport conditions, inducing major differences in the chosen methodology and consequently for its efficiency.

## CONCLUSIONS

Two research topics aiming to a better characterisation of field sites for accurate modelling of groundwater flow and transport conditions were presented. Integrating geoelectrical tomographic profiles in a stochastic generation process of the  $K$ -field yields spatial correlation structure information. Coupled to an inverse modelling procedure, and applying logical “quality” criteria for the selection of the “best” realisations of the  $K$ -field, it leads to an accurate description of the heterogeneity of the medium and to realistic advective isochrones. Another important issue is addressed involving a better modelling of the actual injection function for tracer tests. Describing more physically the complex well-aquifer interactions, leads to more reliable interpretation of tracer tests and estimation of the transport parameters of a studied zone. Results are shown illustrating the influence of these interactions on the measured breakthrough curves. It can be of overwhelming importance for defining optimal remediation techniques.

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## REFERENCES

- Anderson M.P. (1997) Characterization of geological heterogeneity. In: *Subsurface flow and transport* (Proc. of the Kovac's Colloquium), 23-43
- Bidaux, P. & Tsang, C.-F. (1991) Fluid flow patterns around a well bore or an underground drift with complex skin effects. *Water Resour. Res.* **27**(11), 2993-3008.
- Brouyère, S. (2000) Modelling the injection of a tracer in a well : a new mathematical and numerical approach. In *Tracers and Modelling in Hydrogeology* (ed. By A.Dassargues) (Proc. of the TraM'2000 Conference), 25-31. IAHS Publ. n°262.
- Brouyère, S. (2001) Study and modelling of transport and retardation of solutes in variably saturated media. PhD Thesis. University of Liège, 397 p.
- Brouyère, S. & Rentier, C. (1997) About the influence of the injection mode on tracer test results. In: *Tracer Hydrology 97* (ed. by A.Kranjc), 11-17. A.A.Balkema, Rotterdam.
- Dagan, G. (1998) Solute concentration fluctuations in aquifer transport: theory, simulations and field experiments. *Groundwater Quality: Remediation and Protection* (eds M.Herbert & K.Kovar) (Proc. of the GQ'98 Conference), 575-582. IAHS Publ. n°250.
- de Marsily, G., Schafmeister, M.T., Delay, F. and Teles V. (1998) On some current methods to represent the heterogeneity of natural media in hydrogeology. *Hydrogeology Journal* **6**, 115-130.
- Doherty, J. (1994) PEST. Watermark Computing, Corinda, Australia, 122 p.
- Drost, W., Klotz, D., Arnd, K., Heribert, M., Neumaier, F., Rauert, W. (1968) Point dilution methods for investigating ground water flow by means of radioisotopes. *Water Resour. Res.* **4**(1), 125-146.
- Guvanasen, V. & Guvanasen, V. M. (1987) An approximate semi-analytical solution for tracer injection tests in a confined aquifer with a radially converging flow field and a finite volume of tracer and chase fluid. *Water Resour. Res.* **23**(8), 1607-1619.
- Hubbard, S., Rubin Y. and Majer, E. (1998) Estimation of hydrogeological parameters and their spatial correlation structures using geophysical methods. *Groundwater Quality: Remediation and Protection* (eds M.Herbert & K. Kovar) (Proceedings of the GQ'98 Conference), 503-512. IAHS Publ. n°250.
- Koltermann, Ch.E. & Gorelick, S.M. (1996) Heterogeneity in sedimentary deposits: A review of structure-imitating, process-imitating and descriptive approaches. *Water Resour. Res.* **32**(9), 2617-2658.
- Matheron, G., Beucher, H., de Fouquet, C., Galli, A., Guerillot, D. and Ravenne C. (1987) Conditional simulation of the geometry of fluvial-deltaï c reservoirs. *Society of Petroleum Engineers* SPE 16753
- Mc Kenna, S.A. & Poeter, E.P. (1995) Field example of data fusion in site characterization. *Water Resour. Res.* **31**(12), 3229-3240.
- Novakowski, K. (1992) An evaluation of boundary conditions for one-dimensional solute transport, 1. Mathematical development. *Water Resour. Res.* **28**(9), 2399-2410.