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Interpretation and modelling of multi-tracer tests in heterogeneous geological media

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Abstract Quantifying aquifer heterogeneity is critical for understanding contaminant movement and impacts of remediation techniques and for delineating protection zones in accordance with different regulations. To quantify aquifer heterogeneity, different methodologies can be proposed having common research steps including: (1) geological and hydrogeological characterization based on geology, hydrology, morphostructural geology and shallow geophysical prospecting, (2) multi-tracer tests with artificial 'ideal' tracers, and (3) numerical modeling of groundwater flow and the transport conditions. For (3), the model requires an accurate calibration using piezometric measurements for groundwater flow and measured breakthrough curves for transport of solute contaminant. The spatial distribution of the calibrated permeability values is strongly influenced by pumping test results, and by geological, geophysical and hydrological characterizations. The shape and the characteristics of each computed breakthrough curve is fitted on the corresponding experimental curve, so that the spatial distribution of the transport parameters can be assessed. The detected spatial variability (laterally and/or vertically) can justify fully that the heterogeneity should be invoked to explain late arrivals of tracers. However, the vertical variability may induce effects on the breakthrough curve which can also be represented and simulated by lateral heterogeneities. In this paper, examples are given of the computation of aquifer heterogeneity using results from multi-tracer tests in fissured and porous heterogeneous media. The tests are simulated using detailed finite-element models representing the heterogeneous medium including the spatial distribution of parameter values consistent with the geology, hydrology, morphostructural geology, and geophysical prospecting characterizations.

INTRODUCTION

Current concerns over groundwater contamination have motivated applied researches to improve methods for accurately describing and predicting groundwater solute transport. Despite important theoretical and practical progress, adequate characterization of the variability of aquifer properties which considers heterogeneous groundwater flow and transport numerical simulations is difficult. There are two main options that include geostatistical methods and a deterministic framework, using both 'hard data', such as borehole descriptions, and results of direct measurements or tests, and 'soft data', such as geological or geophysical characterizations/interpretations. To statistically assess flow and transport variability, as determined from geology, is certainly not easy. As mentioned by Anderson (1995), "numerous theoretical papers have been published based on a stochastic description of aquifer heterogeneity (Neuman, 1982; Sudicky & Huyakorn, 1991; Yeh, 1992,....) but the central question of whether the stochastic method, which treats aquifer heterogeneity as a random field, is applicable to real aquifers under field conditions, has not been definitively answered." Focusing on the effective transfer time of contaminant, a methodology has been proposed for studying protection zones around pumping wells in a pure deterministic framework (Dassargues, 1995). This methodology consists of: (a) characterization of the geological and hydrogeological conditions based on a complete set of data consisting of geology, hydrogeology, hydrology, morphostructural geology and shallow geophysical prospecting, (b) experimental tracer tests with artificial tracers, (c) modelling groundwater flow conditions with calibration on the measured piezometric surface under both natural and pumping conditions, (d) modelling transport of dissolved contaminants with calibration on measured breakthrough curves, (e) simulations of transport using calibrated and then upscaled parameters, with injections from different places to compute contaminant arrival time at the pumping well, (f) delineation of protection zones based on computed travel times and considering local regulations.

This paper briefly describes some of the difficulties encountered when applying steps (d) and (e) of this methodology and focuses on interpretation of tracer-test results that detail aquifer heterogeneity. Parameter determination by calibration of a flow and transport model (d) is always delicate, particularly regarding to the following difficulties: (1) the groundwater transport model may often induce numerical oscillations or numerical dispersion for conditions, as affected by mesh size, time steps, and excitations, (2) interpretation of measured breakthrough curves and calibration of a groundwater flow and transport model does not converge to one solution. Upscaling of calibrated transport parameters to simulate contaminant injections (e), is not straightforward. These difficulties are illustrated and discussed below.

INTERPRETATION AND MODELLING TRACER TESTS

Difficulties due to numerical dispersion

Classical finite-element or finite-difference methods are not efficient in solving the advection-diffusion equation, because these methods produce numerical dispersion and oscillations in the solution. The solution of the transport equation is fundamentally difficult because hyperbolic terms, representing the convection/advection, and parabolic terms, representing the dispersion, coexist. Numerical methods used to solve the transport equations may be classified into three categories: (1) Eulerian methods, in which a Eulerian form of the equation is solved at the nodes of a fixed grid, require the simultaneous solution of hyperbolic and parabolic terms; (2) Lagrangian methods, in which a Lagrangian form of the equation is solved in grids moving with the fluid, avoid explicit treatment of hyperbolic terms, but often the grid gradually becomes distorted and subsequent computation of partial derivatives is complicated; (3) Eulerian-Lagrangian methods combine the best aspects of the two other categories. This paper does not focus on describing numerical techniques used to solve the transport and flow equations, but when using groundwater transport models, some awareness of numerical problems is needed. For the first category of methods, numerical engineers provide guidance for grid and time-step selection to avoid truncation errors and subsequent numerical dispersion. Expressed in terms of numerical Peclet (*Pe*) and Courant (*Cr*) numbers, the governing equations are:

$$\frac{|\underline{v}| \cdot \Delta l}{D_L} < \; < 2 \Rightarrow Pe < \; < 2 \quad \text{and} \quad \frac{|\underline{v}| \cdot \Delta t}{\Delta l} \leq 1 \Rightarrow Cr \leq 1 \qquad (1)$$

where in 1D, diffusion is dominated by dispersion, so that $D_L = a_L \cdot |\underline{v}|$ in the concerned direction, Δl is the cell dimension or element in the concerned direction, is the time step, $\underline{v}$ is the vector of effective velocity (Darcy's specific discharge divided by effective porosity), D is the component of the mechanical dispersion tensor $\underline{\underline{D}}$ for the solute in the porous medium, and a_L is the longitudinal dispersivity coefficient. In practice, different mesh sizes are used in the finite-element or finite-difference grids to, for example, accurately represent geometrical characteristics of the aquifer, boundaries, piezometers, and pumping wells. Effective velocity can vary markedly in the modelled domain because it is controlled by the prescribed pumping or recharge fluxes, and the effective porosity, i.e., heterogeneity in the modelled zone. In addition, heterogeneous conditions also can be chosen to describe the dispersion process in the medium, involving varying dispersivity coefficients. Consequently, it is difficult to obtain quasi-uniform Peclet and Courant numbers. However, in some zones of the model, conditions are ideal for providing a numerical solution, whereas in other zones, conditions are poor. Numerical dispersion may appear in these other zones, which are not easy to identify except when a model sensitivity analysis is performed.

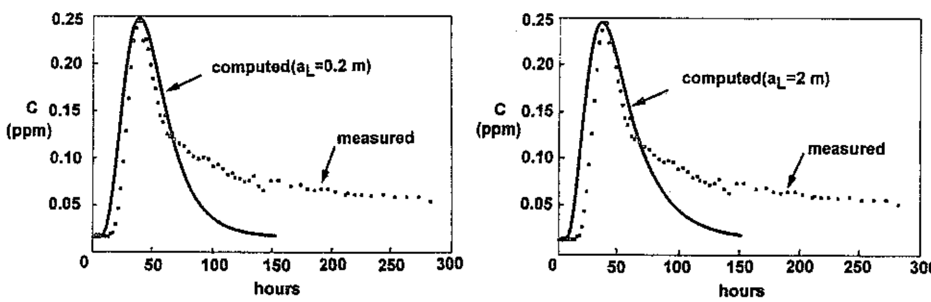

Fig. 1 Observed and computed breakthrough curves using a classical 'upstream' Eulerian method for $a_L = 2$ m and $a_L = 0.2$ m. A large part of the computed dispersion appears to be due to numerical dispersion.

Example

A tracer test was conducted in the alluvial plain of the Meuse River. The LiCl tracer was injected in the water table aquifer when the production well was under maximum pumping conditions. Breakthrough curves of lithium for this well and simulation results, using an Eulerian upstream method, show no significant changes (Fig. 1) with changing longitudinal dispersivity a_L = 2 m and a_L = 0.2 m). These results computed with a Peclet number higher than 2, in a few cells around the pumping well, show that the computed dispersion is largely due to the induced numerical dispersion. If the model does not provide a choice for the Eulerian-Lagrangian solving method, mesh size and time step must be decreased substantially to obtain $Pe < 2$ and $Cr < 1$ everywhere in the model. Results from an hybrid method of characteristics (Eulerian-Lagrangian method) with the same grid and time-step conditions as in Fig. 1, show clearly the effect of the dispersivity value on the computed breakthrough curve (Fig. 2).

Regardless, a sensitivity analysis of the main transport parameters is strongly recommended to avoid misinterpretation of the model results.

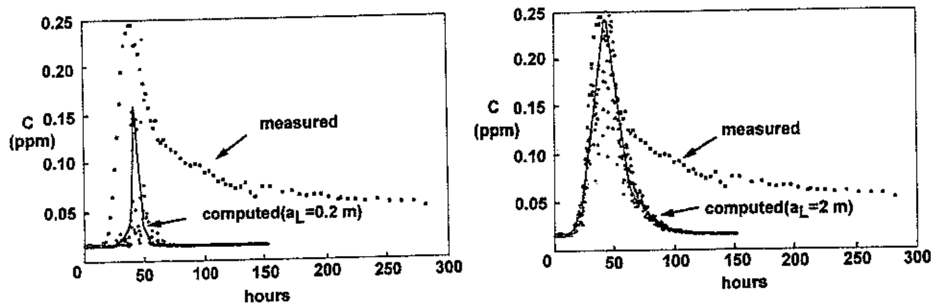

Fig. 2 Observed and computed breakthrough curves using an hybrid method of characteristics for a_L= 2 m and a_L= 0.2 m. The sensitivity of the results to is evident.

Calibration on a measured breakthrough curve

It is well known that the interpretation of a measured breakthrough curve can be multiple. Without 'hard' or 'soft' geological data, all situations of wrong/inconsistent interpretations, induced by 'automatic' calibrations that solve the inverse problem are difficult to identify. As an example, a 3D flow and transport model is applied to simulate tracer tests performed in 2D, i.e., depth averaged, conditions. Although a quasi-infinite number of suitable parameter combinations will allow the transport model to be calibrated, geological data provide information on the different geological layers that reduce the possible of model solutions. Within these strata, facies changes cause flow and transport to vary. Morphostructural analyses provide information on fracture zones in hardened formations or on other physical sedimentological features in loose sediments, and shallow geophysical surveys can augment the geological and morphostructural information. In fact, in the framework of a complete methodology as described here above, one can not choose freely the parameter spatial distributions. Only few of the model solutions are consistent with the 'hard' and 'soft' data.

Example

Comparisons can be made between computed breakthrough curves obtained by calibration of a 2D model on one hand, and by calibration of a 3D model on the other hand, for one set of tracer-test data. The tracer test, with iodide and LiCl injected in two different piezometers, was performed in depth-averaged conditions in the alluvial sediments of the Meuse River. The 2D interpretation, which used the finite-element program AQUA2D (Vatnaskil Consulting Engineers), applies an upstream Eulerian schema to solve the 2D transport equation. The finite-element program SUFT3D developed at the LGIH University of Liège (Dassargues, 1994) with upstream Eulerian and Hybrid Eulerian-Lagrangian schema also is used. The 3D model is applied to three layers corresponding to the different alluvial deposits, i.e., gravels containing different percentages of sand. Values for the main parameters in the vicinity of the pumping well for both 2D and 3D models are listed in Table 1. Corresponding breakthrough curves are shown in Fig. 3 for iodide tracer. In this case, 2D modelling underestimates longitudinal dispersivity, which is attributed to numerical dispersion as explained above. The 3D modelling offers more freedom: (1) to describe the heterogeneity and the spatial variability of the parameters, (2) to simulate the injection of the tracer, and (3) to simulate the arrival of the tracer in the pumping well. With this 3D model, acceptable calibrations occur with many different parameter sets. The hydrogeologist must choose which parameter set is most consistent with the 'hard' and 'soft'geological data. In this case, due to the distinctly different hydraulic conductivities and effective porosities of the various layers of the 3D model, the shape of the breakthrough curve before the tracer maximum is better simulated than with the 2D model. In the case of a more complex measured breakthrough curve as shown in Fig. 4 for lithium, the 2D model can only simulate one of the two measured maxima, whereas the 3D model can be calibrated for each maximum, using different values of flow and transport in the different layers (Table 2).

Table 1 Calibrated parameters of the computed breakthrough curves of Fig. 3.

Model	K (m s^{-1})	n_e	a_L (m)	a_T (m)
2D	0.215	0.048	0.01	0.003
3D, Layer 1	0.027	0.07	1.5	0.15
3D, Layer 2	0.0027	0.07	0.5	0.05
3D, Layer 3	0.0027	0.075	1.5	0.05

Table 2 Parameters of the computed breakthrough curves of Fig. 4.

Model	K (m s^{-1})	n_e	a_L (m)	a_T (m)
2D	0.215	0.058	0.01	0.003
3D, Layer 1	0.027	0.07	1.5	0.3
3D, Layer 2	0.0027	0.07	0.8	0.05
3D, Layer 3	0.0027	0.075	5	1

UPSCALING TRANSPORT PARAMETERS

Difficulties and issues

According to local regulations in Belgium, two main protection zones need to be

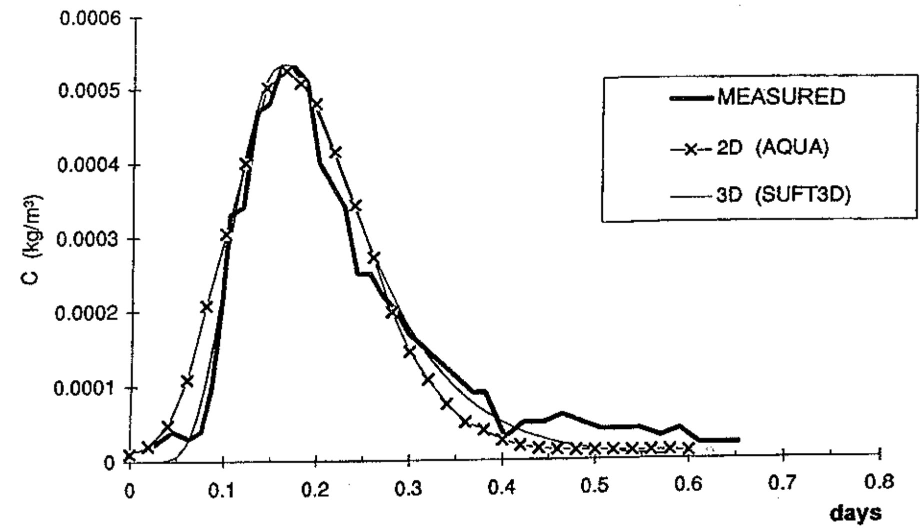

Fig. 3 Observed and computed breakthrough curves using the AQUA2D and SUFT3D models.

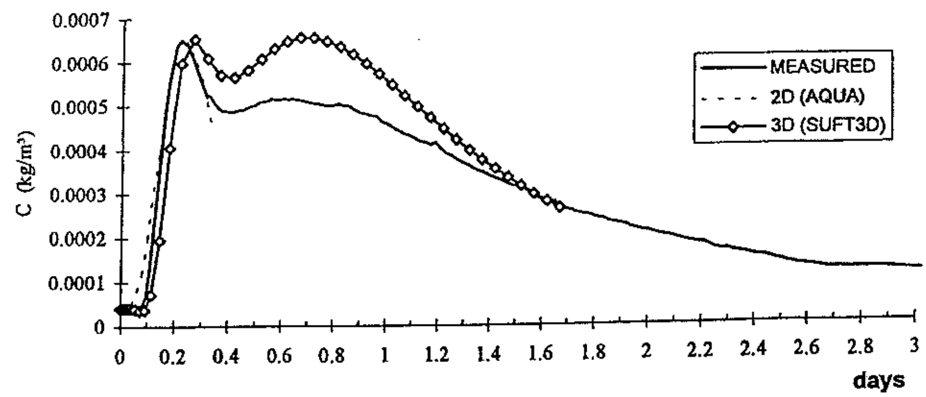

Fig. 4 Observed and computed breakthrough curves usnig the AQUA2D and SUFT3D models.

defined based on contaminant travel time in the saturated zone: (1) "zone IIa" corresponding to 1 d travel time, and (2) "zone IIb" corresponding to 50 d. Applying the methodology described herein, groundwater flow and transport parameters are obtained at a scale corresponding to travel times from a few hours to two weeks. Dispersivity is affected by scale. In fact, two trends are observed in the way that dispersion is included in the models. First, heterogeneity of the modelled domain is not fully described but 'lumped' into a macro-dispersion term. The corresponding dispersivity coefficients are not physically consistent, but they statistically represent the general behavior of the contaminant around its advective mean position. The main advantage of this method is that smaller scale heterogeneities are not known in detail.

The main problem, therefore, is upscaling, because scale effects the detail of the heterogeneities. In the second approach, heterogeneities are accounted for explicitly by varying permeability and effective porosity. In that approach, dispersivity derived from field investigations at a local scale do not have to be upscaled because they are assumed to be representative at the scale used in the model. This latter approach is used here and applied for protection-zone computations. For determination of the 1-d isochrone lines, no major extrapolation of the groundwater flow and transport parameters are needed. However, for computing the 50 day isochrone lines, all of the lithological, morphostructural, geophysical and hydrological data must be integrated. This is a pure deterministic procedure which assumes that the zones, in which preferential flowpaths occur at the scale of the chosen REV, can be detected deterministically and with sufficient spatial resolution.

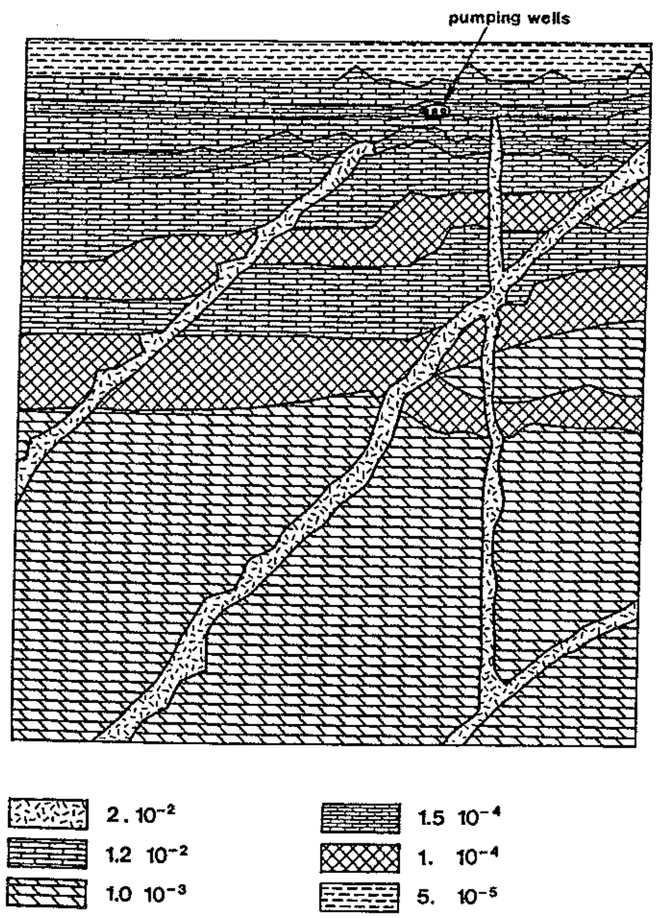

Fig. 5 Map of the transmissivity values ($m^2 s^{-1}$) from calibration at the local scale near the pumping wells and from extrapolation based on geology for the larger scale.

Example

The case described here is located in calcareous layers which are oriented East-West with a 80¡ dip and the northern part of the zone is limited by less pervious layers. Heterogeneities are related to the more fractured/karstified zones detected from a suite of field and laboratory data including 25 boreholes, geophysical methods, and morphostructural analysis, and a piezometric map generated from these data. The local 2D horizontal model using AQUA2D program (Vatnaskil Consulting Engineers) is composed of triangular finite elements with edges ranging from 5 to 100 m. In the fitting process, attention was given to the geological significance of any value or distribution change for flow and transport parameters. As a result of the model calibration on the measured flow and transport, transmissivity was mapped (Fig. 5), and an adjusted anisotropy factor of 0.67 was included to improve the fit of longitudinal hydraulic conductivity along the bank direction.

The predicted transport parameters are as follows:

- n_e=0.01, a_l=30m and a_T/a_L=0.04 extrapolated to the unfractured zones;
- n_e=0.08, a_l=8m and a_T/a_L=0.04 for the main fractured zones (affected by $K = 2 \times 10^{-2}$ m s^{-1}, Fig. 5) as revealed by the geophysical and morphostructural studies. Transport parameters fitted during the calibration on the measured breakthrough curves are only representative for the local-scale transport model. Because no other information is available to upscale the dispersivity values, the extrapolation mainly occurs by introducing detailed transmissivity values over the entire modelled domain. Of course, this extrapolation takes into account the knowledge about geology. Accordingly, no real upscaling of the dispersivity values is performed. Rather, the upscaling is replaced by a highly variable, but geologically consistent, distribution of the transmissivity values added to a simple extrapolation of the calibrated values of the transport parameters.

CONCLUSIONS

After a comprehensive site characterization, including geology, morphostructural geology, geophysical prospecting, and piezometer drilling, local heterogeneity of an aquifer can be characterized somewhat deterministically. However detailed and accurate the set of data, an REV approach must be considered in which the heterogeneity of the aquifer is to be described more or less globally with "equivalent" values for the parameters.

During calibration of the transport model, numerical dispersion can be an annoying factor which can affect the 'calibrated' values of the dispersivity. Consequently, it is essential (1) to perform a sensitivity analysis of the transport parameters and eventually, (2) to use alternate solving methods to minimize the effects of numerical dispersion.

Methods of calibrating flow and transport parameters can be strongly affected by the type of model, i.e., 2D or 3D, offering in theory a multitude of acceptable solutions. The choice between solutions must be consistent with all of the available 'hard' and 'soft' geological data.

If many of these geological data are available, the upscaling procedure for transport parameters can be replaced by a highly variable and consistent field of flow parameters. These highly heterogeneous flow conditions, associated with the extrapolated values of the calibrated dispersivity, will create macro-dispersion at the scale of the entire domain.

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