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From calibration on tracer test data to computation of protection zones: upscaling difficulties in a deterministic modelling framework

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Abstract In order to compute accurately the groundwater protection zones in each particular case and relating to the local hydrogeological conditions of each site, a methodology involving *in situ* tracer tests and flow-transport numerical simulations is commonly used. In the modelling approach, the parameters describing the aquifer (hydraulic conductivity, effective porosity, dispersivities, etc.) are chosen with "equivalent" and depth-averaged values on Representative Elementary Volumes (REV). The difficulty consists in finding a good agreement between the heterogeneous reality of the aquifer and its representation using this REV concept. In each case, calibration of the flow model on measured piezometric maps and calibration of the transport model on observed breakthrough curves (for each tracer) allow the deduction of local parameters of the aquifer. This determination has an advantage over classical analytical interpretations as the aquifer heterogeneity is taken into account for flow and transport parameters. The main problem then consists in obtaining significant parameters at the scale of the volume concerned by pollutant transfer times corresponding to the definition of the protection zones (e.g. 50 days). An upscaling procedure is often necessary and it strongly influences the expected reliability for protection zone computations. Results are shown from two case studies, where a manual upscaling technique is chosen, based on deterministic interpretations of the geological information.

INTRODUCTION

One of the biggest challenges in groundwater modelling is surely represented by the way of describing the effects of spatial variability on the values of the parameters to be entered in models. Quantifying aquifer heterogeneity is critical to understand the movement of contaminants, to study the possibility for their removal, to delineate protection zones around wells or water catchments, etc. In practical cases, how can we characterize adequately the variability of aquifer properties in order to take it into account in the context of numerical simulations of groundwater flow and transport? Despite important theoretical and practical progress in the last years, it is still very difficult to assess this variability statistically on the basis of information derived from common geological environments. 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". Moreover, in fractured media, the question is more complex (Wang, 1991) and very few field data sets are suitable for this kind of study.

Even in non-fractured media, in practical situations, the hydrogeologist is often faced with the following dilemma:

(a) If many and different data are available in terms of geological and hydrogeological information in the studied domain, a very detailed geological interpretation is possible with a reasonable but unquantified error. Then the measured parameters can be correlated or extrapolated consistently with this geological interpretation. A statistical approach can be tried to describe the aquifer heterogeneity but it must include a large amount of "soft" data from the geology in order to condition the system (conditional simulations, indicator geostatistics, etc).

(b) Since only a few data are available, consequently neither a statistical approach nor an accurate geological interpretation can be made.

Up to now, and bearing in mind the need to obtain practical results in terms of effective transfer time of contaminants, a complete methodology has been proposed to water suppliers for studying protection zones around pumping wells (Dassargues, 1995). This methodology includes the following steps: (a) a characterization of the geological and hydrogeological conditions based on a complete set of data related to geology, hydrogeology, hydrology, morphostructural geology and shallow geophysical prospecting, (b) experimental tracer tests with artificial tracers, (c) modelling of the groundwater flow conditions with calibration on the measured piezometric maps with and without pumping, (d) modelling the transport of a dissolved contaminant with calibration on the measured breakthrough curves, (e) simulations of contaminant transport using the calibrated hydrodispersive parameters, with contaminant injections at different places in order to compute the contaminant arrival time at the pumping well, and (f) delineation of the protection zones on basis of the computed times in respect of the local regulations. This complete methodology is entirely applied in a deterministic framework. According to the local regulations in Belgium, two main protection zones are to be defined on basis of the contaminant travel time in the saturated zone: "zone IIa" corresponding to 1 day, and "zone IIb" corresponding to 50 days. For determination of the 1-day isochrone lines, no major extrapolation of the groundwater flow and transport parameters are needed: we are working at the same scale as during the calibration of the model on the data of the *in situ* tracer and pumping tests. The main problems arise when upscaling of the flow and transport parameters is needed for determination of the 50-day isochrone lines. The chosen upscaling procedure is based here on the effective integration of all the information we obtained in the study area, by interpretation of lithological, morphostructural, geophysical and hydrological data. This is a pure deterministic upscaling procedure assuming that the zones (at the scale of the chosen REV) where preferential flow paths occur can be detected deterministically and with a sufficient spatial resolution by interpretation of all the geological, geophysical and hydrological surveys. Two case studies are described below, where such a deterministic upscaling was applied. The studied pumping sites are located respectively in an alluvial aquifer and in a fissured limestone aquifer.

DETERMINISTIC UPSCALING IN AN ALLUVIAL AQUIFER

Lithological, geophysical and hydrological data

Four pumping wells, located in the alluvial plain of River Meuse downstream of the city of Liège (point 1 in Fig. 1.) provide about 8000 m^3 day^{-1} of drinking water. Additionally to seven already existing piezometers, 10 new boreholes were drilled for the purpose of the protection zone study. The lithological information provided by boreholes, added to data from the interpretation of many penetration tests (CPT) and from shallow geophysical surveys (electric and seismic sounding methods), have lead to an accurate definition of (a) the setting and lithology of the geological layers, (b) the geometrical configuration of the aquifer, and (c) the heterogeneity and the limits of its vertical and lateral extension (Fig. 2). The alluvial plain of the River Meuse is characterized by a fluvial sedimentation composed of gravels (average thickness of about 7 m) mixed in a sandy, silty or clayey matrix. High spatial variations in the importance and the composition of the matrix have been detected in the geophysical results and confirmed by the drilling logs. The lateral as well as vertical heterogeneity of the fluvial loose deposits reveals the geomorphological evolution of the course of the River Meuse in the studied area (Calembert, 1964). The shale and sandstone bedrock of Primary age is characteristic of the substratum of the River Meuse valley in that region, and can be considered as the impervious bottom of the alluvial aquifer (Fig. 2). The water in the unconfined aquifer flows in northern direction, with a 0.075% average gradient outside the direct pumping catchment area.

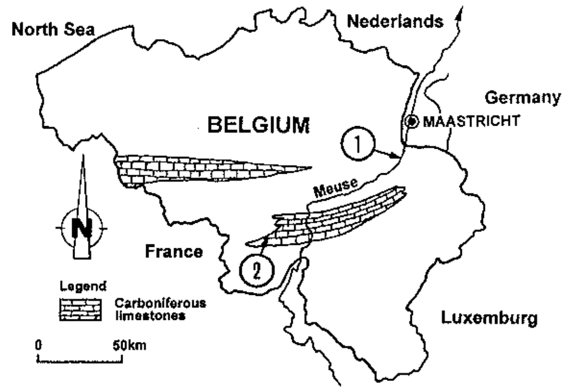

Fig. 1 Location of the studied sites in Belgium.

Local parameters deduced from measurements and model calibrations

The spatial variability of the hydraulic conductivity values in the gravel sediments has been previously studied at a regional scale (Dassargues, 1992). More locally, around the pumping wells, the first values of the hydrodynamic parameters can be obtained from classical interpretation of several pumping tests completed in each production well and

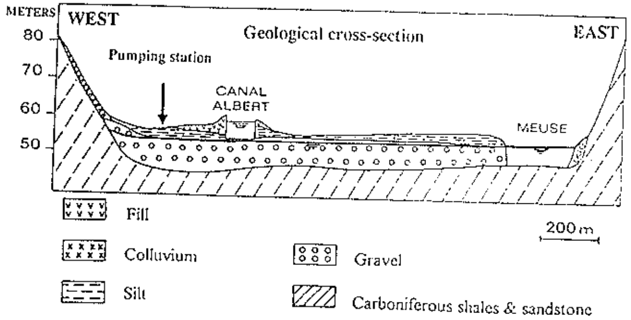

Fig. 2 One of the transverse cross-sections in the alluvial deposits, in the River Meuse valley.

piezometer: transmissivity values range from 1×10^{-4} to 2×10^{-1} m^2 s^{-1} for zones with a high clay content to zones where the gravels are well-sorted. An averaged storage coefficient of 0.10 has been analytically estimated using the Theis method. Using the Dupuit solution in homogeneous and steady-state conditions, an averaged radius of influence for the wells has been estimated to 500 m with extreme values ranging from 230 to 810 m. Given the strong assumptions under which the Theis and Dupuit expressions are valid, all these values can be considered as first estimations only.

To obtain the local hydrodispersive parameters, five different tracers (lithium, iodure, uranine, rhodamine WT, naphtionate) have been injected "instantaneously" in six different piezometers to study the contaminant transport in the saturated zone of the gravel aquifer (Derouane & Dassargues, 1994). The distances between injection points and pumping wells ranged from 27 to 115 m. Some of the experimental breakthrough curves are given in Fig. 3.

A 2D groundwater and transport model covering an area of 4 km^2 with 3000 triangular finite elements has been constructed, with element sides ranging from 200 m to less than 2 m. The finite element code uses the "Streamline Upwind Petrov-Galerkin" (SUPG) method, associated to an implicit time integration scheme. The chosen spatial distribution of the calibrated permeability values, was strongly influenced by the results from interpretation of the pumping tests. During this calibration by trial-and-error method, all the features and information obtained from interpretation of all the geological, geophysical and hydrological surveys are deterministically taken into account. The calibrated transmissivity values are given in Table 1 and Fig. 4.

Concerning the calibration of the contaminant transport model, advection, hydrodynamic dispersion and molecular diffusion were considered. For each simulated injection, a computed breakthrough curve was obtained. The shape and the characteristics of each computed breakthrough curve was fitted by trial and error on the corresponding experimental curve, so that the different values and spatial distribution of the major parameters (effective porosity and longitudinal dispersivity) can be assessed. The main results are shown in Table 1. The asymmetrical appearance presented by each breakthrough curve (Fig. 3) corresponding to late arrivals of pollutant cannot be fitted completely by the model. The spatial variability detected in the alluvial deposits (laterally and/or vertically) justifies fully the suggestion that the heterogeneity should be invoked to explain late arrivals of tracers. However, for the vertical variability, the limited number of specific data do not allow a reliable interpretation of the heterogeneity in the vertical direction. At this stage of the study, the introduction of local lateral heterogeneities into the model has lead however to fair results.

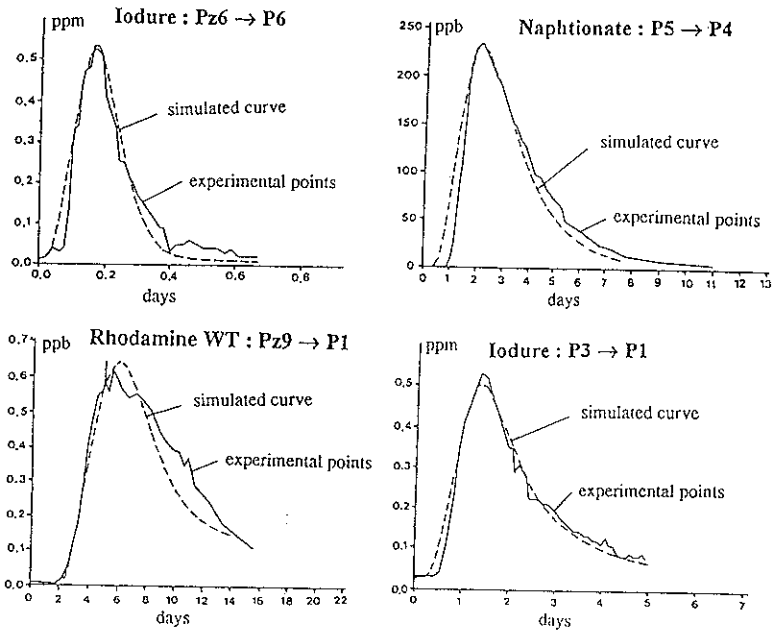

Fig. 3 Measured and computed (fitted) breakthrough curves.

Upscaling the parameters and delineation of the protection zones

At the end of groundwater flow and pollutant transport calibrations stages, the model can be considered as the best representation of the reality at the current investigation stage. Bearing in mind the above mentioned hypotheses, it can be used for provisional studies with situations resulting from various stresses: influence of an increase in pumping rate, evaluation of critical flow rates, intervention means in case of local pollution (optimization of recovery wells, pumping rate, duration, analysis of resident times and transfer velocity of the pollutant, etc.). Moreover, a good assessment of the protection zones around each production well can be provided by the model.

The effective velocity field of contaminant can be considered as reliable in the experimentation area. Indeed, for each tracer test, the hydrodispersive parameters have been calibrated only in the sub-area concerned by the particular tracer tests. Nevertheless, for the delineation of the protection zone IIb (corresponding to a transfer time of 50 days), more important volumes of porous medium are concerned as longer pollutant migration distances (in comparison with those of the tracer tests) are to be considered.

A problem of representative scale comes up (Jensen *et al.*, 1993) and, in the current state of the study, we have preferred to upscale the values of the parameters choosing

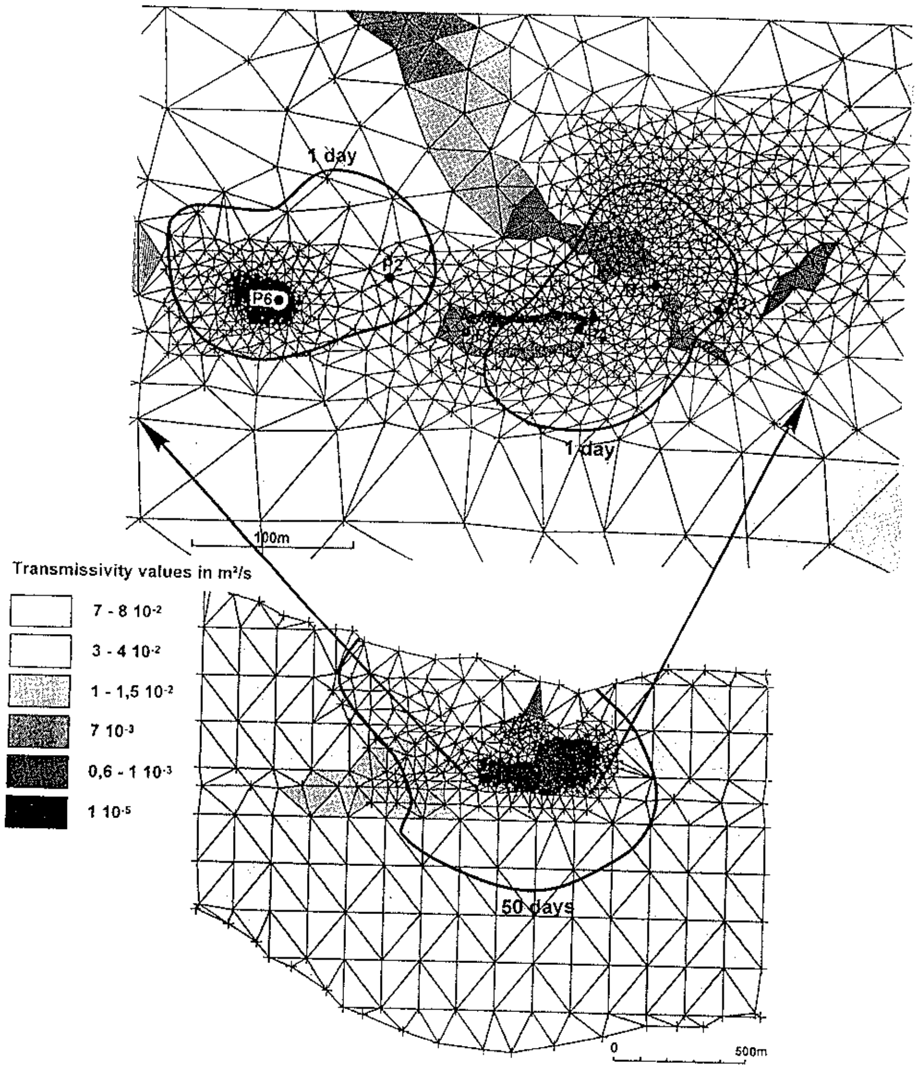

Fig. 4 Map of the transmissivity values as a result of the calibration at a local scale (up), and map of the values chosen in the entire domain (down). Computed 1 day and 50-day isochrone lines around the pumping wells P1, P2, P4 and P6 (providing perimeters of protection zones).

the values in function mainly of the geological knowledge about the site. Doing so, we have extrapolated the unchanged parameters to the whole modelled area as shown for the transmissivity values in Fig. 4. This choice can be justified by the fact the results of the tracer test have provided dispersivity values ranging from 0.01 to 0.95 m. Physically, it means that the local dispersion (mostly at the pore and grain scale) is

Table 1 Hydrodispersive parameters in zones close to the piezometers or wells where tracer tests were performed and computed breakthrough curves were fitted.

Zones near...	T (m^2 s^{-1})	n_e	a_L (m)	a_T (m)	D_m (m^2 s^{-1})
P6, Pz5 and P6	8×10^{-2}	0.048	0.01	0.003	1×10^{-9}
P3	8×10^{-2}	0.072	0.01	0.003	1×10^{-9}
P5 and P4	4×10^{-2}	0.056	0.95	0.22	1×10^{-9}
Pz10	8×10^{-2}	0.059	0.04	0.01	1×10^{-9}
Pz9	8×10^{-2}	0.047	0.60	0.20	1×10^{-9}
Pz8	4×10^{-2}	0.082	0.90	0.25	1×10^{-9}

predominant in this porous medium. Dispersion at a larger scale can then be explicitly taken into account in the model by considering the heterogeneity, as much as possible, in the permeability values. This way of treating the heterogeneity does not take into account the scale effect with increasing dispersivity values (Gelhar *et al.*, 1992), but with the distinction of different permeability and effective porosity values. Ideally, long-lasting tracer tests should be realized from piezometers situated at longer distances from pumping wells in order to justify *a posteriori* this method.

Additionally, in this case study, the hydrodynamic dispersion and the molecular diffusion are turning out to be very weak so that only the dominant advective process has been considered for the isochrone calculations (for the computation of the 50-day isochrone), with extrapolated values of effective porosity ranging from 0.047 to 0.06. The computed isochrone lines are shown at the Fig. 4. Since effective porosity is usually not affected by scale effect, the computed protection zones are expected to be reasonably accurate.

DETERMINISTIC UPSCALING IN A FISSURED LIMESTONE AQUIFER

Lithological, geophysical and hydrological data

The case described briefly here consists in the protection study of three production wells drilled in a small topographical valley corresponding to the northern part of a east-west syncline in Carboniferous layers (south of Belgium) (point 2 in Fig. 1). The direction of the calcareous layers is approximately east-west with a 80 degree dip. The northern part of the studied zone can be considered as limited by sub-vertical layers characterized by strongly lower hydraulic conductivity values. About 25 piezometers have been drilled and measured piezometric maps have been drawn for natural conditions (natural south-north gradient of groundwater flow) and in pumping conditions (3600 m^3 day^{-1}).

Results of the geomorphostructural study, confirmed by shallow seismic and electrical geophysical surveys, have provided information on the main fracture axis in the limestones. The detailed geological survey of the numerous outcrops including mapping of all the collected data has given information on the lithological differences between the successive limestone formations, and on bed and fracture dipping/orientations.

Local parameters deduced from measurements and calibrations

A local 2D horizontal finite element model has been built with the mesh composed of triangular elements with edges of about 100 m in the farthest zones from the pumping wells. The mesh size decreases to 5 m near the pumping wells and where strong heterogeneities have been revealed. Lateral boundary conditions of the flow model consist in prescribed heads (Dirichlet type) boundaries interpolated from the local and regional piezometric measurements, taking into account the geology and the presence of main fracture axes.

Since the natural piezometric conditions are not precisely known, the model has been calibrated on pumping piezometric conditions for two different flow rates (for the three wells). In the model, the distinguished heterogeneities are related to detected fractured zones using information from outcrops geological survey, geophysical methods, geomorphostructural analysis and boreholes. A map of the transmissivity values is deduced (Fig. 5) from the calibration. In the fitting process, particular attention has been given to the geological significance of any value or distribution change for the transmissivity. The main fractured axes have been explicitly distinguished and the different lithologies taken into account. An anisotropy factor had to be introduced in order to take into account that the layers seemed to have a more important longitudinal hydraulic conductivity along the bank direction than transversely. This anisotropy coefficient has been fitted to a 0.67 value.

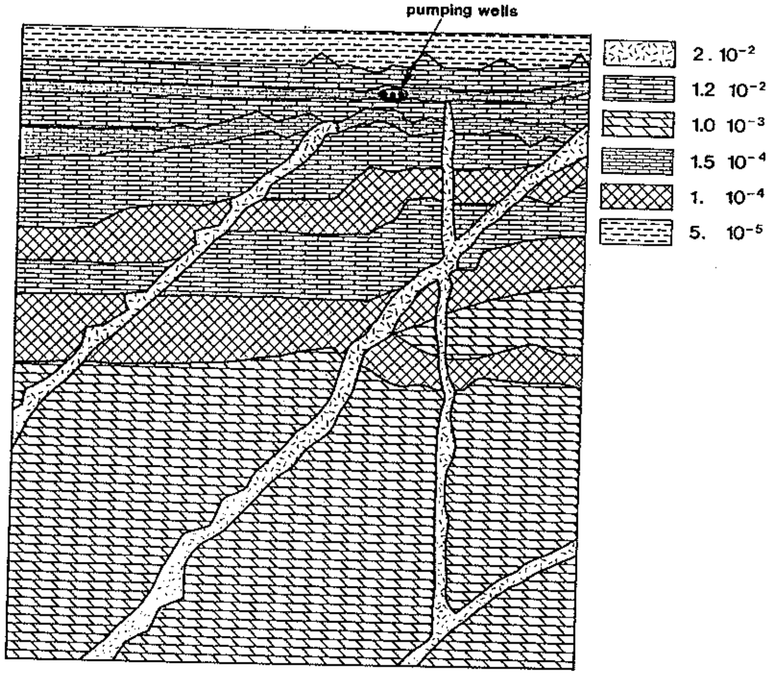

Fig. 5 Map of the transmissivity values ($m^2\ s^{-1}$) from calibration at a local scale near the pumping wells and from extrapolation based on geology for the larger scale.

A multi-tracer test has been performed (Meus & Bolly, 1994), and measured breakthrough curves obtained in each pumping well. Two tracers reached the pumping wells: naphtionate and uranine injected in piezometers respectively located at distances of about 50 and 70 m from the wells. The calibration of the model for the transport conditions has lead to the fitting of the values and distributions of the effective porosity (n_e) and of the longitudinal and transversal dispersivities (a_L and a_T). One of the main limitation to this calibration is that depth-averaged concentrations are considered in a 2D flow-transport model. An average value of 15 m has been chosen, consistently with screened levels in the pumping wells.

Some of the results of the calibration are shown in Fig. 6 in terms of breakthrough curves in the pumping wells. The deduced values for the transport parameters are as follows:

$$n_e = 0.01,\ a_L = 30\ \text{m}\ \text{and}\ a_T/a_L = 0.04$$

$$n_e = 0.08,\ a_L = 8\ \text{m}\ \text{and}\ a_T/a_L = 0.04$$

We have interpreted the first couple of values as corresponding to the limestone matrix (eventually microfissured), while the second is more representative of fractured or slightly karstified zones. Indeed, it seems logical to consider that a more fractured zone presents higher values of porosity with lower dispersivity, and matrix blocks of limestones lower values of effective porosity with a higher dispersivity due to multiple single microfractures.

Upscaling the parameters and assessment of the protection zones

In this case, it was evident that we could not neglect the dispersion component of the transport. Normally, the transport parameters fitted during the calibration on the measured breakthrough curves are only representative for local scale transport model. It has been decided to extrapolate deterministically the local values to the entire

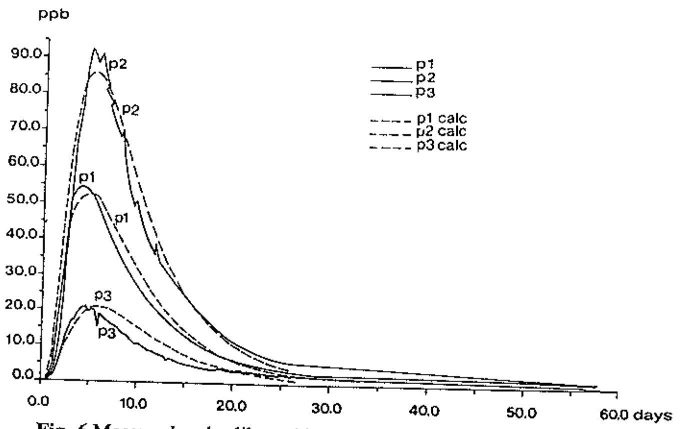

Fig. 6 Measured and calibrated breakthrough curves for naphtionate in the three wells.

modelled domain. This extrapolation takes into account, as logically as possible, the knowledge that we have about the geology. In this way the strong scale effect on the dispersivity values that can be expected (e.g. Gelhar *et al.*, 1992) is explicitly considered by a determinist representation of the heterogeneity. The first set of transport parameters has been extrapolated to the whole supposed unfractured domain and the second set to the main fractured zones as revealed by the geophysical and morphostructural studies. Simulations of the contamination scenario have been computed from 114 points of the meshed domain. For each of these points, a first arrival time is recorded and then by interpolation of the results, a map with isochrone lines can be drawn (Fig. 7) and protection zones corresponding to the existing regulations can be assessed.

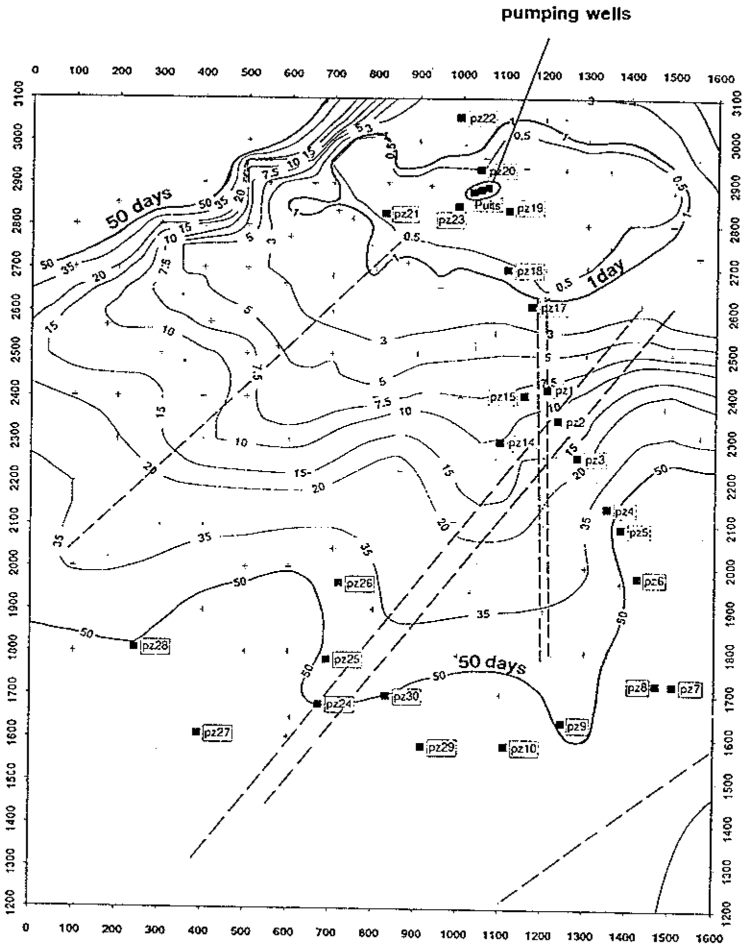

Fig. 7 Computed 1-day and 50-day isochrone lines around the pumping wells (providing perimeters of protection zones).

CONCLUSIONS

Dealing with practical cases it is often particularly uneasy to apply geostatistically-based methods to upscale the groundwater flow and transport parameters. Usually, for local situations, sufficient geological data ("soft data") are available in order to obtain a clear (but to a certain extent always subjective) geological interpretation. Measurements ("hard data") are added and allow a reliable assessment of the spatial variability and heterogeneity in the different layers in order to infer or extrapolate logically the flow and transport parameters needed for the model.

According to the generally accepted definition, dispersion is the result of a statistical distribution of flow paths and velocities around local heterogeneities (at a lower scale). Microdispersion caused by flow around grains is on the order of centimetres whereas the macrodispersion caused by macroscopic heterogeneities is on the order of metres (or more). Two trends are observed in the way of including macrodispersion values in the models.

In the first way, the heterogeneity of the modelled domain is not fully described but "lumped" into a macrodispersion term. The corresponding dispersivity coefficients are not really physically consistent but they represent statistically the general behaviour of the contaminant around the advective mean position. The main advantage of this method lies in the fact that smaller scale heterogeneities need not be known in detail; the main problem consists in upscaling the values.

In the second approach, the main detected heterogeneities are taken into account explicitly with different values of permeability and effective porosity values. In that approach, the dispersivity values obtained by field investigations at a local scale do not have to be really upscaled since we supposed that they are representative at the scale used in the model.

The methodology described here, and applied to two local situations, lies between these two possibilities, trying to add the advantages and to avoid disadvantages. We try to consider as accurately as possible the heterogeneity of the domain. For that part of the work, the role of a good geological background is essential. But as there is no hope of having a detailed knowledge of the medium at a small scale, extrapolations of values are still needed from measured values at a local scale to larger scales; these extrapolations being mainly influenced by the geological information.

The main difficulty lies in the relative definition of that "intermediate scale" at which one can expect to apply this methodology. Of course, this conceptual choice must be made and balanced as a function of the accuracy needed for the results. In the future, the implementation of long-lasting tracer tests should be considered, as far as it could help to solve this problem of the deterministic upscaling of the parameters more accurately.

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