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2D and 3D groundwater simulations to interpret tracer test results in heterogeneous geological contexts

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ABSTRACT: It is well known that the interpretation of tracer tests breakthrough curves can be multiple. It should be difficult to describe all the possible situations of wrong and inconsistent interpretations induced by 'automatic' calibrations solving the inverse problem without introducing any 'hard' or 'soft' geological data. When a 3D flow and transport model is applied to simulate tracer tests performed in 2D (depth averaged) conditions, a quasi infinite number of suitable parameters combinations allow to reach the calibration of the transport model. Geological data must provide informations on the different geological layers to be distinguished in the model. Inside these layers, the observed facies changes can motivate the choice of different values of the flow and transport parameters. Morphostructural analyse provides also informations on more fissured zones (in hardened formations) or on sedimentological features (in loose sediments), and shallow geophysical surveys provide new data or confirmation of the previous informations. In fact, one can not choose freely the parameter spatial distributions. Only few of the combinations are fully geologically consistent with all the collected 'hard data' and 'soft data'.

Due to differentiated values of hydraulic conductivity, effective porosity and dispersivities distinguished in the different layers of a 3D model, computed breakthrough curves can represent any complex shape of the measured curves including double peaks, strong delays, etc.

Comparisons are made between the computed breakthrough curves obtained by calibration of a 2D model and by calibration of a 3D model for a same situation corresponding to tracer tests, performed in depth-averaged conditions, in the alluvial sediments of the Meuse River (Belgium). Conclusions in terms of under- and over-estimation of the interpreted parameters values are drawn.

1 INTRODUCTION

When delineating protection zones which are based on contaminant travel times in the saturated part of aquifers, different methodologies are proposed to take the aquifer heterogeneity into account:

(1) geological and hydrogeological characterisation based on geology, hydrology, morphostructural geology and shallow geophysical prospecting,

(2) multi-tracer tests with artificial tracers, and

(3) numerical modelling of groundwater flow and transport.

During this third step, an accurate calibration of the model is required, using measured piezometric heads for groundwater flow and measured breakthrough curves for transport of solute contaminant.

The spatial distribution and values of the calibrated permeability coefficients must be consistent with pumping test results, and with geological, geophysical and hydrological data sets. 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.

Usually, the detected spatial variability (laterally and/or vertically) can fully justify that heterogeneity should be invoked to explain late arrivals of tracers.

For one set of tracer-test data, 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. Suitable combinations of the groundwater flow and transport parameters which are deduced from both calibrations can be strongly different. Advantage and drawback of each approach can be compared on a same situation. For illustration, in this paper, the discussion will concern the interpretation of tracer tests performed in depth-averaged conditions in the alluvial sediments of the River Meuse. These tracer tests, with iodide and LiCl injected in the same piezometer, have been modelled using 2D and 3D numerical codes.

The alluvial plain of the River Meuse is characterized by a fluvial sedimentation composed of gravels mixed in a sandy, silty or clayey matrix. A complete hydrogeological study has been realized at the pumping station of Vivegnis near Liège in Belgium (figure 1). The aim of the study consists in the accurate delineation of protection zones based on contaminant travel times.

The general methodology includes the determination of the experimental values and the spatial layout for hydrodynamic and hydrodispersive parameters and the use of these parameters in a groundwater flow and contaminant transport model (Biver and Meus, 1992). This model is supposed to take all detected local heterogeneities into account. After calibrations, it can be used to compute the transport travel times from different injection points to the pumping well. A good assessment of the protection zones can then be deduced (Dassargues, 1994).

The average drinkwater production of the site is about 8000 m^3/day, using four pumping wells. More than ten piezometers have been drilled, and are available for measurements and tracer injections. The lithological information provided by those boreholes, added to data from many penetration tests and from geophysical survey (electric and seismic sounding methods), leads to the definition of a main gravel layer with an averaged thickness of 7 meters, overlaid by a 2 meters thick silt layer. The Primary shale and sandstone bed-rock (Namurian and Westphalian ages of Carboniferous formation), is characteristic of the substratum of the River Meuse valley and can be considered as an impervious bottom for the alluvial aquifer (figure 2). At the regional scale, the unconfined aquifer presents a 0.075 percent average gradient towards the North (Dassargues and Lox, 1991).

A first interpretation of pumping test results (following the classical analytical solutions of Theis in transient conditions, and Dupuit in steady-state), have given transmissivity values which range from $1.10^{-4} m^2/s$ to $2.10^{-1} m^2/s$. Transmissivity values lower than 5.10^{-3} m^2/s are found corresponding to zones where the clay content is higher. Transmissivity values higher than 8.10^{-2} m^2/s correspond to clean and well sorted gravels. An averaged storage coefficient of 0.10 was estimated using the Theis solution. This value can be used as a first approximation for the effective porosity of the porous medium. In steady-state conditions, an averaged radius of influence for the production wells was estimated to range from 230 to 810 meters. In transient conditions, a value of 440 meters was calculated. One should keep in mind that the hydrodynamic parameters obtained from those pumping test interpretations are only first approximations, given the strong assumptions under which the Theis and Dupuit expressions are valid. Moreover, these values can only be considered as 'mean values' around the wells.

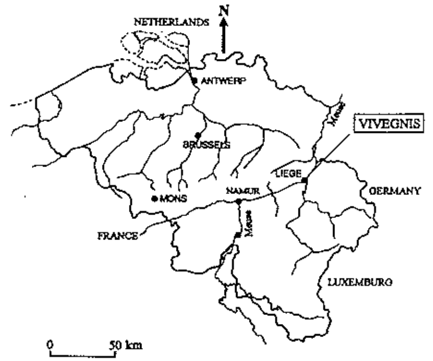

Fig. 1 Location map

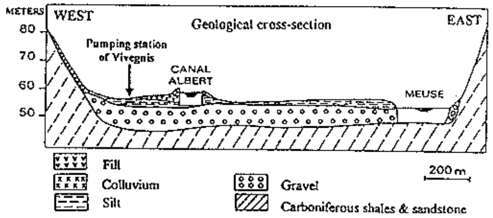

Fig.2 Transversal cross-section in the alluvial deposits of the River Meuse valley.

2 2D AND 3D GROUNDWATER FLOW MODELLING

2.1 *Groundwater flow conditions and boundary conditions*

A 2D regional FEM model using the code AQUA2D (Vatnaskil Consulting Engineers) was previously calibrated in steady state conditions on a measured piezometric map (figure 3) (Derouane, 1994).

In the 3D local model, it is also assumed that stabilized pumping conditions are reached, so that steady state groundwater flow is considered for modelling the alluvial water table aquifer. In the gravels, a vertical sequence was distinguished with, at the bottom, coarse and clean pebbles in a 2 meters thick layer, and finer pebbles with increasing silt and loam content in the 6 meters thick upper part. The silt layer is not taken into account as it lies definitively above the water table (i.e. in the unsaturated zone) in the modelled zone and as only saturated zone of the aquifer is considered here. Moreover, in a first approach and to simplify reinterpretation of the results, homogeneous distributions of the parameters are chosen in each horizontal layer.

The finite-element program SUFT3D (Dassargues, 1994) is used. Dirichlet prescribed piezometric heads are chosen as flow boundary conditions of the domain around the pumping well P6 (figure 3). These values are deduced from the calibrated regional piezometric map (Derouane, 1994) obtained by the 2D regional model. The lower horizontal boundary which corresponds to the bottom of the alluvial aquifer is characterized by no flow. A uniform infiltration flow rate is prescribed on the top boundary of the model.

A three layers discretization is chosen. The lower layer, representing the clean and coarse gravels (2 m thick), is overlaid by two layers, each of them having a thickness of three meters (figure 4). The horizontal discretization was made using two meshing networks (1) a regular grid with 1292 nodes and 864 blocks, (2) an irregular and refined grid with 2604 nodes and 1848 elements (figure 5).

2.2 *Heterogeneity and permeability values*

Due to the different lithological nature of the alluvial sediments, it was arbitrarily decided to maintain a factor ten between the permeability values of layers 2 & 3 and layer 1 (bottom layer). Taking a mean value of the saturated thickness at 7 m, and in order to be consistent with the equivalent value of the transmissivity which was used in this zone of the 2D model, the contrasted permeability coefficients can be found as following:

$$T = 7.K_{eq} = 2K_1 + 5K_2 = 2K_1 + 0.5\,K_1 = 2.5\,K_1 \quad (1)$$

where K_1 is the permeability coefficient in layer 1 and K_2 is the permeability coefficient in the layers 2 & 3 ($K_2 = 0.1\,K_1$).

In the 2D model, an equivalent transmissivity value was calibrated at $6.8\ 10^{-2}$ m^2/s, so that permeability values of $2.7\ 10^{-2}$ m/s and $2.7\ 10^{-3}$ m/s are deduced respectively for K_1 and K_2 (figure 6).

After calibration of the 3D local model, it is

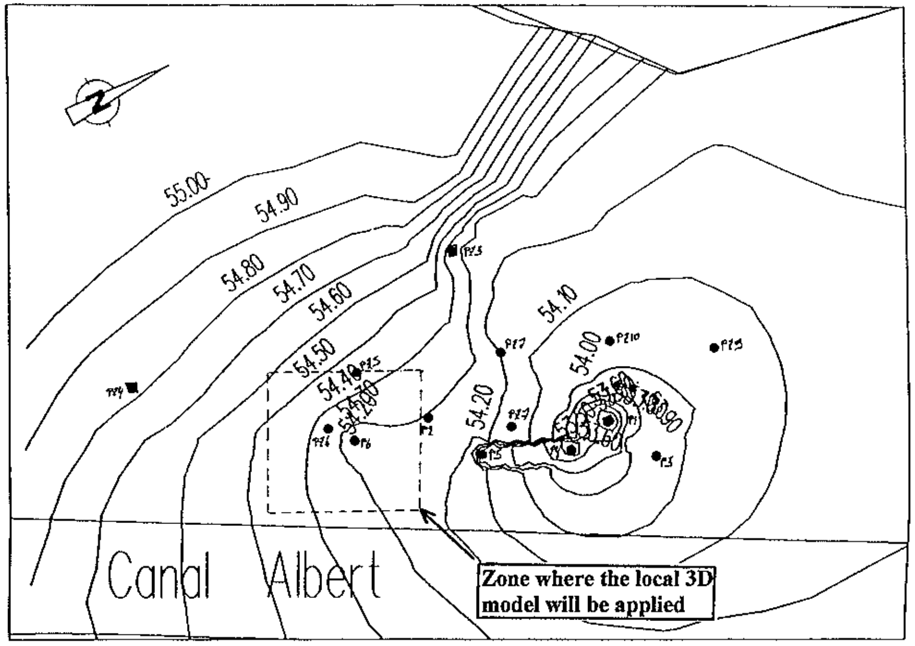

Fig. 3 Calibrated regional piezometric map obtained by 2D FEM groundwater flow modelling.

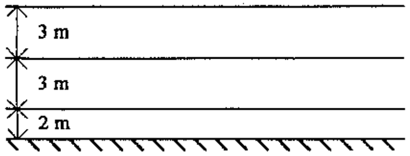

Fig.4 Vertical discretization of the local 3D model.

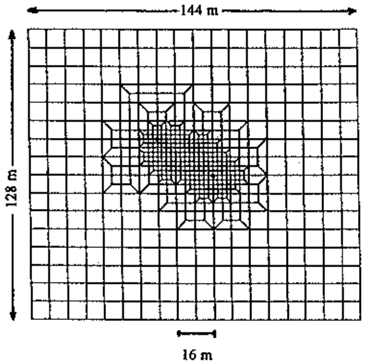

Fig. 5 Horizontal discretization of the local 3D model: refined mesh.

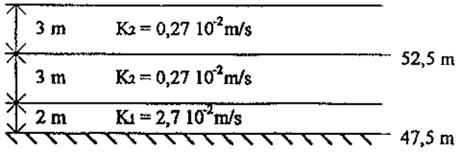

Fig.6 Vertical distribution of the permeability values.

evident that a strong contrast in computed Darcy's specific fluxes is found (figure 7). This contrasted situation will have a overwhelming influence on the transport conditions in the modelled zone.

3 MODELLING TRANSPORT IN 3D

Results from 2D transport simulations are often questionable when the porous medium is vertically heterogeneous. The choice between 2D and 3D modelling must be guided by the aims of the study, the spatial variability of the parameters describing the aquifer, and the available data set. If an accurate representation of the aquifer heterogeneity with a realistic determination of the hydrodynamic and hydrodispersive properties is needed, then a detailed 3D is more adequate. However, the actual spatial distribution of the parameters to be introduced in the model is only badly known so that the uncertainty is still important.

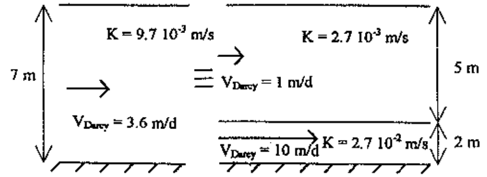

Fig.7 Effect of the chosen heterogeneity on the Darcy's specific fluxes.

A 2D transport simulation is often considered as sufficiently accurate and detailed when interpreting 'depth averaged' tracer and pumping tests. This approach can be accepted when the awaited values for the properties in the different layers are not too contrasted, so that equivalent values can be easily considered.

For both 2D an 3D approaches, the concept of Representative Elementary Volume (REV) is applicable so that the link between actual values and adjusted parameters in the elements of the models is difficult to assess, and in any case, depends strongly on the chosen scale (Gelhar et al., 1992). The effective velocity or advection velocity in the porous medium is given by:

$$\underline{v}_e = -\frac{K}{n_e}\underline{gradh} \qquad (2)$$

where n_e is the effective porosity of the aquifer and $\underline{gradh}$ is the piezometric gradient. When 'depth averaged' conditions are chosen, the transmissivity is used in the groundwater flow computations so that the effective velocity becomes:

$$\underline{v}_e = -\frac{T}{n_e . e}\underline{gradh} \qquad (3)$$

where *e* is the saturated thickness of the aquifer. For a given value of transmissivity (deduced generally from calibration of the groundwater flow model), the effective porosity as well as the saturated thickness influence the effective velocity. Consequently, a 2D calibration on the measured 'depth-averaged' breakthrough curves, cannot provide clear information on the effective porosity. In studies concerning protection zones, the first arrival of contaminant is of big importance. If we consider 2 layers with contrasted permeability values, as in figure 7, a depth averaged 2D approach should compute a global effective porosity value which is three times lower than the value found for the lower layer.

In a 3D transport model, the geometry of the different layers is supposed to be known and equation (2) is used. For given values of permeability in each layer, effective porosity values are found to calculate the effective velocity and to calibrate the computed breakthrough curve on the measured one.

Different breakthrough curves were found as a result of two tracer tests conducted in a same piezometer (figure 8). Injection of iodide and LiCl were performed in different conditions, and at different times. Many scenarios can be invoked to explain the different breakthrough curves which were obtained. One of them consists in invoking the influence of the injection mode on the tracer test results (Brouyère & Rentier, this issue). Another explanation can be given assuming that the largest part of each tracer was actually injected into the aquifer at different levels of the screened piezometer (Carabin, 1995). This last scenario imposes a 3D analysis of the results. A combination of both causes should probably be invoked.

Anyway, having two different measured breakthrough curves, the situation is ideal for testing how a 3D transport model can always be calibrated on measurements by introduction of vertical (and/or lateral) heterogeneities.

For the local 3D simulation of the transport in the radial convergent flow conditions induced by the pumping at the well P6, transport Neumann boundary conditions or 'natural condition of zero dispersive flux' are chosen allowing only an advective flux through boundaries. By this way the injected tracer (in Pz6) can go out of the modelled zone through the lateral boundaries.

The injection simulation is realized considering a constant injection flow rate during 5 time steps of 1 hour. As awaited, the computed breakthrough curve is largely influenced by the choice of the injection nodes in the 3D mesh.

In a first step, the iodide injection (in Pz6) is simulated according to the scheme of figure 8. The computed breakthrough curves at each of the pumping nodes (from bottom to the top: nodes 1 to 3) are given in figure 9. They show the strong influence of the vertical heterogeneity on the results. The less pervious layers (layers 2 & 3) have a transport behaviour which can be qualified as characteristic of 'buffer zones': the tracer reached them mainly by transversal dispersion. The transport parameters which were used, are provided in table1.

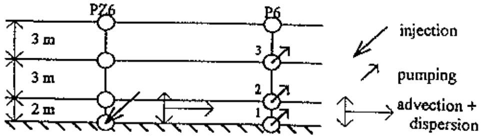

Fig.8 Injection and pumping conditions for the local 3D transport model simulating the tracer test n°1.

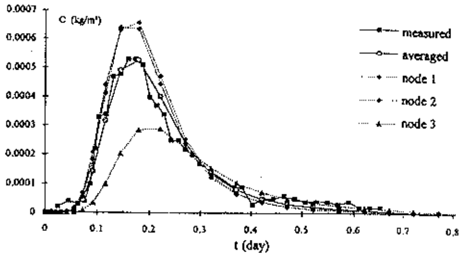

Fig.9 Measured and computed breakthrough curves for tracer test n°1.

Table 1 Transport parameters used to simulate the tracer test n°1 (a_L and a_T are the longitudinal and transversal dispersivities).

Tracer test n°1	n_e	a_L (m)	a_T (m)
layers 2 & 3	0.05	1.5	0.3
layer 1	0.07	1.5	0.3

For calibration on the results of the second tracer test (with injection of LiCl) some changes in the way to inject the tracer were needed. As observed on

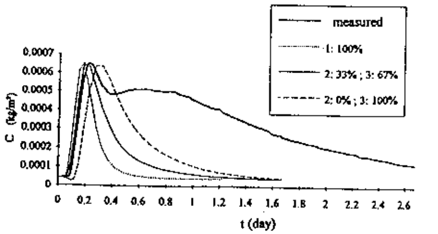

Fig.10 Measured and computed breakthrough curves for tracer test n°2 with different injection schemes (percentages of the total injected mass are mentioned).

figure 10, to simulate the first peak of the measured breakthrough curve, a good fitting can be found by changing only the distribution of the tracer injections at the different nodes of the vertical discretization.

When changing the transport parameters in layers 2 & 3, different breakthrough curves can be computed showing two peaks (figure 11). The injection distribution and the transport parameters which were used for each curve, are given in table 2.

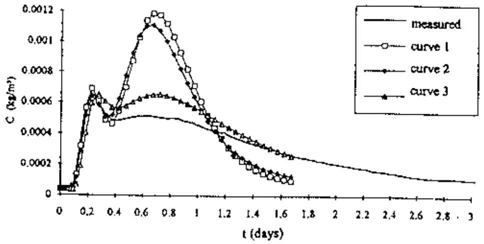

Fig. 11 Measured and computed breakthrough curves for the tracer test n°2 with different transport parameters in layers 2 & 3.

The same changes of transport parameters do not affect strongly the computed breakthrough curves for the tracer test n°1 (figure 12).

In studies concerning protection zones, it is essential to obtain an adequate calibration of the first peak. Having in mind this aspect, the first peak is better simulated with the transport parameters corresponding to curves 1 & 2. Keeping these different changes in the model to simulate again the tracer test n°1, no important discrepancy is found. The greatest changes affected the layer 3, which does not play an important role in the transport results of the tracer test n°1.

Table 2 Injection distribution and transport parameters which are used to compute the curves of figure 11.

Tracer test n°2	n_e	a_L (m)	a_T (m)
layer 3: curve 1	0.08	0.5	0.05
curve 2	0.075	1.5	0.05
curve 3	0.075	5.0	1.0
layer 2: curve 1	0.07	0.5	0.05
curve 2	0.07	0.5	0.05
curve 3	0.07	0.8	0.05
layer 1	0.07	1.5	0.3
Injection distr.	node 1	node 2	node 3
	0 %	3 %	97 %

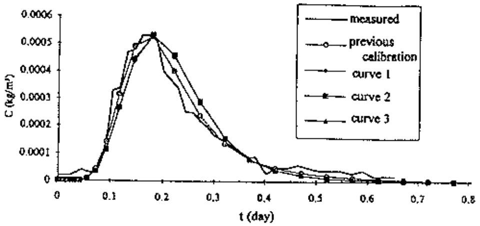

Fig. 12 Measured and computed breakthrough curves for tracer test n°1 with the different transport parameters in layers 2 & 3 .

4 COMPARISONS AND CONCLUSIONS

On basis of the last results, the transport parameters corresponding to curve 2, are considered (table 3) for the best calibration on the first peaks of both tracer tests. Injection distributions on the three nodes of the vertical discretization are not the same: 100 % of the iodide injection in node 1 for the tracer test n°1 and 97 % of the LiCl injection in node 3 for the tracer test n°2.

Table 3 Final transport parameters

Tracer tests n°1 & 2	n_e	a_L (m)	a_T (m)
layer 3	0.075	1.5	0.05
layer 2	0.07	0.5	0.05
layer 1	0.07	1.5	0.15

The comparison of the flow and transport parameters of this 3D model with those obtained previously by calibration of the 2D model (Derouane, 1994), can be made (table 4). Computed breakthrough curves are given in figure 13.

In table 4, the dispersivity values of the 2D model are not consistent. This is due to an important numerical dispersion. Consequently, the 2D computed breakthrough curves (figure 13) show more dispersion than awaited with the values of table 4. It is difficult to establish clear comparisons between the transport parameters obtained with the 2D and the 3D models. The main differences in values of the effective porosity are due to the contrasted value of permeability distinguished in the layers of the 3D model. As mentioned previously, the 'depth averaged' effective porosity can be largely underestimated. This can be very important when considering the delineation of protection zones.

Table 4 Flow and transport parameters obtained by 2D and 3D calibrations.

	K (m/s)	n_e	a_L (m)	a_T (m)
2D	0.0215	0.048	0.01	0.003
layer 3	0.0027	0.075	1.5	0.05
layer 2	0.0027	0.07	0.5	0.05
layer 1	0.0270	0.07	1.5	0.15

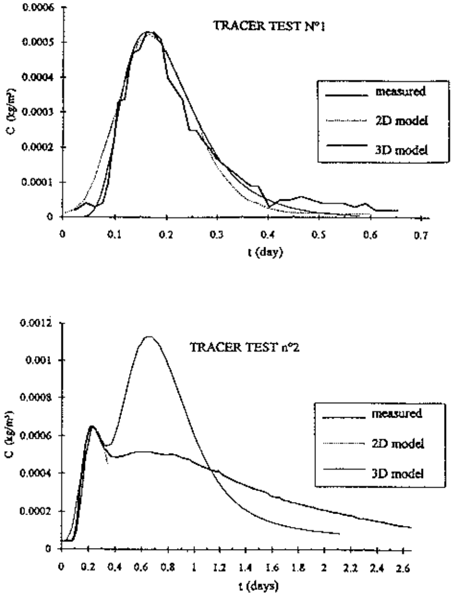

Fig. 13 Comparison of the results obtained with 2D and 3D models.

The first arrival of tracer and the way to reach the first peak are certainly better simulated in 3D than in 2D. However, the 3D model allows to distribute the injection and the pumping on different nodes. These distributions can have a significant influence on the results. The vertical discretization allows to gain more flexibility in the introduction of the spatial variability. To calibrate the model, lateral and vertical heterogeneities can be introduced.

Advances must be considered to obtain better controlled experimental conditions and better numerical representations of the actual conditions. Tracer tests in 3D conditions with adequate use of packers, and a better control of the actual input function into the aquifer should be addressed. For modelling aspects, an explicit representation of the injection piezometer and of the pumping well (with line elements), should help to simulate more accurately the injection and pumping conditions (Lacombe et al., 1995, Sudicky et al., 1995).

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