Detailed calibration of a deterministic transport model on multi-tracer tests: analysis and comparison with semi-analytical solutions

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Abstract Multi-tracer tests were carried out close to a pumping well in fluvial deposits located in the Meuse valley near Liège in Belgium. Detailed investigations with different tracers and injection procedures have provided a very complete data set of measured breakthrough curves at the pumping well. Influence of the tracer nature and of tracer injection conditions on the measured concentrations can be observed.
Heterogeneity of the porous medium - gravels intersected by sandy and silty lenses - was previously investigated using geo-electrical resistivity measurements. In groundwater flow and transport simulations, it is represented deterministically by the choice of various flow and transport parameters in the modeled zone. After calibration on the multiple measured breakthrough curves, the comparison with analytical solutions assuming advection-dispersion in homogeneous radial conditions is particularly interesting.
Conclusions are drawn in three directions, all of them having a strong influence on the calibrated values of the transport parameters and consequently on the further plume simulations: (a) some of the tracers, classically considered as non-reactive tracers, are actually affected by important adsorption/desorption and/or decay processes; (b) accurate control and measurement of effective injection conditions in the aquifer must be conducted in order to be able afterwards to simulate them adequately in the transport model; (c) gravels of fluvial deposits are often erroneously considered as an homogeneous porous medium, important differences are found in terms of flow and transport parameters when heterogeneity is addressed.

INTRODUCTION

When analysing tracer tests results, different results can be found in terms of fitted transport parameters and in terms of computed breakthrough curves when using semi-analytical solutions or a spatially distributed numerical model solving the flow and coupled transport equations in heterogeneous aquifer conditions. The determination of the hydrodispersive parameters by means of a numerical model (MODFLOW & MT3D) is compared to the determination by means of manual and automatic calibration using a semi-analytical solution.

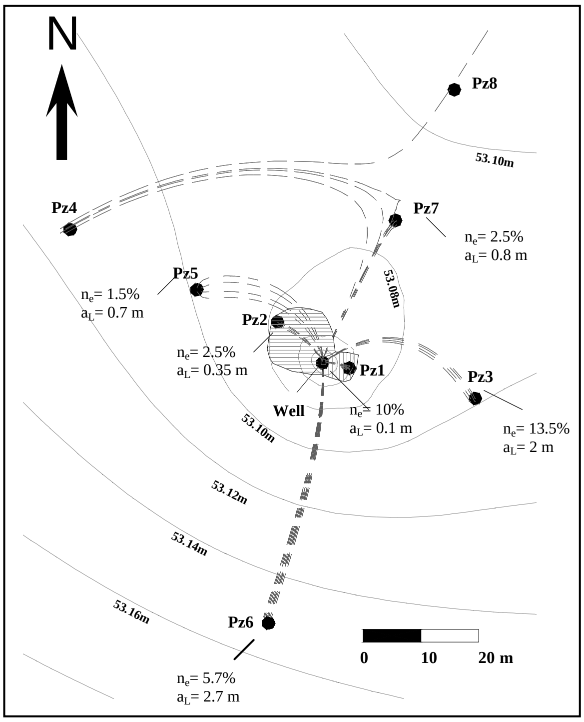
CASE STUDY AND MEASURED BREAKTHROUGH CURVES

The studied site is located in the alluvial plain of the river Meuse near Liege in Belgium. Upper Carboniferous bedrock consisting in shale and sandstone constitutes the impervious basis of the aquifer. Loose fluvial sediments deposited by the river Meuse on that substratum form the main aquifer. The fluvial deposits are composed of gravel bodies imbedded in old channels filled with sandy to silty or clayey sediments. Total thickness of the main gravel layer varies from 3 to 12 meters. The aquifer shows locally confined and unconfined behaviour with a natural piezometric gradient lower than 1/1000. There is one production well (1270 m^3/day), surrounded by 8 piezometers located at distances ranging from 5 m to 50 m. A local and detailed hydrogeological study including groundwater flow and transport modelling was conducted mainly to study the influence of a) the injection procedure, and b) the tracer nature, on measured results of tracer tests (Haerens, 1999). However other concomitant interesting results were found and are commented here below.
Fourteen tracer tests have been performed from 7 different piezometers, using 10 different artificial tracers (fluorescent dyes and saline tracers), and several injection procedures. The tracer tests were performed in “depth averaged conditions” and the following steps were followed during the injection procedure: a) the tracer is diluted in a volume of water, b) this solution is injected in the piezometer and than c) a volume of flush water is injected. During these operations a “circulation system” is active in the injection well to avoid entrapment in the injection well and to homogenise the tracer concentration in the piezometer. Thanks to this system it is also possible to sample during and after each injection in order to follow up the tracer concentration at the injection point. It helps to obtain a better assessment of the actual input function of the tracer in the aquifer and consequently to have a better understanding of the breakthrough curves in the pumping well.
The measured breakthrough curves show a variety of modal transfer times as presented in Fig. 1 for the different injection points.

NUMERICAL MODEL

In order to assess the advective-dispersive parameters, MODFLOW & MT3D (McDonald & Harbaugh, 1984; Zheng, 1991) have been used to simulate the tracer tests: a 2D finite difference flow and transport model is constructed. For determination of hydrodispersive parameters, only injections performed with “so-called” conservative tracers are selected. We are supposing no adsorption/desorption and no decay in our interpretation of tracer tests. In practice, the following steps are performed: (a) hydraulic conductivity values are deduced from the groundwater flow calibration (not changed during the transport calibration); (b) the effective porosity is adjusted with fitting of the simulated peak on the measured first peak; (c) with use of the longitudinal dispersivity and a normation coefficient (multiplying the simulated injected mass), the concentration rising and amplitude of the computed first peak are fitted to the measured one (with eventual return to step b). The measured recovery factor is not reproduced because other processes are included in the measured breakthrough curve creating delay and lower peak. Effective porosity and longitudinal dispersivity (to a lesser extent) are underestimated (Brouyère *et al*., 1999). However, this approach can be considered as consistent when only minimum transfer times have to be computed.
After calibration of the groundwater flow and transport models on the 6 breakthrough curves, a spatial distribution of the transport parameters around the pumping well is found on basis of

local extrapolation (based on all other geological information) of the fitted parameters for each tracer test (Fig. 1). This is a pure deterministic upscaling-extrapolation procedure assuming that heterogeneity can be detected deterministically by interpretation of all geological, geophysical and hydrological surveys (Dassargues *et al.*, 1996). At this stage, and using the calibrated parameters, the computed streamlines for each injection (Fig. 1) show clearly that the actual travel of the tracer between injection and pumping wells cannot be approximated by the linear segment between these two points.



Pz	*d(m)*	*Tr.*	*n_e(%)*	*a_L(m)*	*MT(h)*
Pz1	4.7	N	10	0.1	0.7
Pz2	10.3	C	2.5	0.35	1.1
Pz3	27.2	I	13.5*	2*	41.3
Pz4	50.0	U	/	/	103.3
Pz5	25.1	I	1.5*	0.7*	4.7
Pz6	46.1	I	5.7*	2.7*	23
Pz7	27.6	U	2.5*	0.8*	22.2

a_L/a_T = 0.1 for all simulations
*: parameter values outsides the zones for Pz1 and Pz2

Pz: injection piezometer
D: distance to well in m
Tr: tracer: **N**: nitrate; **C**: chloride; **I**: iodide; **U**: uranine
n_e: effective porosity in %
a_L: longitudinal dispersivity in m
a_T: transversal dispersivity in m
MT: modal transfer time in h

Fig. 1 Fitted parameters and advective streamlines from each injection point to the pumping well.

SEMI-ANALYTICAL PROCEDURE

A semi-analytical solution for advection-dispersion solute transport in a converging radial flow (Sauty *et al.*, 1992) is widely used with the well-known CATTI code for interpretation of tracer tests with instantaneous injection. Both manual and automatic (least-square based) calibrations can be performed to determine the hydrodispersive parameters. Manual calibration is essentially based on the first arrival and on the peak concentration of the experimental breakthrough curve (like it was done with the numerical model. Automatic calibration takes the whole breakthrough curve into account: first arrival, peak and tailing. It uses a least mean squared method for parameter optimisation. Parameters chosen for optimisation are effective porosity n_e (%), longitudinal dispersivity a_L (m) and recovery factor F (%). Using a numerical recovery factor (for both calibration techniques available in CATTI) is here the way of normalising the curves to be fitted.

COMPARISON OF RESULTS

As it can be observed in Table 1, different results are obtained using the three methods. Differences between the results obtained with the numerical method and the semi-analytical method can essentially be explained by the assumptions inherent to the latter method. As this method uses an approximate solution for advective-dispersive solute transport in a converging radial flow, the flow paths from injection point to pumping well are supposed to be rectilinear and the influence of a regional gradient is not taken into account. As obtained from the numerical model it is clear that some of the flow paths are far from rectilinear, for example the trajectory Pz3-pumping well (Fig. 1). Although the fitted curves present a better agreement (Fig. 4), the semi-analytical solution is leading to an overestimation of the effective porosity since this method calculate the hydrodispersive parameters using a shorter (rectilinear) distance than in reality. Even if rectilinear flowpaths are considered for the tracers injected at Pz6 and Pz7 there is a significant difference in results. For the transport Pz6-well the regional gradient adds an extra component to the radial converging flow not taken into account with the semi-analytical method, leading to an underestimation of the effective porosity. At the contrary for the transport Pz7-well, the regional gradient counteracts the radial convergent flow to the pumping well, leading to a slower transport to the well than in pure radial convergent flow. As a result an overestimation of the effective porosity by the semi-analytical model is observed.

Table 1 Transport parameters obtained by calibration of the numerical model and by manual and automatic calibration of the semi-analytical solution.

		Pz1	**Pz2**	**Pz3**	**Pz5**	**Pz6**	**Pz7**
NUMERICAL	n_e	10%	2.5%	13.5%	1.5%	5.7%	2.5%
	a_L	0.1 m	0.35 m	2 m	0.7 m	2.6 m	0.8 m
	a_L/a_T	0.1	0.1	0.1	0.1	0.1	0.1
SEMI-ANALYTICAL	n_e	10.5%	3.25%	25.2%	1.65%	3.2 %	8%
Manual calibration	a_L	0.54 m	0.75 m	5.02 m	0.32 m	3.9 m	1.5 m
	F	0.75	0.47	0.41	0.40	0.39	0.19
SEMI-ANALYTICAL	n_e	10.8%	3.44%	24%	1.75%	4.6%	19.6%
Automatic calibration	a_L	0.54 m	0.95 m	4.4 m	0.5 m	9.25 m	8.25 m
	F	0.70	0.43	0.41	0.51	0.60	0.51

Differences between manual and automatic calibration are resulting from the fact that automatic calibration uses all experimental data including the tailing of the breakthrough curves. As no retardation should have occurred ("conservative" tracers do not experience too much sorption processes), this tailing is here probably resulting from vertical heterogeneity of the aquifer (Dassargues *et al.*, 1997). Consequently, automatic calibration presents the poorest fitting of first arrivals as shown in figures 2 and 3.

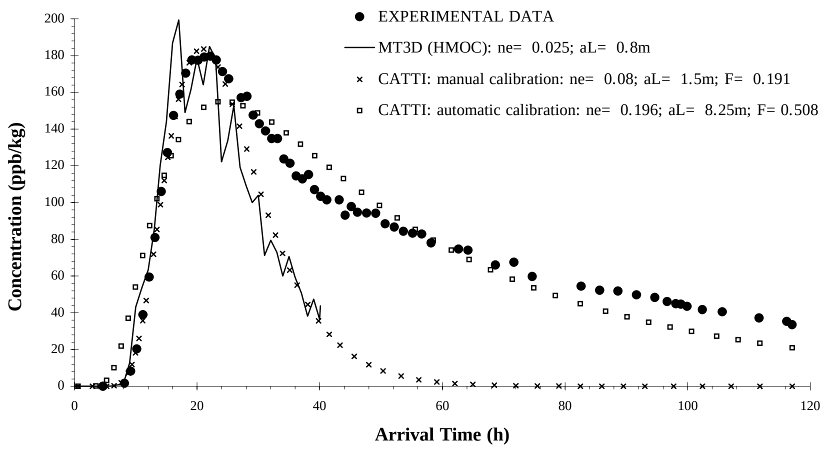


Fig. 2 Comparison of the results obtained with numerical modelling and semi-analytical solutions for injection at piezometer Pz7.

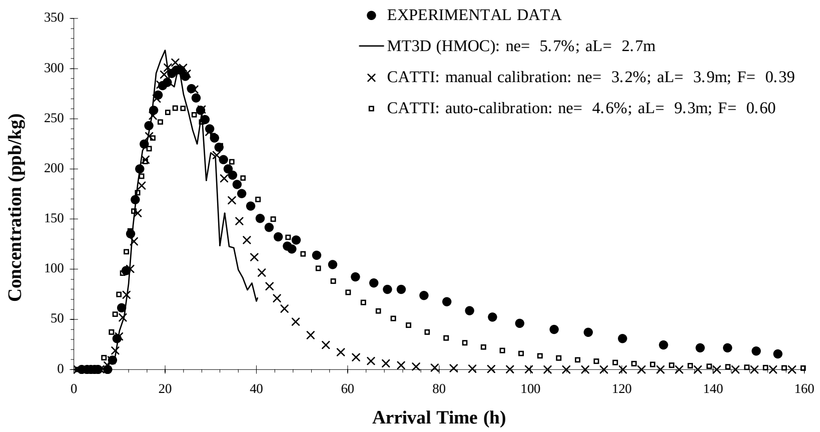


Fig. 3 Comparison of the results obtained with numerical modelling and semi-analytical solutions for injection at piezometer Pz6.

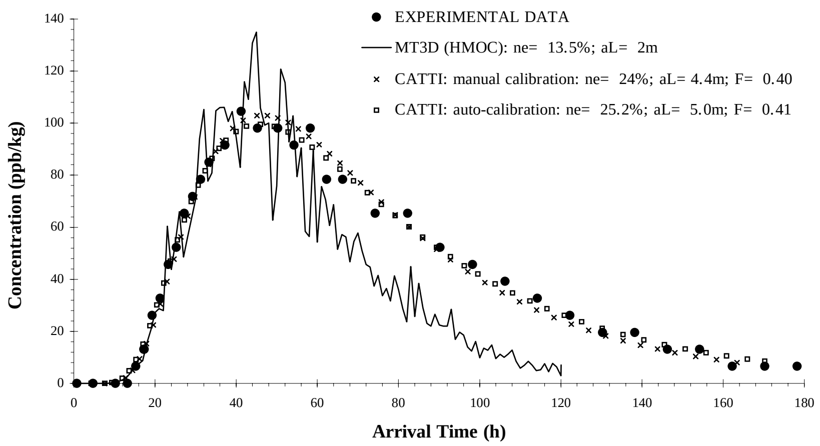


Fig. 4 Comparison of the results obtained with numerical modelling and semi-analytical solutions for injection at piezometer Pz3.

CONCLUSION

Assessment of transport parameters (effective porosity and dispersivity) from measured breakthrough curves depends strongly on the used interpretation tool. Estimation using semi-analytical solutions can lead to unreliable results, even when beautiful fitted breakthrough curves are found. Assumptions inherent to these solutions should be checked thoroughly before use: even a very weak piezometric gradient can influence radial converging flow by modifying the flow paths and the flow velocities leading to over- and underestimation of the transport parameters. On the contrary, when using a 2D numerical model taking the regional gradient and the 2D heterogeneity into account, more reliability can be awaited for the fitted parameters. Still more reliability and accuracy can be reached using full 3D groundwater flow and transport models, but the whole tracer test (injection and sampling) must then be carried out in full 3D controlled conditions (Gelhar *et al.*, 1992).

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