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USING TRACER TESTS AND NUMERICAL SIMULATIONS TO ASSESS PROTECTION ZONES IN HETEROGENEOUS AQUIFER

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Abstract

Tracer tests have been carried out in a chalky aquifer in the eastern part of Belgium. The methodology of the tests, especially concerning the control of the input of tracers into the aquifer, was chosen in order to allow accurate "a posteriori" simulations.

The transport parameters of the advection-dispersion equation are investigated assuming that the Representative Elementary Volume (R.E.V.) concept can be used. The parameters are deduced from accurate calibration computations to the observed breakthrough curves, using numerical finite element simulations. The spatial variability of the hydraulic conductivity in the investigated field is treated as determinist heterogeneities in the two-dimensional finite element model. Moreover, an important "immobile water" effect is accounted for representing the double porosity (pores and fractures) of the chalk.

Then, from transport simulations using the same finite element code, isochrone lines may be determined for the arrival of ideal, chemically nonreactive, miscible pollutants at the main pumping well. These results provide the necessary informations for a good assessment of the groundwater protection zones around the well.

Key-words: tracer test, numerical simulation, heterogeneous aquifer, protection zones.

Résumé

Des essais de traçages ont été réalisés dans un aquifère crayeux de l'Est de la Belgique. La méthodologie de ces essais, et particulièrement le contrôle de l'injection des traceurs, a été choisie de manière à permettre par la suite une simulation numérique adéquate.

Les paramètres de transport de l'équation d'advection-dispersion sont recherchés en se plaçant dans les hypothèses du concept de Volume Elémentaire Représentatif (V.E.R.). Les paramètres sont déduits de la calibration précise des simulations sur les courbes de restitution, en utilisant un modèle par éléments finis. Les variations spatiales du coefficient de perméabilité dans la zone testée sont traitées de façon déterministe comme des hétérogénéités dans le modèle à deux dimensions formé d'éléments finis. De plus, il est tenu compte d'un important effet d'eau 'immobile', représentant les processus de transport dans ce milieu à double porosité.

Ensuite, à partir de simulations de transport de contaminants utilisant le même modèle, des lignes isochrones peuvent être déterminées pour caractériser l'arrivée, au puits de pompage concerné, de substances polluantes idéalement dissoutes et non-réactives dans l'eau. Ces résultats fournissent les informations nécessaires pour une bonne estimation des zones de protection autour du puits.

Mots clés: essais de traçages, simulations numériques, aquifère hétérogène, zones de protection.

1.Introduction

It is essential to characterise the hydro-dispersive parameters of an aquifer at a particular field site in order to simulate... and try to predict the movement and the spreading of a contaminant plume at the considered location. For example, from the experimental tests and investigations, we have to find the field-scale dispersivity values which are most often greater than values determined in laboratories. Sometimes this "gap" can reach several orders of magnitude and it is usually considered as a consequence of the influence of natural heterogeneities producing irregular flow and transport patterns at the field scale (Gelhar et al., 1992).

In the study from which this paper is drawn, tracer tests have been conducted at different locations of the same chalky aquifer: the 'Hesbaye aquifer located near the city of Liège in Belgium. The purposes were (1) to examine the transport processes of a full-miscible contaminant in such an heterogeneous and fissured chalky aquifer; (2) to determine the values of the transport parameters in such conditions using analytical and numerical simulations of the tracer tests; (3) to compare with some of the values obtained at the laboratory scale; (4) to assess the prevention and protection zones to be delineated near the future pumping wells at the considered locations.

With these goals in mind and at a particular site of this 'Hesbaye aquifer', the following points will be particularly developed in this paper: (1) a description of the groundwater flow system in this chalky aquifer; (2) the experimental procedure adopted for the tracer tests; (3) the theoretical concepts and the conceptual options chosen for the simulations of the field tests; (4) the calibrations on breakthrough curves and the results of the simulations; (5) some conclusions with regard to the assessment of protection zones.

2.Groundwater flow system

The Hesbaye aquifer is represented by a chalk outcrop of 350 km^2 lying to the North of the River Meuse near Liège (figure 1). It provides by collecting galleries and pumping wells about 60000 m3/day of drinking water for Liège and its suburbs. Recently, a complete set of data relating to the geology, hydrology, geomorphology and geophysics has been collected. A three-dimensional finite element model of the flow in the aquifer has been developed by the University of Liège (Dassargues et al., 1988) to forecast changes in the heights of the water level and to provide additional interpretation about the main drainage axes in the aquifer (Dassargues, 1991). The geological sequence may be summarised as follow:

- Recent alluvial and colluvial deposits, up to 5 m thick;
- Quaternary and Tertiary sands and loess, 2-20 m thick;
- Residual conglomerate, 2-15 m thick;
- Maastrichtian chalk locally referred to as 'upper chalk'. It has been exposed to weathering and hence it is fractured, 10-15 m thick;

- Thin (less than 1 m) layer of hardened Upper Campanian chalk (or 'hardground');
- Campanian chalk, compact massive white chalk, referred to as 'lower chalk', with many fracture zones providing preferred flow routes for groundwater; 20-40 m thick;
- 'Smectite de Herve', a layer of hardened calcareous clay of Campanian age, about 10 m thick, that forms the impermeable base of the chalk aquifer.

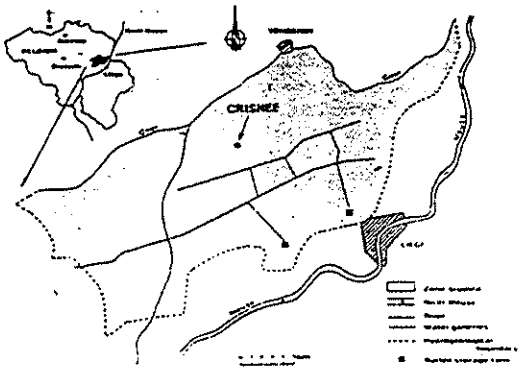

Figure 1 : Location of the 'Hesbaye aquifer' near the city of Liège in Belgium.

Values for the hydrodynamic parameters of the groundwater flow have been obtained initially from pumping tests and then carefully calibrated in the model. For the hydraulic conductivity of the chalk layers, values between 1.10^{-5} and 1.10^{-3} m/s are found and for the effective porosity assimilated to the storage coefficient (as we are in water table conditions) values from 1.10^{-2} to 1.10^{-1} are deduced.

The complex geometry of the layers and the full heterogeneity with regard to the parameters, depending on the fissuration degree, are taken into account to some extent by a full 3D finite element mesh following the different limits and sub-limits of the layers. Of course the Representative Elementary Volume (REV) theory and conceptual approach has been chosen to deduce the parameters to introduce in each finite element of the 3D mesh. The model has been calibrated against historical data from 1951 until 1992 (figure 2).

In each location where a tracer test has been conducted, a complete local investigation had to be completed previously with among other techniques: geophysics, drilling of piezometers and pumping tests.

A local 2D horizontal flow model using also the Finite Element Method (FEM) has allowed to calibrate accurately on natural conditions

(natural gradient of the piezometric heads) and on the pumping test results (drawdowns of the piezometric heads), taking into account the detailed local heterogeneity of the chalky formation near the well. Figure 3 shows the corresponding computed piezometric maps and the Darcy's specific discharge maps for natural and pumping conditions at one of the tested location at the site of Crisnée in the catchment area of the 'Hesbaye aquifer' (Biver, 1993).

For this particular site, we can observe (figure 3.b) that the computed fluxes are greater in the north-east zone where the chalk is more fissured as it has been previously detected by refraction-seismic investigations. One can remark also that even in permanent pumping conditions, there are still some fluxes going out of the detailed study zone. In these locations where water is going out of the zone, it will not be allowed to prescribe imposed concentrations for the numerical simulations describing the transport problem.

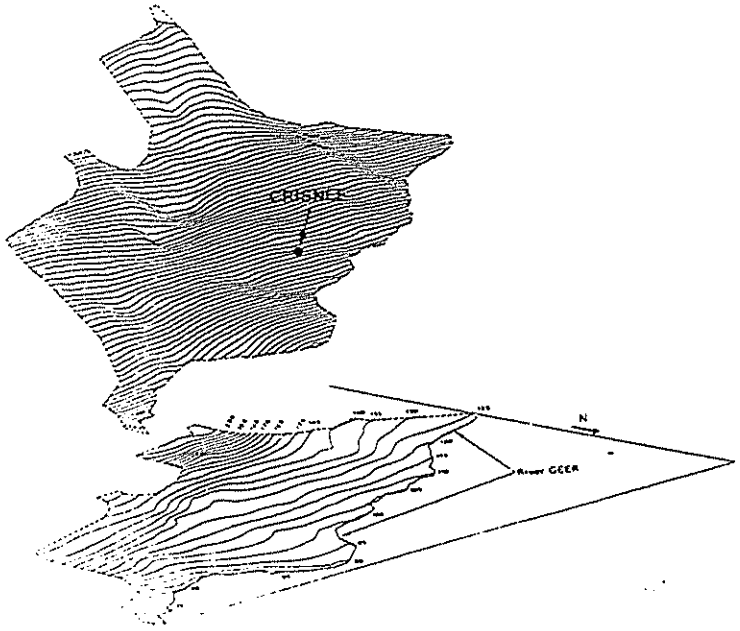

Figure 2 : Example of calibrated computed map of groundwater levels in the 'Hesbaye aquifer', corresponding to the end of 1984 (modified after Dassargues & Monjoie, 1993)

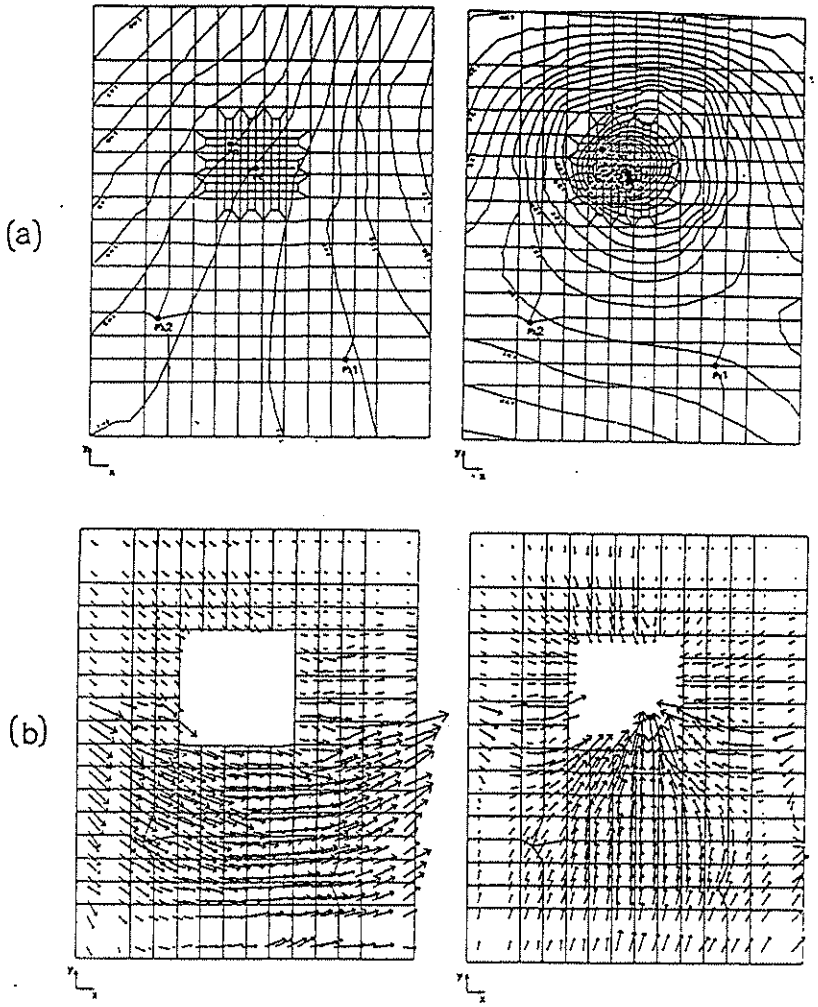

Figure 3 : (a) Computed piezometric maps in natural (left) and in pumping (right) conditions
(b) Computed vectors of the specific discharge (Darcy's law), in natural (left) and in pumping (right) conditions.

3.Experimental procedure or tracer test methodology

After 18 hours of stabilised pumping in PE (figure 3.b), the tracers have been injected in the Pz1 and Pz2 piezometers located respectively at 54.4 m and 47.7 m from PE. Another tracer has been also injected in the well PR situated at a distance of only 9.7 m from PE. Details about the methodology of these tracer tests can be found in the PhD thesis of Meus (1993).

Injections were carried out in Pz1 with uranine, in Pz2 with lithium chloride (LiCl) and in PR with naphtionate and potassium iodide (KI). As the distance between the pumping well and this last injection well is very short with regard to the influence radius of the pumping, the restitution at the pumping was very fast and complete and nearly not influenced by the dispersion process. So that we can consider that it is really a pure convection problem which can be simulated by many simple codes calibrating on the effective porosity parameter additionally to the classical hydrodynamic parameters (permeability coefficient K and effective storage coefficient S_s).

Hereafter emphasis will be given on the interpretation of the tracing test results from the piezometers Pz1 and Pz2.

The injections can be considered as instantaneous at the level of the tested aquifer by using an injection tube coupled with water injection above and below. It is a converging radial flow tracer test in the sense of Gelhar et al. (1992), and the monitoring equipment allowed only a two-dimensional analysis of the concentrations. In these conditions we are working with what is usually called depth-averaged (mixed vertically) concentrations and as Gelhar et al. (1992) have pointed out, we will underestimate the tracer concentration and as a result the longitudinal dispersivity will be probably overestimated.

The recorded breakthrough curves in the pumping well PE (figure 4) show that the restitution of the lithium from Pz2 and of uranine from Pz1 are quite different in time.

In a first attempt of interpretation, this fact can be explained by the different piezometric gradients between Pz1-PE and Pz2-PE. The heterogeneity of the aquifer (which corresponds to an heterogeneous field of permeability coefficients in the calibration of the numerical flow model) leads to different flow conditions around the pumping well and as a matter of fact the results of the transport processes in this aquifer are quite dependent of these flow conditions.

These differences in the flow conditions (figure 3) when pumping in PE can also explain the quite different observed breakthrough curves and additionally also the lower mass recovery factor found for uranine.

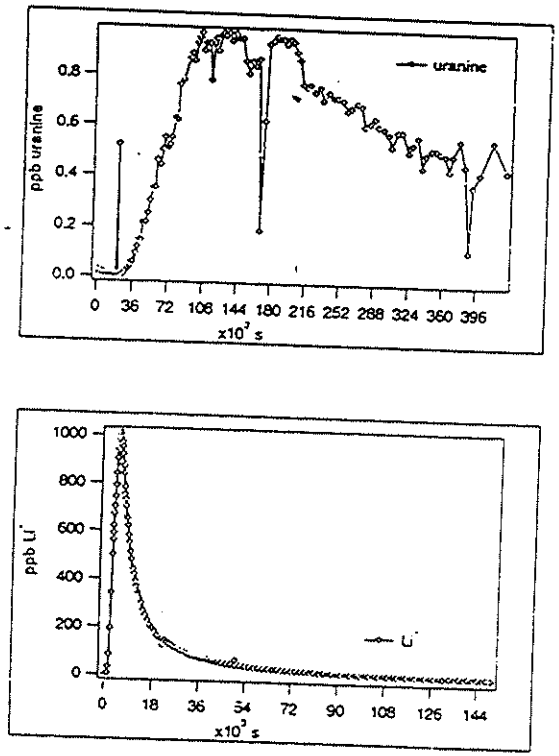

Figure 4 : Breakthrough curves at the pumping well PE for uranine and lithium.

4.Theoretical concepts for the numerical simulation

Determinist finite element models have been used for groundwater flow and transport simulations. The 3D flow model of the whole 'Hesbaye aquifer' has been previously described (Dassargues et al., 1988). The computer code which has been used is called LAGAMINE developed at the Civil Engineering Department of the University of Liège (M.S.M. Dpt) in collaboration with the Laboratory of Engineering Geology, Hydrogeology and Geophysical Prospecting of the same University (L.G.I.H.). This code uses a standard Bubnov-Galerkin formulation. In this method, the same interpolating functions are used for both the weighted residuals system and the local

description of the unknown field (piezometric heads). More details can be found in Charlier et al.(1988) and Biver (1993).

As low concentrations of miscible tracers are concerned, we can assume that flow and transport simulations can be uncoupled: no density or viscosity effects interacting on flow are taken into account.

The 'Hesbaye aquifer' is a double porosity medium: (1) porosity of pores and (2) porosity of the fissures. The permeability coefficients relative to the porosity of the pores have been estimated on basis of laboratory tests (Biver, 1991) to 1.10^{-8} m/s. On the contrary, the global permeability coefficients are varying between 1.10^{-5} and 1.10^{-3} m/s as mentioned previously.

In consequence, it is possible to describe the transport of a solute contaminant with a determinist system of classical advection-diffusion equations (applied to an equivalent porous medium) considering that the pore water can be qualified as 'immobile' water (figure 5) (Bear & Verruijt, 1987, Biver & Dassargues, 1993).

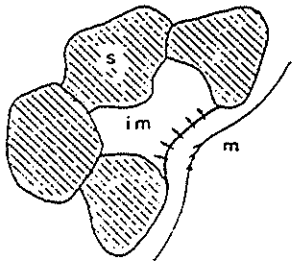

Figure 5 : Schematic representation of 'immobile' water (im) as a distinct phase.

Adsorption, reactive processes and degradation are very low in this fissured and porous chalky aquifer (Biver, 1993), and their effects on the transport of the solute can be neglected. So that the transport equations can be simplified to obtain the following system:

$$\begin{cases} \dfrac{\partial C_m}{\partial t} + div(\underline{v}.C_m) - div(\underline{D_h}\,\underline{grad}C_m) + \alpha_m(C_m - C_{im}) = 0 & (1.a) \\ \dfrac{\partial C_{im}}{\partial t} + \alpha_{im}(C_{im} - C_m) = 0 & (1.b) \end{cases}$$

where

C_m = mobile water volume concentration

C_{im} = immobile water volume concentration

$\underline{v}$ = vector of the average effective velocity

$\underline{D_h}$ = hydrodynamic dispersion tensor

$\alpha_m = \alpha_d^* / n_e$

$\alpha_{im} = \alpha_d^* / \theta_{im}$

with α_d^* (s^{-1}) = transfer constant between 'mobile' and 'immobile' water

n_e = effective porosity of the multiporous medium corresponding to the volume of 'mobile' or moving water

θ_{im} = volumetric portion corresponding to 'non-effective' porosity filled by 'immobile' water

This system includes two mass balance equations: one for 'mobile' water, the second for 'immobile' water with a transfer constant α_d^* (included in the definitions of α_m and α_{im}) representing globally (and averaged on the R.E.V.) all the interactions between 'mobile' and 'immobile' water.

As a first approximation, these interactions can be considered as dominated by diffusion processes (figure 5) between 'immobile' and 'mobile' water, but additionally, on basis of experimental results on the 'Hesbaye' chalk, Biver (1993) has found that also dispersion and linear adsorption occur. So that we have chosen a linear form similar to classical Fickian laws to obtain the term $\alpha_m(C_m - C_{im})$ in the mass balance equation of 'mobile' water and the term $\alpha_{im}(C_{im} - C_m)$ in the mass balance of the 'immobile' water.

The movement of the tracer at the average effective velocity $\underline{v}$ (m/s) of the water is expressed by the convective term: $div(\underline{v}.C_m)$. The effective averaged velocity ($\underline{v}$) is obtained from the Darcy's specific discharge ($\underline{q}$) divided by the effective porosity (n_e) :

$$\underline{v} = \underline{q} / n_e \qquad (2)$$

Using the fact that $div(\underline{v}) = 0$, this convection term is reduced to $\underline{v}.\underline{grad}C_m$.

The mechanical dispersion corresponding to the spreading of this ideal chemically nonreactive conservative solute in an homogeneous fluid (water) is presumed to be Fickian, i.e. the dispersive mass flux is proportional to the concentration gradient. The term $div(\underline{D_h}\,\underline{grad}C_m)$ represent the net dispersive spreading flux due mainly to the variations of the velocities around

the average convective position. In isotropic porous media, this flux is characterised by the tensor $\underline{D_h}$ (m^2/s). Neglecting the molecular diffusion coefficient because of the high awaited velocities due to the high permeability values in this chalky aquifer, the dispersion tensor is completely defined by the longitudinal and lateral dispersivities a_L and a_T (m). Moreover, it is difficult at a macroscopic scale to differentiate clearly the diffusion effects from the dispersion effects.

In two dimensions the three components of the dispersion tensor can be reduced to :

$$\begin{cases} D_{h_{xx}} = (a_L v_x^2 + a_T v_y^2)/|v| \\ D_{h_{yy}} = (a_T v_x^2 + a_L v_y^2)/|v| \\ D_{h_{xy}} = D_{h_{yx}} = (a_L - a_T).v_x.v_y/|v| \end{cases} \quad (3)$$

The classical finite element method, using the Bubnov-Galerkin scheme, is not efficient to solve the advection-diffusion equation. If this method is tried some spurious wiggles are found. In fact, there is a fundamental difficulty in the solution of this transport equation because of the simultaneity of the advection and dispersion processes; they contribute to the total mass transport of the solute very differently. As mentioned above, the convection is a transport along streamlines of the flow and the dispersion is a transport by spreading both along and between these characteristic lines

Mathematically, this means that we have simultaneously hyperbolic terms representing the convection/advection, in the same equation with parabolic terms of the dispersion. The integration of this kind of equation is still a problem that no numerical method has yet fully overcome (Yeh, 1993)

The numerical methods which are used for solving the transport equations may be classified into three categories: (1) Eulerian methods where an Eulerian form of the equation is solved at the nodes of a fixed grid, requiring the simultaneous solution of hyperbolic and parabolic operators; (2) Lagrangian methods where a Lagrangian form of the equation is solved in grids moving with the fluid, avoiding the explicit treatment of hyperbolic terms but involving often a set of points (moving grid) which becomes gradually very distorted during the motion and the computation of partial derivatives is then very complicated; (3) Eulerian -Lagrangian methods where one try to combine the best aspects of the two other categories.

Two of these methods have been introduced by Biver (1993) in the LAGAMINE code:

(1) An Eulerian method called 'Full Upwind Petrov Galerkin method' (F.U.P.G.) (for details see Yu & Heinrich, 1986 and 1987, and Biver, 1993). The weighting functions are modified to obtain more representative

weighted residuals: they are off-centred in space and in time to give more importance to upstream areas to avoid numerical dispersion effects.

(2) An Eulerian-Lagrangian method called 'Hybrid Eulerian Lagrangian Method' (H.E.L.M.) (for details see Yeh, 1990 and Biver, 1993). A particle-tracking method is applied to the convection component of the transport, and classical weighting functions are kept for the remaining terms of the equilibrium.

Using these two methods, Biver (1993) has established a criterion deduced from the respective limitations of each method. It is based on the Courant number (Cr) characterising the studied problem:

$$Cr = \left|v_{averaged}\right| . \Delta t \Big/ \Delta l \quad (4)$$

where $\left|v_{averaged}\right|$ = the modules of the averaged convection velocity in the finite element

Δt = the time step used in the numerical simulation

Δl = the finite element length in the direction of $v_{averaged}$

The stability of the F.U.P.G. method requires that $Cr < 1$, and the H.E.L.M. is really efficient and accurate when $Cr > 1$. The combination of the two methods in the same code allows very flexible choices in term of time steps for the user.

5.Results and calibration of the numerical model

The discretized finite element meshes are presented at the figure 6 for the transport simulation of lithium from Pz2 and of uranine from Pz1.

According to the reduced transport equation described above, the remaining transport parameters to calibrate are: a_L, a_T, α_d^*, n_e and θ_{sw}. However, the 'averaged' two-dimensional analysis of the concentrations introduces in the calibration an additional subjective parameter: the mean aquifer thickness (e_m) concerned by the tracer plume. One of the usual approach consists in choosing the same thickness for the plume that for the injection thickness (e_{inj}) in the injection piezometers. But it is only a very rough approximation of the reality and in our calibration we have chosen to change this value in some places where the vertical fissuration of the chalk aquifer has probably induced important spreading of the tracer in the vertical direction. Of course the estimation of the convective velocity of the tracer is strongly affected by this simplification of the reality and it can be the cause of the imperfect agreement found between the calibrated and measured breakthrough curves (especially for the lithium) and also the main reason (additionally to the heterogeneity of the aquifer) why the calibrated transport parameters are so different for lithium and for uranine.

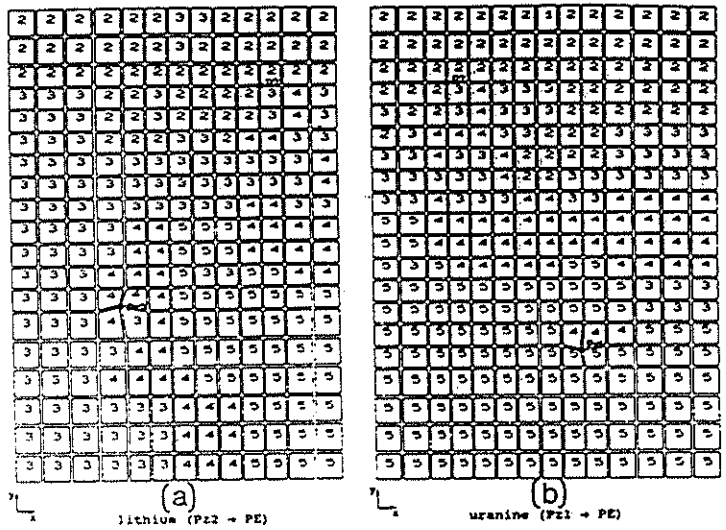

Figure 6 : Finite element meshes and 'materials' of the discretizations for lithium and uranine tracer tests transport simulations.

Other tracer tests performed previously (Biver & Meus, 1992, Meus, 1993, and Biver, 1993) have provided some order of magnitude of the transport parameters in the chalk in other parts of the same aquifer. Taking into account those results, five different 'materials' are distinguished on basis of the values of their transport parameters (tables 1 and 2).

Transport parameters	material 1	material 2	material 3	material 4	material 5
α_T (m)	0.05	0.25	0.32	0.50	0.65
α_L (m)	0.5	2.50	3.20	5.00	6.50
α^*_L (s^{-1})	1.10^{-7}	$1.2\ 10^{-7}$	$2.5\ 10^{-7}$	5.10^{-7}	6.10^{-7}
n_e (%)	0.3	0.5	1.0	1.5	2.0
θ_m (%)	8.0	10.0	13.0	18.0	20.0
e_m (m)	15.0	7.5	4.0	4.0	4.0

Table 1 : Calibrated transport parameters for the lithium tracer test between Pz2 and PE.

Transport parameters	material 1	material 2	material 3	material 4	material 5
α_T (m)	0.05	0.32	0.5	0.7	0.95
α_L (m)	0.5	3.20	5.0	7.0	9.5
α^*_L (s^{-1})	1.10^{-7}	$3.7\ 10^{-7}$	$6.7\ 10^{-7}$	$7.9\ 10^{-7}$	$1.5\ 10^{-6}$
n_e (%)	0.3	1.5	2.7	5.3	11.3
θ_m (%)	8.0	19.0	24.0	31.0	42.0
e_m (m)	15.0	10.0	15.0	15.0	15.0

Table 2 : Calibrated transport parameters for the uranine tracer test between Pz1 and PE.

Nevertheless, the 2D spatial distribution of both tracers in the mobile water reflects clearly two different behaviours (figure 7) due mainly to the heterogeneity of the aquifer.

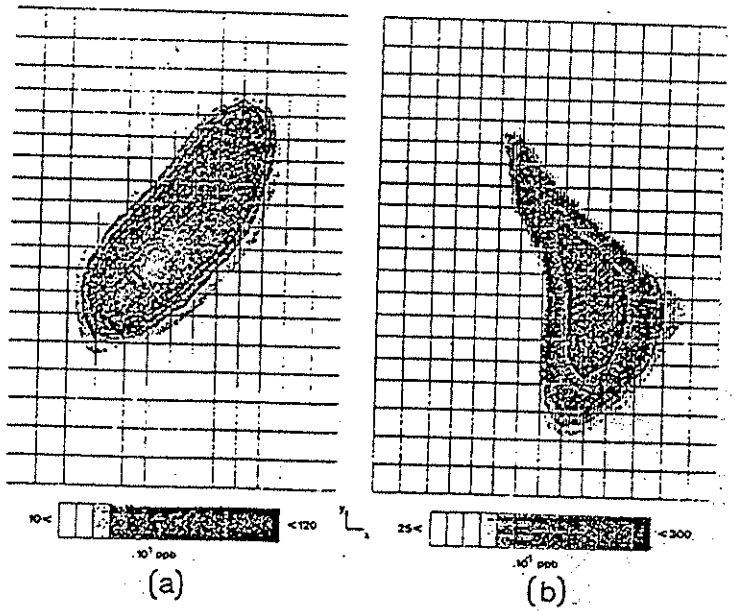

Figure 7 : Computed concentrations in the 'mobile' water
(a) for the lithium after 12 hours $\Delta C_m = 100 ppb$
(b) for the uranine after 100 hours $\Delta C_m = 2.5 ppb$.

The computed plume of injected lithium (figure 7.a) has a regular shape with a long ridge. This shape is largely due to the fact that the migration velocity of the tracer decrease strongly when passing successively in the zone with lower fracturation (lower permeability coefficient).

The computed plume of injected uranine (figure 7.b) is wider and is spreading in two main directions. One of them corresponds to a fissured axe between Pz1 and PE, the second direction corresponds to the regional groundwater flow.

When looking to the immobile water concentrations, one can remark (figure 8) that the high concentrations in tracers are simulated as staying in each case in a zone very close to the injection piezometer.

Figure 9 shows the total transport fluxes of tracer mass. Comparing the computed fluxes to the Darcy's fluxes of figure 3, we can deduce that they are mainly dominated by the convection process.

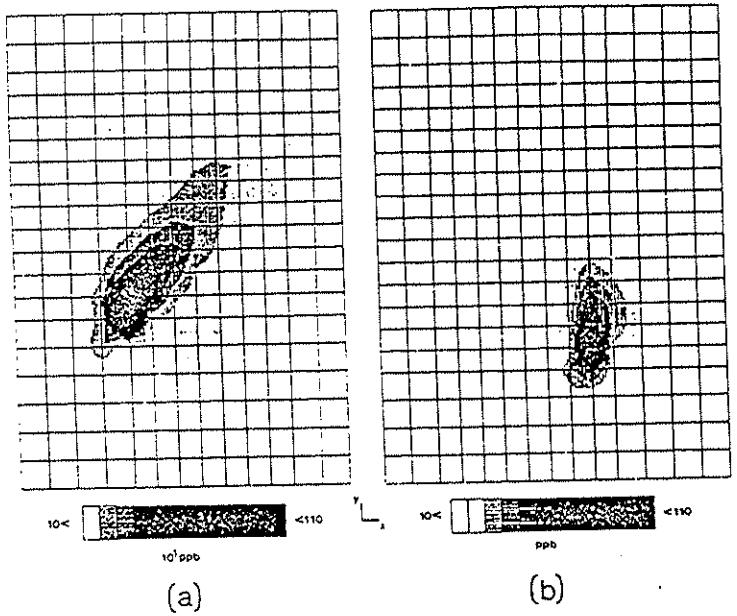

Figure 8 : Computed concentrations in the 'immobile' water
(a) for the lithium after 12 hours $\Delta C_{im} = 100 ppb$
(b) for the uranine after 100 hours $\Delta C_{im} = 10 ppb$.

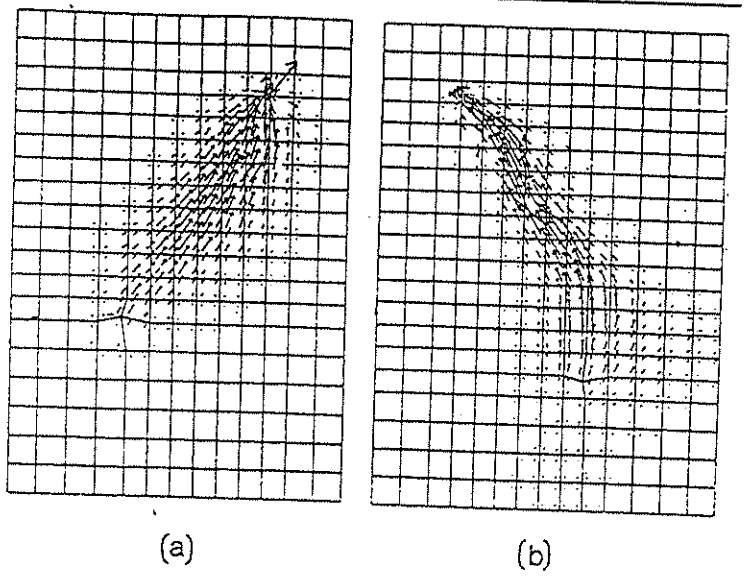

Figure 9 : Computed total transport mass fluxes
(a) for the lithium after 12 hours ($f_{max} = 8.8\ 10^{-4} kg/m^2/s$)
(b) for the uranine after 100 hours ($f_{max} = 1.1\ 10^{-4} kg/m^2/s$)

Comparing maps of 'mobile' and 'immobile' water concentrations, we can remark that a large amount of tracer is provisionally captured in the 'immobile' water near the injection piezometer. In the breakthrough curves (figure 10) it induces a long tail in the curve as the pollutant is slowly restored from the 'immobile' water into the 'mobile' water.

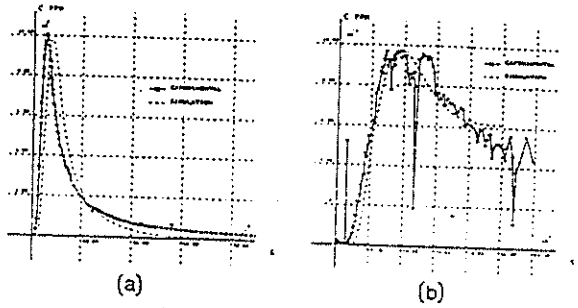

Figure 10 : Experimental and calibrated breakthrough curves in PE.
(a) for lithium
(b) for uranine

6.Conclusions and assessment of protection zones around the tested well

From tracer tests results added to other geological, geophysical and hydrogeological investigations, first conclusions have been made on the heterogeneous nature (due essentially to local fracturations) of this double porosity aquifer in the Cretaceous chalks of Belgium.

Numerical simulations using adapted finite element methods have been preferred to analytical solutions in order to include in the models a maximum of the available informations. The spatial heterogeneity of the aquifer has been taken into account for both flow and transport simulations. Additionally, the double porosity effect is included in the simulated interactions between 'mobile' and 'immobile' water.

The transport parameters are deduced from the calibration on the experimental breakthrough curves. It is reasonable to think that we can use them for the assessment of the protection zones around the pumping well. But we are not allowed to use these coefficients at the regional scale as it is evident that a strong scale effect can be predictable in this kind of aquifer.

In order to establish isochrone lines which are usually used in the definition of the protection zones, we could now make some repetitive simulations of injections at different nodes of our discretized mesh As results we will obtain the different breakthrough curves at the pumping well (for each injection) and the maps of concentrations at the time that we choose On basis of all these results it will be possible to draw the isochrone lines of the protection zones taking into account the heterogeneity and the double porosity characteristics of the aquifer

7.Acknowledgements

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