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COMPUTATIONAL METHODS IN WATER RESOURCES X

Volume 1

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USING A NUMERICAL MODEL OF TRANSPORT BASED ON A DETERMINISTIC THEORY TO INFER WELL PROTECTION ZONES IN A CHALKY AQUIFER.

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The aim of this paper is to show how tracer test results may be used to determine isochrone lines around a pumping well, for a specified input of solute, in the chalky aquifer of Hesbaye (Belgium).
The use of a deterministic numerical model is interesting as it includes not only convection (as usual), but also the other main transport processes. The influence of the input function is discussed and a methodology to apply this model at a regional scale is given as a conclusion.

INTRODUCTION

The chalky aquifer of Hesbaye is an important water resource in Belgium. It is the main water supply for the town of Liège and its suburbs. In recent years, risks of accidental or diffuse pollutions due to agricultural practices and hazardous waste disposal have increased. For this reason, it is important to define protection zones around pumping wells in order to prevent water pollution and to adapt water production if such a problem occurred.
This paper, divided in three parts, describes a methodology to achieve this goal. In the first part, we give a brief account (see references for details) of tracer tests interpretations performed to obtain transport coefficients of the chalk and to characterize heterogeneities around the well of Crisnée (a production well near a little village of the Meuse valley). In the second part, emphasis is put on the numerical model. The numerical methods used to solve the equations are described. In the third part, we discuss the results obtained by using the same model to quantify the time arrival of a pollutant spill coming from different locations in the neighbourhood of the well.

TRACER TESTS INTERPRETATIONS

Below the site of Crisnée, we observe a typical geological sequence of Hesbaye cretaceous formations: under recent alluvial and colluvial deposits, lays a residual conglomerate with a clayey level at the base. Beneath this level, the chalky aquifer is semi-confined. The aquifer has been tested by a high rate pumping test (125 m^3/h). After stabilisation (18 hours), tracers (uranine and lithium chloride) have been injected in the nearby piezometers (Pz1 and Pz2, see figure 1). These tests have been interpreted in terms of a heterogeneous medium, due to the occurrence of a major fractured zone in the vicinity (figure 1). The geometrical description of heterogeneities has been defined on the basis of a geophysical prospecting on the site.

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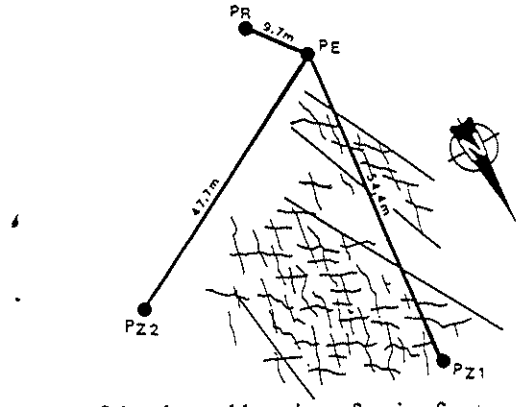


Figure 1: Equipment of the site and location of major fractured zones (Crisnée)

Using the numerical simulator (described below), the following flow and transport characteristics have been obtain by Biver (1993 & and 1994) resulting from detailed calibration procedures.

coefficient	range (from weakly to highly fractured zones)
K (permeability coefficient)	$1\ 10^{-5} \rightarrow 5\ 10^{-5}$ m/s
n_{eff} (effective porosity)	0.5 → 10.0 %
n_{im} ("non effective" porosity)	10 → 40 %
α_d^* (transfer coefficient for dual porosity effect)	$1.0\ 10^{-7} \rightarrow 1.5\ 10^{-6}$ m/s
a_T (transversal dispersivity)	0.1 → 1.9 m
a_L (longitudinal dispersivity)	0.5 → 9.5 m

Table 1: Flow and transport coefficients obtained from calibration of Crisnée tests.

Those coefficients correspond to the following mass balance equations:

$$div(-K.grad\,h) = div(n_{eff}.\vec{v}) = 0 \qquad (1a)$$

$$\frac{\partial c_m}{\partial t} + \vec{v}.grad\,c_m - div(\underline{D}.grad\,c_m) + \alpha_m.(c_m - c_{im}) = 0 \qquad (1b)$$

$$\frac{\partial c_{im}}{\partial t} + \alpha_{im}.(c_{im} - c_m) = 0 \qquad (1c)$$

with $\alpha_m = \alpha_d^* / n_{eff}$

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

$(\underline{D})_{ij} = a_T.|\vec{v}|.\delta_{ij} + (a_L - a_T).v_i.v_j / |\vec{v}|$

In this system, one can recognize in (1a) the well-known steady state flow equation, written in terms of piezometric head (h) as the aquifer is considered to be confined. Equation (1b) is the transport equation which describes the variation of concentration c_m in the moving fluid (say in the fractures). It takes into account convective and dispersive fluxes, but also a dual porosity effect involving the so-called "non moving" fluid, located mainly in the pores of the chalk. The mass balance in the pores is given by (1c), describing the variation of concentration in this "non moving" fluid (c_{im}).

NUMERICAL MODEL.

The system defined by equations 1a,b,c has been solved with a finite element method, implemented in the LAGAMINE code (developed in the Civil Engineering Department of the University of Liège). The complete methodology can be summarized as following:

1°) The flow equation (1a) is uncoupled and treated classically with a standard Bubnov Galerkin weighting of the residuals (already implemented in the code).
We write:

$$\int_V div\left[-K.grad\left(N_i(\vec{x}).h_i\right)\right].N_j(\vec{x}).dV = 0 \qquad j = 1,\ldots,N \qquad (2)$$

with $N_i(\vec{x})$ the interpolating function for node i of the finite element mesh,
h_i the nodal piezometric head,
N the total number of nodes,
V the simulation domain.

The solution provides the effective velocities ($\vec{v}$), defining the convective flux in (1b)

2°) The mass balance equation in the "non moving" fluid can be solved analytically as it is demonstrated below.
Let us discretize c_m on each time step $\Delta t = t_{n+1} - t_n$. We have:

$$c_m = c_m^{t_n}.N1(t') + c_m^{t_{n+1}}.N2(t') \qquad (3)$$

with $N1(t') = 1 - t'/\Delta t$

$N2(t') = t'/\Delta t$

$t' = t - t_n$

Then, (1c) can be written as:

$$\frac{\partial c_{im}}{\partial t'} + \alpha_{im}.c_{im} - \alpha_{im}.\left(N1(t').c_m^{t_n} + N2(t').c_m^{t_{n+1}}\right) = 0 \qquad (4)$$

which can be solved analytically versus time.

We obtain:

$$c_{im}(t') = c_{im}^{t_n}.\exp(-\alpha_{im}.t') + c_m^{\cdot\, t_n \rightarrow t_{n+1}}.t' + \left(c_m^{t_n} - c_m^{\cdot\, t_n \rightarrow t_{n+1}} / \alpha_{im}\right).(1 - \exp(-\alpha_{im}.t')) \qquad (5)$$

with $c_m^{\cdot\, t_n \rightarrow t_{n+1}} = \dfrac{c_m^{t_{n+1}} - c_m^{t_n}}{\Delta t}$

Result (5) in equation (1b) provides a single transport equation in terms of c_m :

$$L(cm) = \frac{\partial cm}{\partial t} + \bar{v}.\,grād\,cm + other\ terms \qquad (6)$$

3°) The single transport equation (6) is the most difficult to solve due to the convective component ($\bar{v}.grād\,c_m$). If a standard Bubnov Galerkin method is applied, it leads to instabilities which manifest as spurious wiggles on the concentration profiles. To avoid this effect, without introducing artificial dispersion, two new methods have been programmed.

• The first method uses modified weighting functions, in order to obtain more representative weighted residuals. These weighting functions are off-centred in space and time to give more importance to upstream areas without numerical dispersion effect. For this reason, it is called the Full Upwind Petrov Galerkin method (F.U.P.G.). Mathematically, we can write:

$$\int_{\Delta t}\int_{V} L(cm).W_j(\bar{x},t').dV.dt' = 0 \qquad j = 1,\ldots,N$$

$$\Rightarrow \int_{\Delta t}\int_{V} L\left(N1(t').c_m^{tn} + N2(t').c_m^{tn+1}\right).W_j(\bar{x},t').dV.dt' = 0 \quad j = 1,\ldots,N \qquad (7)$$

with $W_j(\bar{x},t') = N_i(\bar{x}).W^t(t') + \Delta W_{j1}(\bar{x}).W^t(t') + \Delta W_{j2}(\bar{x}).\Delta t/2.\partial W^t(t')/\partial t'$

$\Delta W_{j1}(\bar{x}) = \alpha.\Delta l/2.\bar{v}_m/|\bar{v}_m|.grād\,N_j(\bar{x})$

$\Delta W_{j2}(\bar{x}) = \beta.\Delta l/2.\bar{v}_m/|\bar{v}_m|.grād\,N_j(\bar{x})$

$W^t(t') = 4.N1(t').N2(t')$

$\alpha = \coth(Pe/2) - 2/Pe$

$\beta = Cr/3 - 2.\alpha/(Pe.Cr)$

$Pe = |\bar{v}_m|.\Delta l/D_L$ = Peclet number of the considered finite element

$Cr = |\bar{v}_m|.\Delta t/\Delta l$ = Courant number of the finite element

$\bar{v}_m$ = average convection velocity on the finite element

Δl = finite element length in $\bar{v}_m$ direction.

From these expressions one can see that weighting functions are off-centred with two coefficients (α and β) which are optimized to avoid numerical dispersion (Yu and Heinrich 1987).
This numerical scheme is able to treat convection dominated problems as well as dispersion dominated ones if the stability condition $Cr < 1$ is respected. For high convection velocities, this restriction may induce an excessive time discretization refinement. But in our practical case, this limitation is rarely prohibiting.

• The second method, the Hybrid Eulerian Lagrangian Method (H.E.L.M.), treats the convection component with a particle-tracking routine. This allows us to keep

the classical weighting functions in the remaining equilibrium. It can be summarized as following.
Time variation of concentration observed in Frenet axes (moving with convected particles) can be written:

$$\frac{dcm}{dt} = \frac{\partial cm}{\partial t} + \bar{v}.grād\,cm \qquad (8)$$

Result (8) in equation (6) gives: $$L'(cm) = \frac{dcm}{dt} + other\ terms \qquad (9)$$

This equilibrium leads to the following scheme:

$$\int_{\Delta t}\int_{V} L'(cm).N_j(\bar{x},t').dV.dt' = 0 \qquad j = 1,\ldots,N$$

$$\Rightarrow \int_{\Delta t}\int_{V} L'\left(N1(t').c_m^{tn} + N2(t').c_m^{tn+1}\right).N_j(\bar{x}).W^t(t').dV.dt' \quad j = 1,\ldots,N \qquad (10)$$

with $W^t(t') = \delta(t'=\Delta t)$ = collocated function in t_{n+1} (better for large time steps)

$$\frac{dcm}{dt} = \frac{c_m^{tn+1} - c_m^{*tn}}{\Delta t}$$

c_m^{*tn} = Lagrangian concentration of the particle; it is the concentration which could be observed at time t_{n+1} if the transport was purely convective; it is obtained by reverse particle tracking of global nodes and of intermediate hidden nodes if it is necessary (Yeh 1990).

This new approach is well suited to convection dominated problems but can take into account a non negligible dispersion. It gives better results for larger time steps and requires the condition $Cr > 1$. Time step length is only restricted by dispersion or immobile ("non moving") water effect.

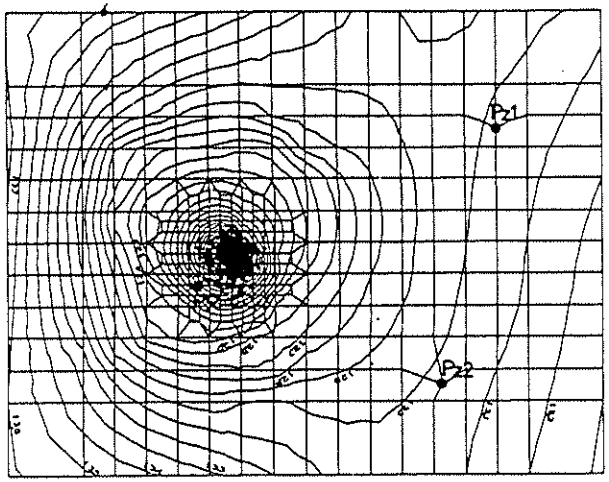
It is clear that those two methods are complementary. Covering all ranges of Cr allows the user to choose time discretization in terms of physical phenomena and not in terms of the numerical scheme's stability. For not purely convective problems, it is even possible to use both methods together with mixed grids (H.E.L.M. and F.U.P.G. finite elements).

Tests have been made in that direction (Biver 1993). However, for previous and subsequent applications, the F.U.P.G. method has been proved to be more efficient.

ASSESSMENT TO WELL PROTECTION ZONES.

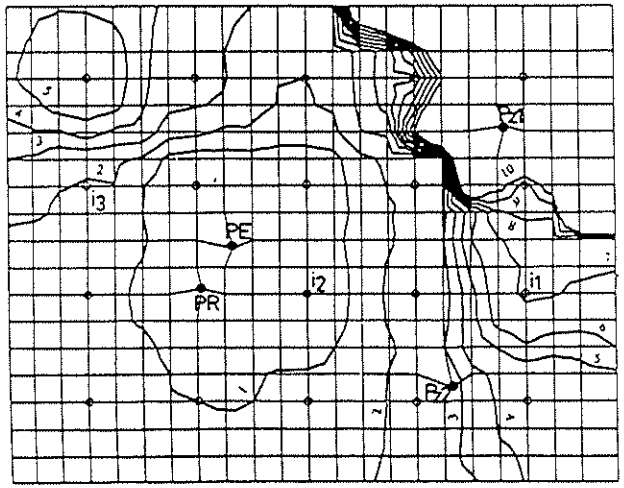
Once the numerical model has been calibrated on pumping tests and tracer breakthrough curves, we can keep flow results, transport coefficients, and discretization to infer aquifer behaviour in some prediction situations.

A local pollution with nitrates, at a rate of 1.2 kg/hour, stopped after 5 hours, has been simulated in 20 locations covering all the area around the well. An injection flow rate of 0,25 m³/hour has been considered. The concentration of the spill is supposed to be 10 g/l. The injected surface varies with the effective porosity and the thickness of the fissured zone at the injection point. Its order of magnitude is around 0.5 m². To model the transfer at the injection point, and to quantify the real input function of pollutant in the aquifer, a special finite element has been used. It takes into account the convection velocity variation in the injection area (which leads to a mixed boundary condition for the dispersive flux).



dh = 0.1 m

a) Piezometric head contours (permanent flow).



dt = 1 hour

b) Isochrone lines for a concentration of 10 mg/l at the pumping well (injection of 10 gr/l during 5 hours at a rate of 0,25 m³/h).

Figure 2: Numerical results in pumping conditions (125 m³/h).

With simulation based on the piezometry represented on figure 2a, we can calculate the isochrone lines corresponding to the arrival, at the pumping well, of the very first significant concentrations (i.e. 10 mgr/l or 10 ppm). This result is presented on figure 2b, it is obtained by interpolating the values for the simulated injections. These contour lines are more objective than those which could be obtained by particle tracking. They reflect the three main components of transport in the chalky aquifer of Hesbaye (convection, dispersion, and immobile water effect).
After a quick look, one can see that the zone which is preferentially affected by the pollution around the well is in the direction of piezometer PR. However this zone does not correspond to the known fractured area. This is due to the regional flow of the aquifer which inhibits the pumping flow in this area and which increases it near piezometer PR. For the same reason, a part of the aquifer is totally unaffected by this particular pollution.
If we examine in details the results for 3 injection points (figure 3 a, b, and c,), we can understand that, on the basis of the breakthrough curves, it is possible to generate a great number of isochrone lines associated to different criteria. For instance, if our concentration limit is raised to 50 mgr/l (which is the standard for nitrate pollution in Belgium), the safe zone will be greater including the area represented by injection i_1. This kind of sensitivity analysis is not possible with the particle tracking method.

Moreover, by drawing the isoconcentration curves, we can have an idea of the pollution spreading; it is even possible to define, from those results, the limits of the polluted zone and its evolution in time.

CONCLUSION

We have presented here a methodology, based on a 2D deterministic numerical model, tc determine protection zones around a pumping well in a double porosity medium. This method requires more data than the classical particle tracking method but is more rigorous and also flexible to the choices made by the interpreter (concentration limit and pollutant input function).
However, some work still remains:
- the generalisation of the model in 3D to improve our interpretations.
- applying such a methodology to quantify the main movements of nitrates, at the regional scale, in the saturated zone of Hesbaye aquifer.

If the first improvement is relatively obvious, the second is much more difficult. Indeed, nitrate transport in the fractured chalk of Hesbaye is subject to a scale effect problem which is still to be solved. It is more predictable than in a karstic zone but is still due to a fracture network, unlike a simple porous medium. On the available evidence it is unclear whether a continuum exists at high distances; but in our opinion, this may be the case. More tracer experiments are needed to characterize this scale effect. A study of fracture distribution in chalk could also be helpful to define precisely the representative element o volume for transport at regional scale.

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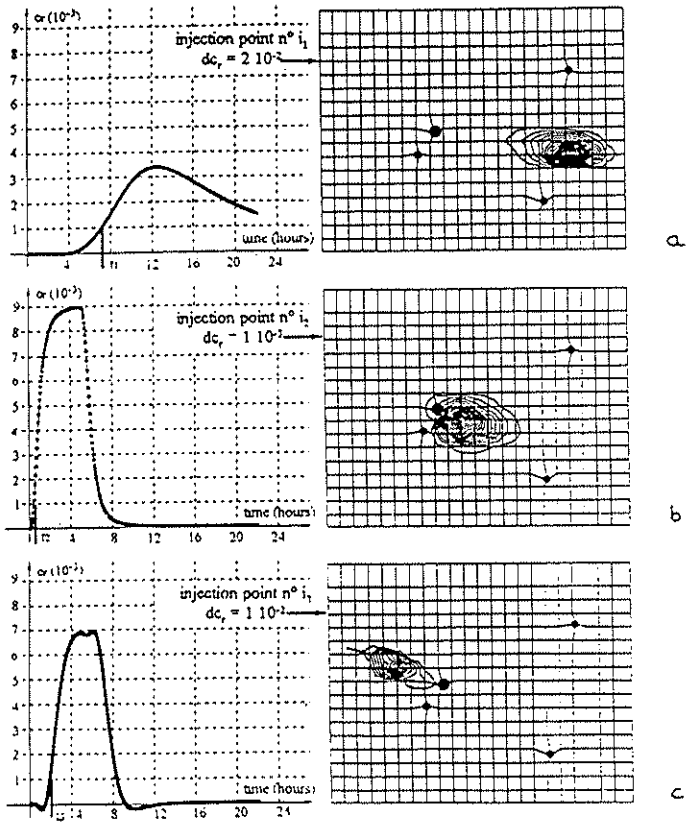

Figure 3: Detailed results of three simulated injections.

REFERENCES

Bear J. & Verruijt A. (1987), "Modelling ground water flow and pollution", Reidel Publ. Company. 415 p.

Biver P. (1994), "Numerical simulation of tracer tests to quantify, at a macroscopic scale, transport processes in a multiporous aquifer", to be published in the proceedings of the I.A.H.R. International Symposium on Transport and Reactive Processes in Aquifers (Zurich, 11-15 April 1994).

Biver P. (1993), "Etude phénoménologique et numérique de la propagation de polluants miscibles dans un milieu à porosité multiple (application au transport des nitrates dans l'aquifère crayeux du Crétacé de Hesbaye)", Ph.D.: University of Liège.

Meus Ph. (1993), "Hydrogéologie d'un aquifère karstique dans les calcaires carbonifères (Néblon Anthisnes, Belgique); apport des traçages à le connaissance des milieux fissurés et karstiques", Ph.D.: University of Liège.

Yeh G.T. (1990), "A Lagrangian-Eulerian method with zoomable hidden fine mesh approach to solving advection-dispersion equations", Water resources research 26: 1133-1144.

Yu C.C. & Heinrich J.C. (1987), "Petrov-Galerkin methods for the multidimensional time dependent convective-diffusion equations", International journal for numerical methods in engineering 24: 2201-2215.