

Are deterministic numerical models helpful to delineate groundwater protection zones in karstic aquifers?

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ABSTRACT: In karstified media, the main difficulty consists in finding a good adequation between the heterogeneous reality of the aquifer and its representation using "equivalent" parameters in the framework of the Representative Elementary Volume (REV concept). The parameters describing the aquifer (hydraulic conductivity, effective porosity, dispersivities, ...) chosen with "equivalent" or averaged values on the REV, do not describe with accuracy the reality of the aquifer but they represent globally the behaviours of the different zones of the aquifer.

A practical case study is described where a finite element model using the REV concept has been realised. The study was asked by a Belgian water supply company, exploiting three wells producing about 3000 m³/day from a limestone karstified aquifer. More than 10 piezometers have been drilled, pumping and multi-tracer tests have been completed and interpreted. The finite element model used to simulate the transport and filtration processes has been realised using the code AQUA. The results of the study show the difficulty to represent adequately the particular behaviour of the aquifer.

From this example, many lessons can be drawn about the advantages and the limitations of the application of a REV based model in karstic hydrogeological conditions. Emphasis is given to the consequences on the way of considering the delineation of protection and prevention zones around production wells in karstic aquifers.

1 NUMERICAL MODELS APPLIED TO KARSTIFIED AQUIFERS

As recalled by Bear (1993), the modelling activities on a case study are conducted primarily to achieve the following activities: (1) to predict the future behaviour of the studied aquifer in response to new solicitations, (2) to provide informations required in order to comply with local regulations, (3) to obtain a better understanding of the aquifer system from the geological, hydrogeological and chemical point of view, (4) to provide informations for the design of future observation networks and field experiments.

The geologic medium is not an engineering system, and to characterize it in detail and deterministically, so many boreholes would be necessary that it would be no longer the same medium as at the beginning (Tsang *et al.*, 1994). The modelling approach is a part of the whole program of investigations coupling site characterisation and predictive assessment to know with a better reliability the groundwater flow and solute transport processes occurring in the studied medium.

Models describing the movement of contaminants through the discontinuous and highly heterogeneous karst media can be classified in four groups: models based on the REV approach, models based on a discrete approach, geostatistical models and black box mathematical models.

1.1 REV approach

When dealing with numerical models used to simulate local or regional groundwater flow and transport situations, the classical approach is to consider the aquifer as a continuous porous medium. It is practically realised using the concept of Representative Elementary Volume (REV) described very clearly by many authors.

This concept needs to consider the continuum approach at a macroscopic level at which quantities can be measured and boundary-value problems can be solved (Bear & Verruijt, 1987). Of course, one still has to choose the appropriate size for the averaging volume.

using this "discrete approach" in a model, the main dependent variables are defined and calculated only in the conduit areas effectively described (discretized) in the model.

A more complete and accurate solution consists in combining a discrete model to represent explicitly the main karst conduits and the more important fissures, with a classical model assuming continuity with equivalent flow and transport parameters in order to represent the matrix of the aquifer as a porous medium. One of the difficulties is due to the quite different time scales. For flood events in karst conduits the scale is in the order of hours whereas in porous media they are in the order of days, weeks and months (Trösch & Zurbrigg, 1993).

Modelling academic cases, Rossier & Kiraly (1992) have varied the density, the topology and the dispersivity of the karst network which is draining the fissured and slightly karstified volumes, to simulate flow and tracing tests for different theoretical aquifers with different karstification degrees.

1.3 Geostatistical approach

The "geostatistical approach" consists in generating by a stochastic method some karstic media statistically equivalent to the studied aquifer. On basis of all available data, conditional simulations tend to reconstitute different karstic media having in common a similar behaviour with respect to the measurements and data. Normally, this approach satisfies the constraints required by hydrogeological applications (Jaquet & Jeannin, 1993). The generated media are equiprobable and, the uncertainty and the confidence interval of each parameter of the model can theoretically be known, if the assumption (often admitted) that the committed errors on the model parameters can be considered as normally distributed (Gaussian law). Consequently, the uncertainty of the provided solution can also be computed.

1.4 Black-box models

In highly karstified aquifers, it is sometimes very difficult to adopt a "physically consistent" model using any of the techniques described above. The reason is always the insufficient knowledge of the real functioning karst system and the general lack of accurate topological and geometrical data concerning the main karst conduits. In that case, simulations of the whole karstic system are usually

in the fissured media and "a fortiori" in the karstified media, the main difficulty consists in finding a good adequation between the highly heterogeneous reality and the REV concept. The parameters describing the characteristics of the aquifer (permeability coefficient, effective porosity, dispersivities,...) chosen with "equivalent" or averaged values on the REV, do not describe with accuracy the reality of the aquifer as they represent globally the behaviour of the different zones of this aquifer. The lack of precision in the representation of the reality depends strongly on the scale at which the problem is considered. It is evident that this "averaging procedure" of the aquifer properties on a volume of aquifer (sometimes very large), is as much the less accurate as the studied problem is strictly a local situation treated with large REV. However, the "local scale" or "regional scale" are relative definitions.

For fissured and slightly karstified aquifers, this approach has been used widely to simulate flow and solute transport problems with regional 3D or quasi-3D finite difference and finite element models for flow and transport. In these models, some cells or elements can be characterized by very contrasted parameters depending on the local fissuration/karstification degree. For local flow/transport studies using finite element, special finite elements have been developed (Dassargues *et al.*, 1988): "conduit elements" (1D pipe elements) and "fault element" (2D plane elements) which can be placed in the 3D space of the aquifer.

For karstic aquifers, the "continuum and REV approach" has also been applied at a regional scale (Calvache & Pulido-Bosch, 1993 and Combes *et al.*, 1992). Pulido-Bosch and Padilla (1988) provided some indications on a methodology based on correlation and spectral analysis which has been used to determine if the karstic aquifer could be simulated adequately by a "REV model" using the concept of porous medium.

1.2. Discrete approach

In the case of highly karstified aquifers, the continuum assumption could be difficult to accept and models are used where the karst conduits and the main fissures are represented explicitly, using a "discrete approach". Of course in this case, many accurate data are needed (geometry, apertures, rugosity, filling,...) for each individual fissure and conduit) and must be located exactly in the 3D space of the aquifer. As a consequence, these last models can only be built at a local scale of study. When

Table 1

Flow	local scale	fissured or slightly karstified aquifers REV - (discrete)	karstified aquifers REV - (discrete)	black-box - discrete
regional scale	REV - geostatistical	REV - geostatistical	REV - geostatistical	REV - geostatistical
local scale	REV - (discrete)	REV - (discrete)	REV - (discrete)	REV - (discrete)
Transport regional scale	REV - geostatistical	REV - geostatistical	REV - geostatistical	REV - geostatistical

realized calibrating "black-box" models. These models are used to assess the transient behaviour of the karstic system in terms of water quantity. When a solute transport is considered by convection, supposed as highly dominated by convection.

Kernel functions are used to predict transient flow/transport behaviour of the karstic system (Doertlinger, 1993). Interpretation of tracer tests using convolution treatments has been realised by Dzikoński & Crampon (1994). "Precipitation-runoff" models are used at a regional scale and multi-reservoir "black-box" models can be coupled to snow-melting processes (Mania *et al.*, 1991).

In function of these few statements, the table 1 has been built describing the different kind of models which are used according to the different situations to be modelled.

2 PROTECTION ZONES DELINEATION

Nowadays, regulations about protection and prevention zones around pumping wells or collecting galleries are enacted in order to maintain or to restore the quality of groundwater near springs or in the vicinity of drinking water production wells.

With respect to the case study described here below, we can mention that three kinds of protection zones are defined in Walloon Region of Belgium: (a) the water supply zone (zone I) where the water supply installations are lying at the circumference of which a 10 meters radius is added in all directions, (b) the first prevention zone (zone IIa) is defined as the distance in each direction corresponding to a 24 hours transit time of pollutant in the saturated zone (in karstic areas the zone IIa includes all the preferential points of infiltration, as sinkholes,...), (c) the second prevention zone (zone IIb) is defined as the distance in each direction corresponding to a 50 days transit time of pollutant, (d) the observation

zone (zone III) is the whole alimentation basin catchment area. A list of restricted activities established for each protection zone "intervention codes" are foreseen in an accidental spill.

However, in practice it is still very difficult to determine on a rigorous and scientific basis effective zones which are to be protected in particular case. Moreover, misunderstanding or inadequate determination of the zones are often due to an insufficient knowledge of the real ground conditions, especially with regard to a heterogeneities and complex processes contaminant transport in porous and fractured media. Usually regulations protection and prevention zones are mainly based on transfer time of contaminants in the saturated porous aquifer.

In practice, each aquifer system will react differently to individual contaminants and pollution scenarios (Andersen & Gosk, 1987). It is evident that aquifer vulnerability has to be assessed in each studied case; even if this general concept applied to a "universal contaminant" has significant limitations in rigorous scientific terms (Fitzpatrick, 1993).

How could we calculate or compute parameters of different zones in each case considering that the factors that control groundwater flow and transport are mainly influenced by heterogeneities of the ground?

Generally, the question is asked as follows: can we practically determine the parameters of different protection zones in each case, considering that the factors that control the groundwater and transport are mainly influenced by heterogeneous nature of the geological layers. Entire considered soil or rock masses are saturated, but different lithologies and more fissuration and fracturation may occur having important influence close to the pumping creating highly contrasted groundwater velocities. In function of these velocities different processes of the contaminant transport more or less emphasized.

3 CASE STUDY

The particular case described briefly here is located in Carboniferous layers composed of Tournai and Viséan limestones in the southern part of Belgium (figure 1). From three production wells drilled in a small topographical valley corresponding to the northern part of a East-West syncline, at

The piezometric map shows a natural South-North gradient of the aquifer. In the further parts of the study, we also had to take an East-West drainage along the valley at the North of the wells to explain what was observed on the results.

The determinist approach is chosen for groundwater and transport simulations. As low concentrations of tracers are concerned, we assume that flow and transport simulations can be uncoupled: no density or viscosity effects interacting on flow are taken into account. The flow and transport parameters of the flow and advection-dispersion equations are investigated assuming that the REV concept can be used.

A local 2D horizontal model based on the Finite Element Method (FEM) has been developed with the AQUA program (Vatnaskil Consulting Engineers). The meshing network is composed of triangular finite 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. The size of the finite elements are to be reduced near the main solicitation zones in order to avoid numerical instabilities and wiggles in the transport computations. Lateral boundary conditions of the flow model consist in prescribed heads (Dirichlet type) boundaries interpolated, and in some cases extrapolated, from the local piezometric measurements, taking into account the geology and the presence of main fracturation axes.

This has allowed to calibrate on natural conditions (natural gradient of the piezometric heads) and on the pumping test results (measured drawdowns in the piezometers). The distinguished heterogeneities are related to the more fractured/karstified zones detected by boreholes, geophysical methods and the morphostructural analysis.

As a result of the model calibration on the flow conditions, a map of the transmissivity values is deduced (figure 3). In the fitting process, a particular attention has been given to the geological significance of any value or distribution change for the transmissivity. 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 transversally. This anisotropy coefficient has been fitted to a 0.67 value.

A multi tracer test have been performed (Meus & Bolly, 1994), and measured breakthrough curves obtained in each pumping well.

Two tracers reached the pumping wells: naphthalene and uranine injected in piezometers respectively located at distances of about 50 m and

70 m from the wells. Unfortunately, only measured breakthrough curves relative to naphthalene in the three pumping wells, allow quantitative interpretation (Meus & Bolly, 1994).

The calibration of the model for the transport conditions has led to the fitting of the values a distributions of the effective porosity (n_e) and of longitudinal and transversal dispersivity (α_L and α_T). One of the main limitation to the calibration is that depth-averaged concentrations considered in a 2D flow-transport model. Consequently, an effective thickness of the aquifer to be chosen and, in this studied case, it particularly uneasy to determine its arbitrary value. During the calibration process, this effective thickness has been fitted to 15 m. This value is more or less consistent with the screened levels in the pumping wells.

The simulated injection mass of the tracer was taken equal to the effective recovery factor of the naphthalene (43 %) since the transport simulation do not take into account any adsorption or immobile water effect. Additionally, it is still possible that certain amount of the tracer would not be transported towards the wells because of undetected fractured (more draining) zones.

Some of the results of the calibration are shown in figure 4 in terms of breakthrough curves in the pumping wells. The deduced values for the transport parameters are distributed as follows:

$$- n_e = 0.01, \alpha_L = 30m \text{ and } \alpha_T/\alpha_L = 0.04$$

$$- n_e = 0.08, \alpha_L = 8m \text{ and } \alpha_T/\alpha_L = 0.04$$

4 USING THE MODEL TO ASSESS PROTECTION ZONES

Among other facilities, the AQUA software proposes to the user to compute automatically the isochrone contours around a pumping well. The procedure is based on a backward particle tracking technique along the streamlines. Of course, the isochrone lines are computed only considering the advective component of the transport.

In our case study, it seems evident that we cannot neglect the dispersion component of the transport. Multiple simulations are completed, each of them considering the contaminant injection in one node of the meshed zone, in order to compute for each point the minimum transfer time of the pollutant to the wells. However, this procedure requires to define more precisely what is the first arrival at the pumping wells.

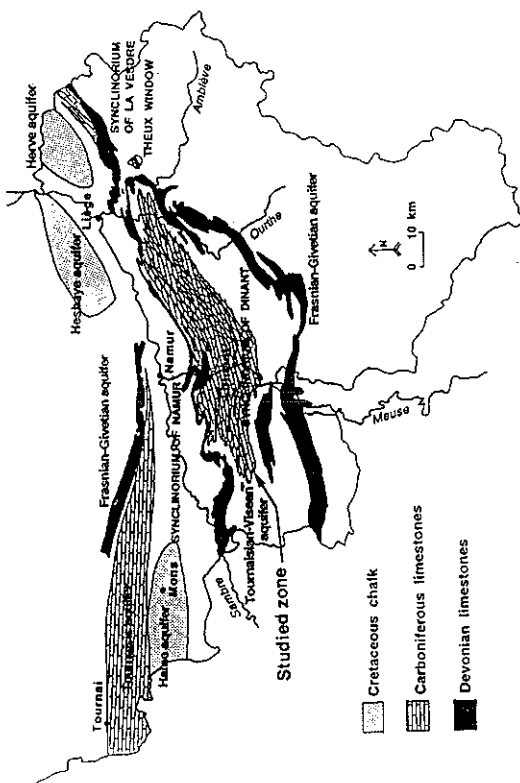


Fig. 1 Location map of the studied zone (modified after Dassargues et al., 1995)

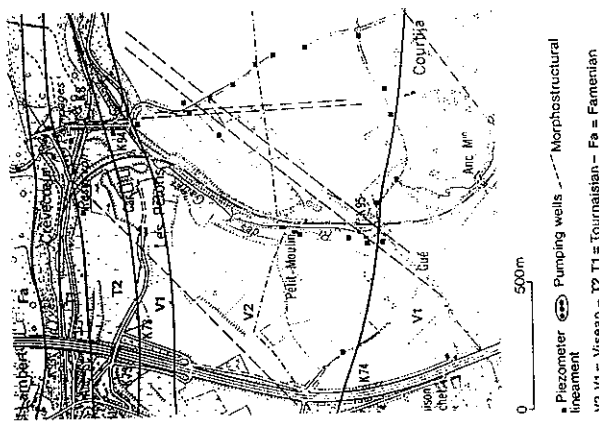


Fig. 2 Geological map, morphostructural lineaments and location of wells and piezometers.

150 m³/h is pumped out of the limestone formations (figure 2). The direction of the calcareous layers is approximately East-West with a 80 degree dip. Occurrences of slightly karstified features has been revealed in quarries located nearby. The northern part of the studied zone is limited by sub-vertical less pervious layers of Famenian age. About 25 piezometers have been drilled and a measured piezometric map have been drawn taking into account all these data.

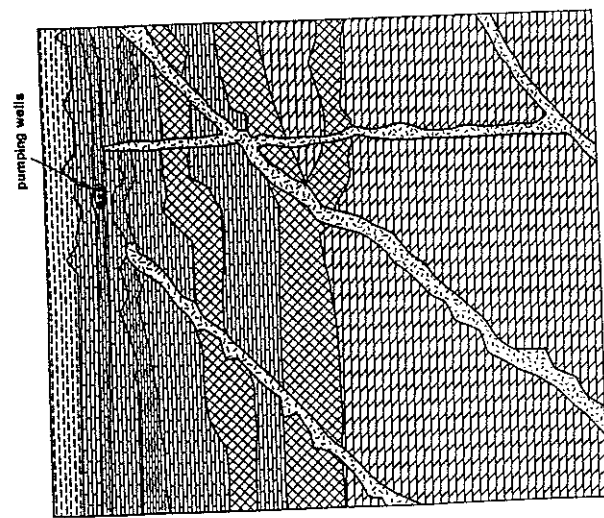


Fig. 3 Map of the transmissivity values (m^2/s) obtain by calibration on both natural and pumping conditions and taking into account the more fractured zones and the different lithologies.

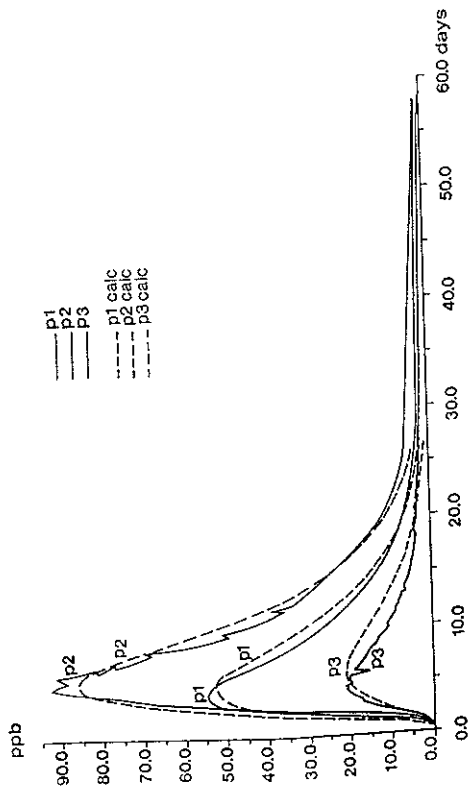


Fig. 4 Measured and calibrated breakthrough curves for naphionate in the three wells.

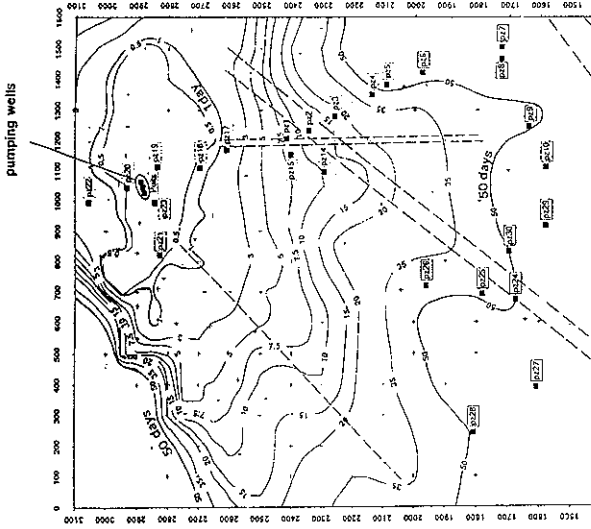


Fig. 5 Computed isochrone contours around the wells.

The regulation do not mention any information about that point. There are two possibilities. (1) Taking a defined percentage of the maximum recovery concentration of pollutant (or a percentage of the recovered mass). This option presents the advantage that the defined concentration level is independent of the injected mass of pollutant, but the disadvantage consists in considering sometimes very high concentration levels corresponding already to unacceptable contamination in the wells. (2) Choosing an absolute concentration level which can correspond to drinking water standards, then the transfer time depends on the injected mass and the nature of the considered contaminant.

In this study case, for the simulations and the assessment of the protection zones, a pollutant mass of 5000 kg and a first arrival concentration of 10 ppb have been chosen.

The transport parameters fitted during the calibration on the measured breakthrough curves are only representative for local scale transport model. Since we have no other information about the way to upscale our results, we decided to extrapolate the local values to the entire modelled domain. Of course, this extrapolation takes into account, the more logically as possible, the knowledge that we have about the geology, but it is certainly not the reality because it is well-known that a strong scale

effect can be awaited when dealing with disperser values.

The first set of transport parameters has been extrapolated to the whole supposed unfractionated domain and the second set to the main fractured zones as revealed by the geophysical morphostructural studies.

Simulations of the contamination scenario have been computed from 114 points of the model domain. For each of these points, a first arrival time is recorded and then by interpolation of the resulting map with isochrone lines can be drawn (figure 5). Protection zones corresponding to the existing ones can be assessed.

5 CONCLUSIONS

With regard to the legal prescriptions, the adequate methodology has to be chosen in order to assess as far as possible the protection zones to be considered at a particular site of water withdrawal. After a complete collect of available data concerning geology, morphostructural geology, geophysics, prospecting, piezometer drilling... the heterogeneity of a studied aquifer can be characterised. If the set of data is exceptionally detailed and accurate a discrete approach can be considered, but most often the heterogeneity of

aquifer is still to be described more or less globally and in the framework of the REV approach, "equivalent" values for the parameters are used.

Considering the practical case study described here above, the REV approach used for modelling purposes is conceptually far from the reality. However, at the scale of interest (100 to 1500 m from the pumping wells), it seems that a REV flow and transport model can provide relatively consistent results if the meshing network can be detailed in the zones where heterogeneities have been revealed. This detailed discretization can then be used to distinguish in the model many small zones with contrasted parameters of flow and transport, describing by this way the main fractured/karstified zones of the domain.

Many problems remain unsolved due to the unsatisfying or inadequate assumptions imposed or chosen in the framework of this REV approach: (1) the use of 2D depth-averaged concentrations and simulation parameters, (2) the implicit smoothing of the piezometric heads and of the velocities due to the use of "equivalent" values in REV instead of highly contrasted values in smaller volumes.

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