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## Evaluating predictive reliability of groundwater models by sensitivity analysis

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### Abstract

The sensitivity analysis method used in linear systems with a limited number of unknown parameters has been generalized to groundwater flow and transport models. The main problems were that in groundwater models the results are not linear functions of the parameters and the number of parameters may - in theory - amount to several thousands. Moreover the calibration errors (on hydraulic heads or concentration for instance) are often highly spatially correlated. To take into account these difficulties a new approach has been developed: the number of parameters has been drastically reduced by defining zones with homogeneous parameters. The equations have been locally linearized and the variogram of the calibrations errors has been integrated. The resulting covariance matrix of the parameters is obtained after running the model several times to determine the derivative of the results (heads, flows, concentrations) with respect to the parameters. When the model is used for prediction, after modifying the boundary conditions (recharge, pumpings, pollutant spreading), the new derivatives are calculated. Combined with the covariance matrix - which is invariant - they yield the confidence limits of the predictions.

The model has been applied with success to 5 aquifers (monolayer, multilayer, steady-state or transient state) and to a tracer test in a fractured formation.

### 1. Introduction

The simulations and forecasts obtained with a groundwater model - as with any physical model are deterministic: a unique response is given in reaction to a given input. As a matter of fact the response is a function of the inputs but also of the model parameters (hydraulic conductivity, storage coefficient). The inputs are usually known with accuracy: abstraction rates, specified hydraulic heads, etc. On the other hand, the model parameters are usually estimated by pumping tests or tracer tests in a limited number of locations, and are determined by calibration over the rest of the aquifer. If the observations are not accurate, or are affected by external phenomena not taken into account by the model (error of synchronization, barometric effect, spatial variability), the calibration will be approximate and the parameters will be affected with uncertainty. This will induce uncertainty on the forecast established with the model. It does not suffice to calibrate a model but it is better to provide the standard deviation associated to the identified values. Similarly it is necessary to provide the standard deviation, or the confidence limits, associated to a forecast. A mapping of the standard deviation makes it possible to determine the locations where it is recommended to get new measurements in priority. A general method of calculation of standard deviation of the parameters of a model and of forecasts has been described in detail by Leijnse (1982) and Thiery (1989). The adaptation of

this method to distributed models as groundwater models (Cooley, 1979; Lavenue and Pickens, 1992) evokes 2 specific problems: parameters are distributed (one or several in each cell of the model) and the observations for calibration are data fields with autocorrelations in 2 or 3 dimensions and possible autocorrelation in time.

This paper presents a method to determine conditional confidence limits on model parameters (hydraulic conductivities, storage coefficients, dispersivity, porosity...) and on forecasts obtained with the model (hydraulic heads, drawdown, spring discharge, concentration, density, etc.). These confidence limits are conditional because they depend on the hydrogeological hypotheses which are not changed (for instance: monolayer model, steady state). The definition of the parameters may not be changed: if 5 zones of hydraulic conductivity have been previously defined, the analysis determines the accuracy of the hydraulic conductivity in each zone but keeps the number of zones and the extension of each zone.

## 2. Methodology

### 2.1. Notations

|                                  |   |
|----------------------------------|---|
| <b>a</b>                         | = optimal parameter   |
| <b>a<sub>q</sub></b>             | = parameter derived from sample <b>q</b>  |
| <b>d</b>                         | = distance between observations (lag)   |
| <b>D<sub>a</sub></b>             | = $a - a_q$ = error for parameters <b>a</b>   |
| <b>e</b>                         | = difference between observation ( <b>y<sub>obs</sub></b> ) and simulation ( <b>y<sub>c</sub></b> ) |
| <b>g</b>                         | = variogram of errors   |
| <b>g<sub>0</sub></b>             | = nugget in variogram   |
| <b>K</b>                         | = hydraulic conductivity  |
| <b>k</b>                         | = decimal logarithm of hydraulic conductivity   |
| <b>n</b>                         | = number of observations  |
| <b>n<sub>e</sub></b>             | = equivalent number of independent observations   |
| <b>p</b>                         | = number of observations  |
| <b>r</b>                         | = range of variogram  |
| <b>R</b>                         | = correlation coefficient between observations  |
| <b>RI</b>                        | = radius of influence   |
| <b>r<sub>ij</sub></b>            | = correlation coefficient between parameter <b>i</b> and parameter <b>j</b>                         |
| <b>s<sub>a</sub></b>             | = standard deviation of parameter <b>a</b>  |
| <b>s<sub>e</sub></b>             | = standard deviation of error <b>e</b>  |
| <b>s<sub>e</sub><sup>2</sup></b> | = variance of error = sill of variogram   |
| <b>s<sub>r</sub></b>             | = relative standard deviation (%)   |
| <b>t</b>                         | = transposed of matrix  |
| <b>x</b>                         | = location  |
| <b>x<sub>f</sub></b>             | = location for a forecast   |
| <b>y<sub>c</sub></b>             | = calculated (simulated) value with the model   |
| <b>y<sub>obs</sub></b>           | = observed value (hydraulic head)   |
| <b>ρ<sub>ij</sub></b>            | = correlation coefficient between error <b>i</b> and error <b>j</b>                                 |

### 2.2. Standard deviation parameters

It is assumed that a model **M** depends on **p** parameters **a**. The model is calibrated on **n** observations **y<sub>obs</sub>** which make a sample **q** of **n** values (hydraulic heads or concentrations...) at locations **x<sub>i</sub>**. The optimal parameters **a<sub>q</sub>** are determined from this sample by calibration. They

are dependent on the sample  $\mathbf{q}$ . The aim of the sensibility analysis is to determine the distribution of the parameters  $\mathbf{a}_{\mathbf{q}}$ .

Let:

$$Da = a_{\mathbf{q}} - \mathbf{a}$$

$e_i = y_{\text{obs}} - y(\mathbf{a}, x_i)$  = simulation error (with true parameters  $\mathbf{a}$ ) at location  $x_i$

$$e_{\mathbf{q}i} = y_{\text{obs}i} - y(a_{\mathbf{q}}, x_i)$$

$$S_{\mathbf{q}} = \sum_i (e_{\mathbf{q}i})^2$$

Deriving  $S_{\mathbf{q}}$  successively with respect to each parameter  $\mathbf{a}_{\mathbf{q}}$ , neglecting the terms of second order, and taking into account that  $\mathbf{a}_{\mathbf{q}}$  is the optimal parameter, Thiery (1989) shows that one obtains the following system:

$$[B] \cdot [Da] = {}^t[A] \cdot [e] \quad (1)$$

where:

${}^t[A]$  = matrix  $\mathbf{p}$  lines,  $\mathbf{n}$  columns = derivative of  $y$

$[B]$  = square matrix  $\mathbf{p} \cdot \mathbf{p}$  made of the sums of products of 2 derivatives

$[e]$  = vector of  $\mathbf{n}$  simulation errors  $e_i$

The variance-covariance matrix of the parameters writes:

$$[VA] = [r_{ij} \cdot sa_i \cdot sa_j]$$

where:

$r_{ij}$  = correlation coefficient between parameters  $\mathbf{a}_i$  and  $\mathbf{a}_j$

$sa_i$  = standard deviation of parameters  $\mathbf{a}_i$

$$[VA] = [Da] \cdot {}^t[Da] = [B]^{-1} \cdot {}^t[A] \cdot [e] \cdot {}^t[e] \cdot [A] \cdot [B]^{-1} \quad (2)$$

If the errors  $e_i$  are all independent, the following relation holds:

$$[e] \cdot {}^t[e] = se^2 \cdot I_n \quad \text{where } I_n = \text{identity matrix } (n \cdot n) \quad (3)$$

Relation (2) may be simplified as :  $[VA] = se^2 \cdot [B]^{-1}$  (4)

When using a model, relation (3) never holds because the errors are not independent. There are periods when all computed values (heads) are too high (e.g. because the aquifer recharge is overestimated) and there are regions of the model where all heads are too low (e.g. because the hydraulic conductivity is too large).

$$[e] \cdot {}^t[e] = [e_{ij}] = [\rho_{ij} \cdot se^2] \quad (5)$$

It is a large  $\mathbf{n} \cdot \mathbf{n}$  symmetrical matrix with variance of errors on the diagonal and covariances between errors on the other elements. In a time series,  $\rho_{ij}$  may depend only on the lag  $\mathbf{d}$  between the observations:

$$\rho_{ij} = \rho_1^{\mathbf{d}} \quad \text{where } \mathbf{d} = |i - j|, \quad \rho_1 = \text{autocorrelation of lag 1}$$

For a spatial series, the variogram  $\mathbf{g}$  may be used:

$$e_{ij} = g(\mathbf{d}) \quad \text{where } \mathbf{d} = \text{distance between 2 observations locations}$$

$$g = \text{variogram of the errors}$$

Thiery (1989) shows that it is possible to define an equivalent number  $\mathbf{n}_e$  of independent errors.

Relation (4) is then transformed into:

$$[VA] = (\mathbf{n}/\mathbf{n}_e) \cdot se^2 \cdot [B]^{-1} \quad (6)$$

The number of independent errors is determined from the variogram considering the disk centred on an error and containing all the errors related by a correlation coefficient  $\mathbf{R}$  greater than 0.5. Inside this disk all the errors are considered as dependent and only one independent error is counted. The radius  $\mathbf{d}$  of this disk is defined by:

$$0.5 = R = 1 - g(\mathbf{d}) / se^2 \quad (7)$$

### 2.3. Standard deviation on the forecast of the model

After calibration of the model and estimation of the standard deviation of the parameters, it is possible to simulate modifications (new abstractions, new boundary conditions, different infiltrations). It is also possible to study another variable  $y$ . For instance, the model may be calibrated on observed hydraulic heads but may be used to forecast a flow, a concentration, a density, a temperature or a spring discharge. The forecast of the model may be relative to a new location  $\mathbf{x}_f$  where no observation was available for calibration. It is assumed that the calculated values  $\mathbf{y}_c$  are locally linear functions of the parameters  $\mathbf{a}$ . In order to obtain such a linear relation, it is possible to change the variable. For instance if  $y$  is the drawdown and  $T$  the transmissivity one can use  $\mathbf{a} = 1/T$  in order to get a quasi linear relation. Thiery (1989) shows that the variance  $\text{syc}^2$  of the forecast  $\mathbf{y}_c$  is given by:

$$\text{syc}^2 = \sum_j \sum_k \underbrace{r_{jk} \cdot sa_j \cdot sa_k}_{\text{fixed term determined by the calibration}} \cdot \underbrace{(dy / da_j) \cdot (dy / da_k)}_{\text{term depending on the location}} \quad (8)$$

This variance  $\text{syc}^2$  is only due to the uncertainty of the model parameters. The total variance  $\text{syp}^2$  of the error between a forecast value  $\mathbf{y}_c$  and an observed value  $\mathbf{y}_{obs}$  must integrate the variance of calibration error  $\text{se}^2$  which is independent on  $\mathbf{y}_c$  (and may be due to errors in  $\mathbf{y}_{obs}$ ):

$$\text{syp}^2 = \text{syc}^2 + \text{se}^2 \quad (9)$$

### 2.4. Standard deviation by Monte Carlo simulations

In some situations it is not possible to get a linear relationship between  $\mathbf{y}_c$  and  $\mathbf{a}$ . For instance  $\mathbf{y}_c$  may be :

- the maximum pollutant concentration in a zone or the maximum concentration during a period
- or the tranfert time of a pollutant
- or the position of a given path line.

In these cases it is possible to use Monte Carlo simulations. The problem reduces to the generation of sets of  $\mathbf{p}$  parameters with a given variance-covariance matrix. this generation can be done easily by a Principal Components Analysis (PCA) of the variance-covariance matrix. From  $\mathbf{p}$  parameters, one gets  $\mathbf{p}$  principal components [C1...Cp] which are independent from each other.

It is easy to generate a set of random principal components (of given variances). This set of generated components is then used to get the corresponding set of  $\mathbf{p}$  parameters by a simple linear relationship. Each set of  $\mathbf{p}$  parameters is used to generate the corresponding model simulation. The statistical analysis of all the simulation gives the statistical analysis of the forecast variable  $\mathbf{y}_c$ .

## 3. Practical implementation

### 3.1. Parameters of the model

The method described in the previous part may be applied only to a number of parameters much lower than the number of observations. This is due to the fact that, in a linear system without constraint, the system is undetermined and the confidence limits are infinitely large if the number of parameters is greater than or equal to the number of observations. Another reason is that the sensitivity analysis of  $\mathbf{p}$  parameters needs  $\mathbf{p}$  runs of the model which is expensive in term of CPU time. The number of parameters is drastically reduced by zonation for each type of

parameter. These zones may be determined from geology or - in steady state - by the head gradient method as described by Thiery (1994a). In each zone (of hydraulic conductivity or storage coefficient or infiltration coefficient for instance) a unique value is determined by automatic calibration as described by Khan (1986), Kessler (1987), Thiery (1993a, 1994b).

### 3.2. Observation series

The sensitivity analysis may be performed in steady state or in transient state. In steady state the observations are usually a map of hydraulic heads or observations of heads in a limited number of locations. The observations may also be of another type e.g. a concentration map or a temperature map. In transient state the observations may integrate also time-series of evolution of hydraulic heads or of spring discharge at a limited number of locations.

### 3.2. Relative standard deviation

When a parameter (e.g. the hydraulic conductivity  $K$ ) has a log-normal distribution it is better to analyse the uncertainty of  $k$  the (decimal) logarithm of this parameter :  $k = \log(K)$ .

The analysis will be analyzed and will yield  $s_k$  the standard deviation of  $k$ . We define the relative standard deviation  $s_r$ , which is expressed in percent, by :  $s_r / 100 = 10^{s_k} - 1$ . The distribution of  $k$  being gaussian, the true value of  $k$  has a probability of 95% to be in the range  $k \pm 1.96 s_k$ . Taking the antilogarithm,  $K$  has a probability of 95% to be in the range :

$$[K/10^{1.96s_k}, K \cdot 10^{1.96s_k}] \quad \text{which corresponds to :}$$

$$[K / f, K \cdot f] \quad \text{with } f = (1 + s_r/100)^{1.96} \quad (10)$$

## 4. Application to 5 actual aquifer systems with field data

The method described above has been applied to the field data of 5 aquifer systems studied by BRGM and described in Table 1. Fig. 1 displays the observed hydraulic heads of the aquifers and the boundaries with prescribed heads (marked by a cross).

Table 1 Description of the actual aquifers

| Name     | Number of cells | Size of the cells (m) | Number of layers | Number of times steps<br>SS=Steady State | Localisation            |
|----------|-----------------|-----------------------|------------------|--|-------------------------|
| Thau     | 701             | 1000                  | 1                | SS                                       | Herault (F)             |
| Cailly 1 | 378             | 500                   | 1                | SS                                       | Normandy (F)            |
| Cailly 2 |                 |                       |                  | 5  |                         |
| Breil    | 536             | 32                    | 1                | SS                                       | Aude (F)                |
| Malta    | 964             | 500                   | 1                | SS                                       | Mediterr.               |
| Sarthe   | 1196            | 1000                  | 2                | SS                                       | Sarthe (F)<br>two-layer |

### 4.1. Determination of optimal parameters

The optimal parameters of each aquifer have been determined as follows:

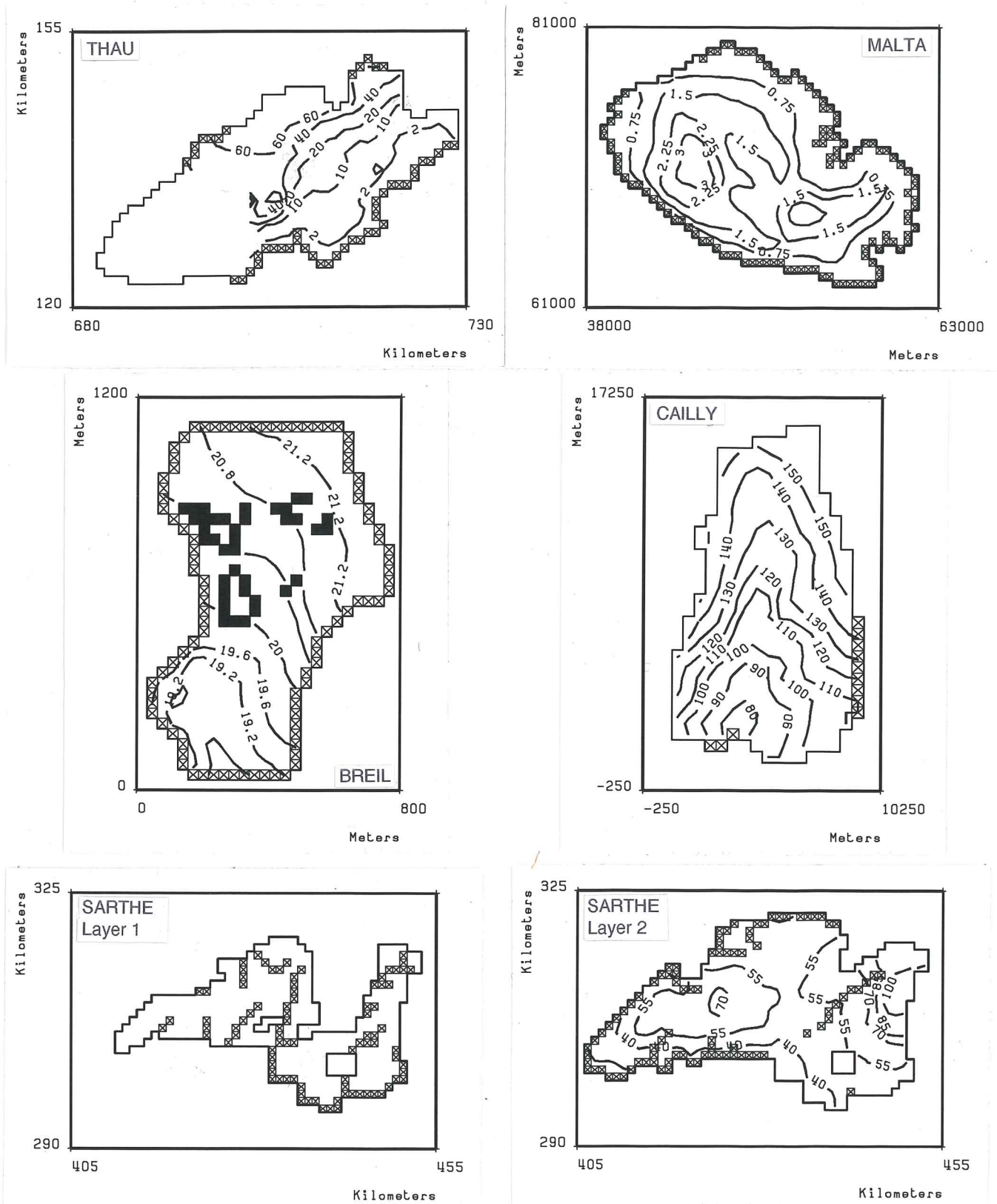


Fig. 1 - Description of 5 aquifers with observed heads and boundary conditions (specified heads are pointed out by a cross [x]).

- determination of homogeneous zones of hydraulic conductivities by inverse modelling (Thiery, 1994a) except for Sarthe aquifer where zones have been determined from geology;
- automatic calibration by zones with MARTHE model (Thiery, 1990, 1993b, 1994c) according to the method described by Khan (1986) and Kessler (1987) and improved by Thiery (1993a, 1994b).

For each aquifer, 3 to 5 zones of homogeneous hydraulic conductivity have been identified. The hydraulic conductivity of these zones is given in Table 2 (the figures given in the table must be multiplied by the unit factor given in column 8).

Table 2 Hydraulic conductivities resulting from calibration

| Aquifer<br>Identif. | Zone number |      |      |      |        |         | Unit<br>(m/s)     | Number<br>of zones |
|---------------------|-------------|------|------|------|--------|---------|-------------------|--------------------|
|                     | 1           | 2    | 3    | 4    | 5      | 6       |                   |                    |
| Thau                | 0.071       | 0.5  | 3.11 | 6.99 | 23.0   | (0.143) | $5 \cdot 10^{-6}$ | 5                  |
| Cailly              | 5.5         | 21   | 133  | 1323 | -      | -       | $10^{-6}$         | 4                  |
| Breil               | 0.52        | 13.7 | 72   | 196  | 1390   | (9000)  | $10^{-5}$         | 5                  |
| Malta               | 32          | 50   | 247  | 301  | (7980) | -       | $10^{-6}$         | 5                  |
| Sarthe              | 1.8         | 14   | 78   | -    | -      | -       | $5 \cdot 10^{-6}$ | 3                  |

## 4.2. Analysis of errors

After calibration the characteristics of the simulation errors have been analyzed. They are given in Table 3. The normalized residual (column 5) is the ratio of the mean square of errors  $se^2$  divided by the observed variance. The histograms of errors for each aquifer are given in Fig. 2. It appears that the distribution is symmetrical and may be considered as Gaussian. The experimental variograms have been computed with VIVA software (Seguin, 1992) and a spherical variogram has been fitted for each aquifer. Fig. 3 shows that the fit is very satisfactory. The range  $r$ , the nugget  $g$ , and the sill  $se^2$  has been determined. The variogram equation is:

$$g(d) = (se^2 - g_0) \cdot [1.5 (d/r) - 0.5 (d/r)^2] + g_0 \quad (11)$$

where  $d$  is the lag

Table 3 - Analysis of calibration errors.

| Aquifer  | Mean<br>error<br>(m) | RmSE<br>(m) | Stand. dev.<br>observ.<br>(m) | Normalized<br>residual<br>(%) | Number<br>independent | Range of<br>variog.<br>(m) | Nugget<br>( $m^2$ )<br>(%) | Radius<br>of Infl.<br>(m) |
|----------|----------------------|-------------|-------------------------------|-------------------------------|-----------------------|----------------------------|----------------------------|---------------------------|
| Thau     | -0.34                | 3.9         | 26.8                          | 1.4                           | 65                    | 3850                       | 1.93 13                    | 1235                      |
| Cailly   | -0.22                | 2.24        | 22.4                          | 1.0                           | 61                    | 1850                       | 0                          | 703                       |
| Breil    | -0.004               | 0.08        | 0.82                          | 0.93                          | 443                   | 282                        | 0.034 56                   | 0                         |
| Malta    | 0.00                 | 0.26        | 0.78                          | 10.8                          | 23                    | 4400                       | 0                          | 1685                      |
| Sarthe 1 | -0.42                | 4.6         | 19.2                          | 5.4                           | 175                   | 5400                       | 6 27                       | 1350                      |
| Sarthe 2 | 0.34                 | 5.2         |                               |                               |                       | 5150                       | 4 19                       |                           |

## 4.3. Determination of the number of independent observations

The radius of influence  $RI$  of one observation is defined by:  $0.5 = 1 - g(RI) / se^2$ . The number of independent observations  $NI$  is the ratio of the total area  $A$  of the aquifer divided by the area  $D$  of one independent disk of radius  $RI$ .

$$NI = A / D$$

$$A = N \cdot a^2$$



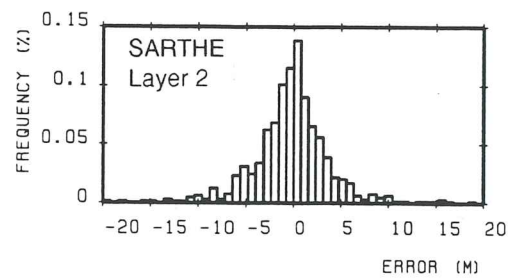
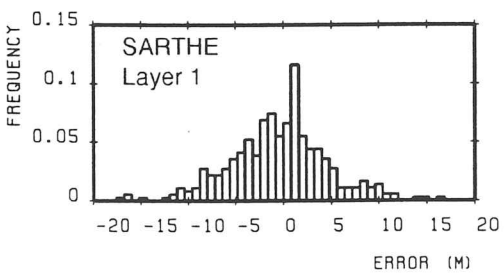
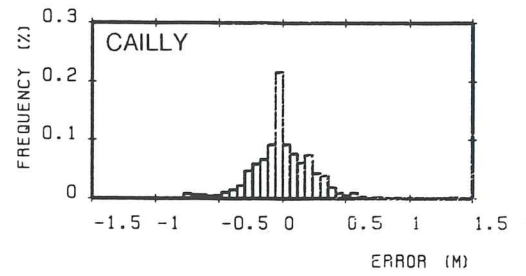
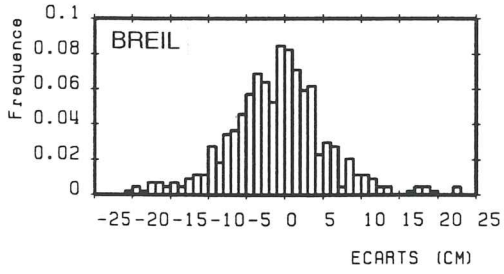
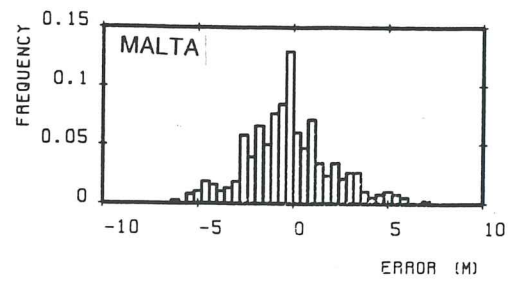
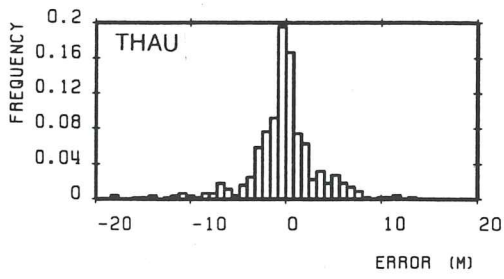


Fig. 2 - Histograms of calibration errors for 5 aquifers.

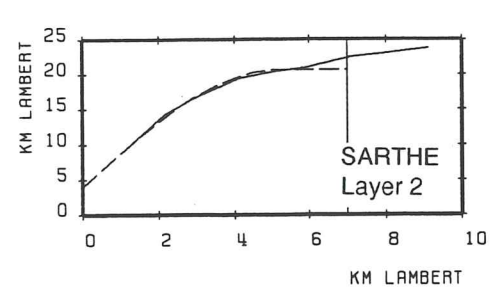
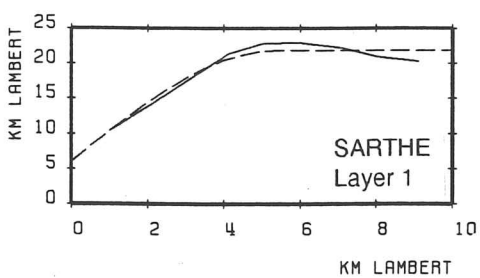
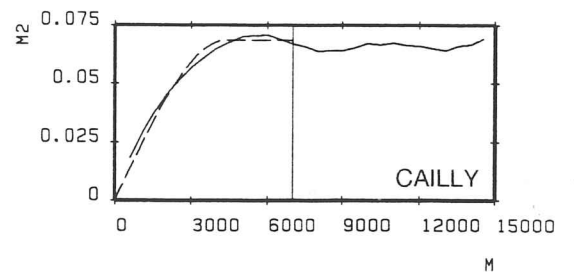
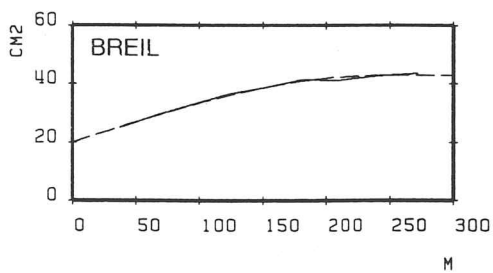
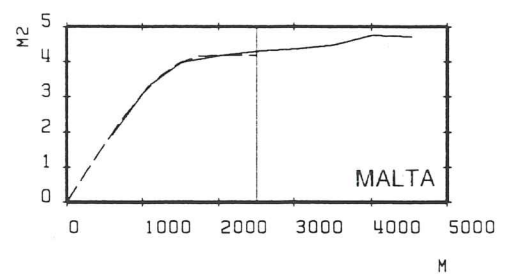
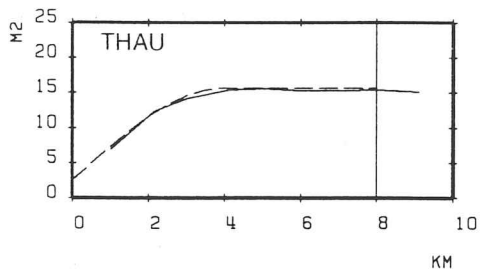


Fig. 3 - Variograms of errors for 5 aquifers.

$$D = \pi \cdot RI^2$$

$$\text{which yields : } NI = N \cdot a^2 / (\pi \cdot RI^2)$$

where:

N = total number of cells

a = size of one cell (assumed to be square)

NI, r, g<sub>0</sub> and RI are given in columns 6-9 of Table 3.

#### 4.4 - Standard deviation of the parameters

Taking into account the number of independent observations, the standard deviations of the parameters have been determined from the derivative of the computed hydraulic heads with respect to each parameter. Table 4 displays these standard deviations in percent. Most of the time the standard deviations are on the order of magnitude of 20% which means that the confidence limits at 95% relative to an hydraulic conductivity **K** is: [K/f, K • f] with  $f = 1.20^{1.96}$  which yields: [0.70 K, 1.43 K]. In some zones (e.g. zone 1 for Breil aquifer, or zone 5 for Malta) the hydraulic conductivity is nearly undetermined.

Table 4 - Relative standard deviation of hydraulic conductivity (%).

| Aquifer | Zone number |    |    |    |          |    |
|---------|-------------|----|----|----|----------|----|
|         | 1           | 2  | 3  | 4  | 5        | 6  |
| Thau    | 15          | 7  | 18 | 21 | 56       | 21 |
| Cailly  | 9           | 5  | 9  | 22 | -        | -  |
| Breil   | 18000       | 21 | 7  | 5  | 8        | -  |
| Malta   | 51          | 19 | 22 | 56 | infinite | -  |
| Sarthe  | 8.7         | 10 | 28 | -  | -        | -  |

#### 4.5. Validation of the method

The validation has been performed by Monte Carlo simulations with Cailly aquifer data. The optimal set of parameters has been considered as being the true solution. The corresponding simulated hydraulic heads **HS** have been calculated and compared to the observed hydraulic heads **HO**. The error of calibration  $ES = HS - HO$  has been considered as a random error due to external reasons (measurements errors, incorrect recharge or runoffs evaluation, etc). Twenty maps of possible observed heads **HO<sub>i</sub>** have been generated, computing, by random generation, 20 different possible maps of errors **ES<sub>i</sub>** respecting the standard deviation and the spatial autocorrelation of errors. The optimal parameters corresponding to the 20 maps of hydraulic heads, have been determined by automatic calibration. The standard deviation of each parameter has then been computed from the 20 sets of parameters and compared to the standard deviation determined directly by the method described in this paper. Table 5 compares the computed relative standard deviations to the realisation obtained by the 20 Monte Carlo simulations. Table 6 compares the computed correlations between parameters to the correlations obtained by the Monte Carlo simulations.

These tables show that the standard deviation of the parameters and the correlations computed are correct. This validation proves that :

- (i) the hypothesis of approximate local linearity between hydraulic conductivity and computed hydraulic head is acceptable.
- (ii) the estimation of the equivalent number of independent observation is correct.

Table 5 Cailly hydraulic conductivity : verification by Monte Carlo simulations

| Zone number | Central value<br>( $10^{-6}$ m/s) |                         | Relative standard deviation<br>(%) |                         |
|-------------|-----------------------------------|-------------------------|------------------------------------|-------------------------|
|             | Optimal value                     | Monte Carlo simulations | Sensitivity analysis               | Monte Carlo simulations |
| 1           | 5.5                               | 5.3                     | 9                                  | 8.5                     |
| 2           | 21                                | 21                      | 5                                  | 6                       |
| 3           | 133                               | 137                     | 9                                  | 13                      |
| 4           | 1 323                             | 1271                    | 22                                 | 30                      |

Table 6 Correlation between parameters

|          | Sensitivity analysis | Monte Carlo simulations |
|----------|----------------------|-------------------------|
| r (1, 2) | - 0.54               | - 0.68                  |
| r (2, 3) | - 0.45               | - 0.36                  |
| r (3, 4) | - 0.38               | - 0.61                  |
| others   | < 0.2                | < 0.2                   |

#### 4.6 - Influence of the number of parameters

For Thau, Malta and Sarthe aquifers, 2 sensitivity analysis have been performed :

- the first one with a large number of hydraulic conductivity zones as initially determined by a hydrogeologist;
- the second one with a small number of zones determined by inverse modelling.

Table 7 compares the median relative standard deviation for each scheme in each aquifer. It shows that for each aquifer the relative standard deviations are approximately doubled when using the larger number of zones. This obviously advocates for using the minimum number of parameters necessary to get an acceptable simulation.

Table 7 Standard deviation of parameters using different number of zones

| Aquif  | Number of zones | Median of relative standard deviation of parameters |
|--------|-----------------|---|
| Thau   | 11              | 51 %  |
|        | 6               | 20 %  |
| Malta  | 11              | 98 %  |
|        | 5               | 51 %  |
| Sarthe | 12              | 36 %  |
|        | 3               | 10 %  |

#### 4.7. Sensitivity analysis for other parameters

Up to here we gave examples of sensitivity analysis of hydraulic conductivity. However the method is general and may be applied to other parameters such as specific yield (in transient state), infiltration factors etc. It is also possible to analyse the sensitivity to parameters controlling pollution transport : e.g. the dispersivity, the cinematic porosity or the retardation coefficient. In this case the observations of hydraulic head are replaced by observations of concentration of pollutant in the aquifer.

In order to prove the applicability of the method we applied it to the data of Finnsjon site (Sweden) which belong to INTRAVAL international tests. The data are relative to the injection of a tracer (In-Edta) in a borehole at an average rate of 2.9 g/day.

The concentration is monitored in another borehole situated 137 meters apart, which is pumped at a rate of 2 l/s creating a convergent flow.

The system is modeled in 3D by 7 000 cells in 5 layers (Schwartz 1993) and the concentration is calculated by a method of characteristics (MOC). Three parameters are determined by automatic calibration :

- $\alpha_L$  the longitudinal dispersivity
- $\alpha_T$  the transverse dispersivity
- R the retardation coefficient

The optimal simulation and the 95 % confidence limits, compared to the observations, appear in fig. 4 and the resulting parameters are displayed in table 8. The number of selected observation is 31 and the mean square of errors is equal to 1.24 mg/l.

Table 8 Finnsjon tracer test parameters

| Parameter  | Optimal value | Relative standard deviation | Correlation | Matrix |   |
|------------|---------------|-----------------------------|-------------|--------|---|
| $\alpha_L$ | 26.8 m        | 25.4 %                      | 1           |        |   |
| $\alpha_T$ | 2.3 m         | 49.1 %                      | - 0.56      | 1      |   |
| R          | 1.19          | 5.8 %                       | - 0.37      | - 0.12 | 1 |

This table shows that the best determined parameter is the retardation coefficient (relative standard deviation equal to 5.8 %). The transverse dispersivity is determined with less accuracy and its correlation with the longitudinal dispersivity is equal to - 0.56 which means that an underestimation of  $\alpha_L$  may be partly compensated by overestimation of  $\alpha_T$ .

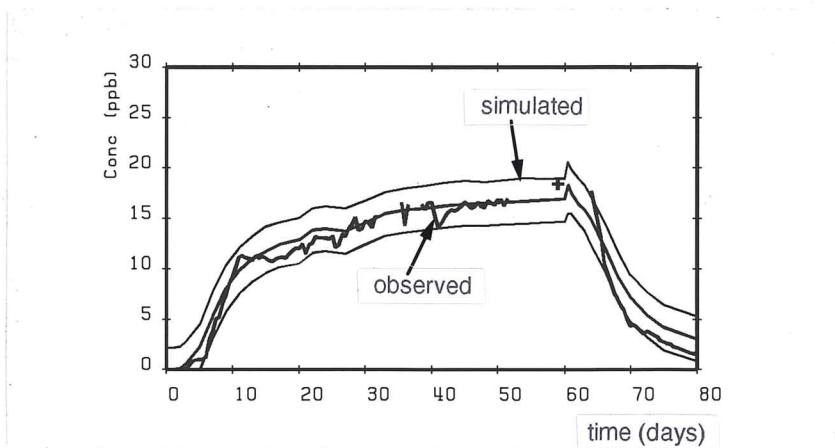


Fig. 4 - Finnsjon tracer test : comparison of simulated and observed concentrations with 95 % confidence limits.

#### 4.8. Standard deviation of predictions

The standard deviations and correlations between parameters have been used to compute the standard deviations of the calculated hydraulic heads. Fig. 5 displays the map of the standard deviations of heads for every aquifer. As it could be expected the standard deviations are smaller near the limits with specified heads. The standard deviations are - in the average - rather small because the situations correspond to the calibration. The standard deviation may be

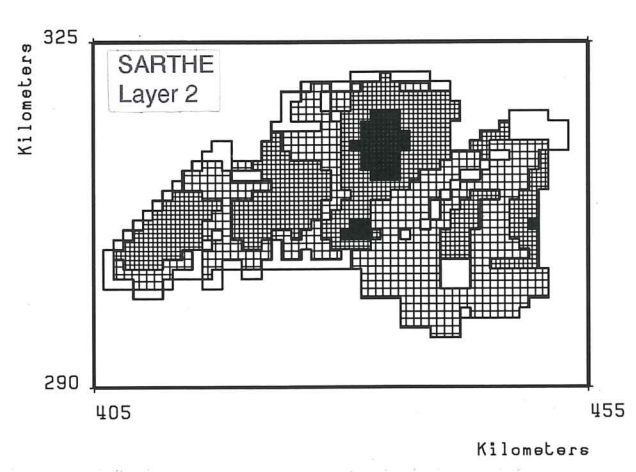
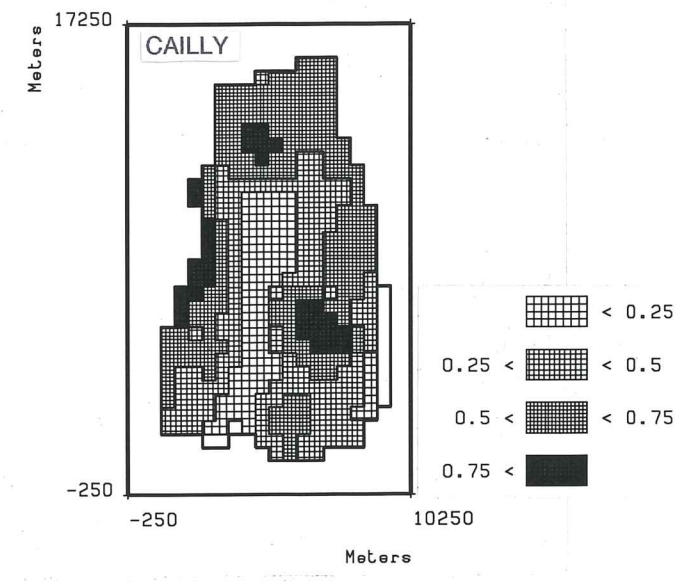
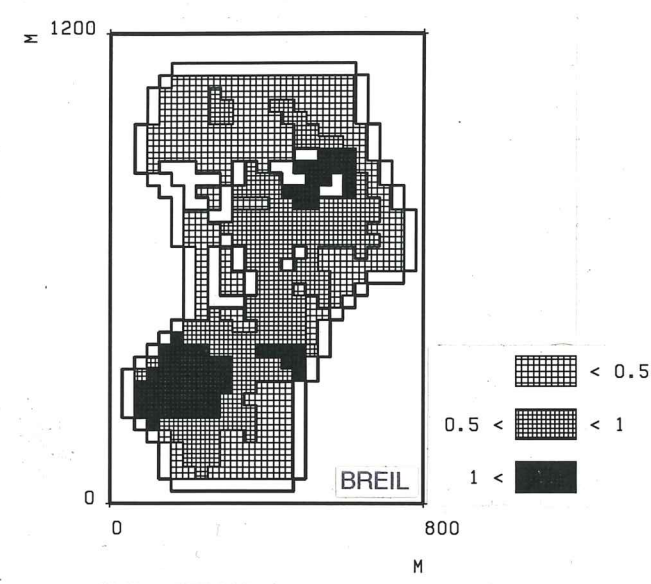
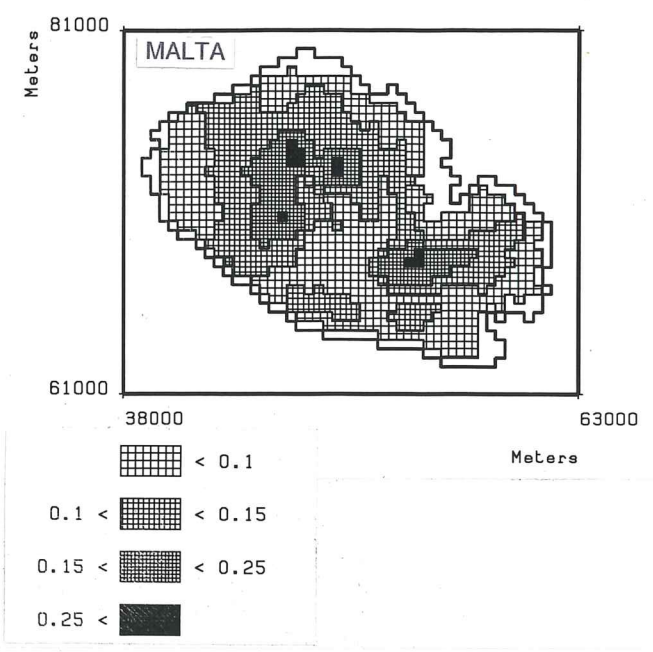
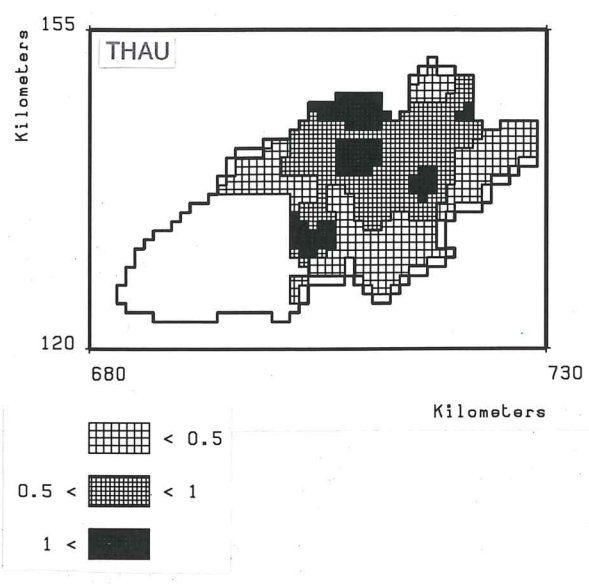


Fig. 5 - Standard deviation of simulated hydraulic for 5 aquifers.

computed for other situations: higher recharge or new pumping. The uncertainty of the heads would have been much larger. When the number of zones is increased the average standard deviation of hydraulic heads is approximately doubled:

Table 9 Average standard deviation of hydraulic heads (m)

|                | Thau | Malta | Sarthe |
|----------------|------|-------|--------|
| 3 to 6 zones   | 0.61 | 0.107 | 0.50   |
| 11 to 12 zones | 1.54 | 0.195 | 0.89   |

For Thau aquifer, fig. 6 shows that the area where the standard deviation of the computed hydraulic head is greater than 1 m is much more reduced when using 6 zones of hydraulic conductivity (determined by inverse modelling) than when using 11 zones (selected a priori by a hydrogeologist).

For Finnsjon system a simulation has been made with a variable injection rate of tracer (from 3.4 to 1.4 g/day) and a variable pumping rate (from 0.8 to 2.5 l/s) in the monitored well. Fig. 7 displays the computed concentration at the pumped well and the 95 % confidence limits determined using the variance-covariance matrix of the 3 parameters. It appears that the uncertainty due to the parameters is equal to about 3 mg/l and is variable during the monitored period. It is minimal at the beginning (before the breakthrough) and at the end of the simulation.

## 5. Conclusions

A method of sensitivity analysis has been described. This method is associated with a kriging technique in order to determine an equivalent number of independent observations used for the calculation of the standard deviation of the parameters. This number, which is usually in the range 5% to 20% of all observations for the 5 studied aquifers, is assumed to be 100% by many authors which is incorrect. The standard deviation of the model parameters and the intercorrelations are calculated from the derivative of the computed hydraulic head or concentration with respect to each parameter. It has been shown that the number of parameters should be kept to a minimum in order to obtain well determined values. The analyzed parameters were hydraulic conductivities, dispersivities and retardation factors but the method is general. It has already been applied to other parameters such as storage coefficients and infiltration factors. Instead of hydraulic heads or pollutant concentrations, the calibration variable may be water content, pressure, salinity or temperature. The standard deviation of the forecasts are derived from the standard deviation of the parameters but Monte-Carlo simulations may also be used after generation of parameters.

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This is BRGM contribution n°95018

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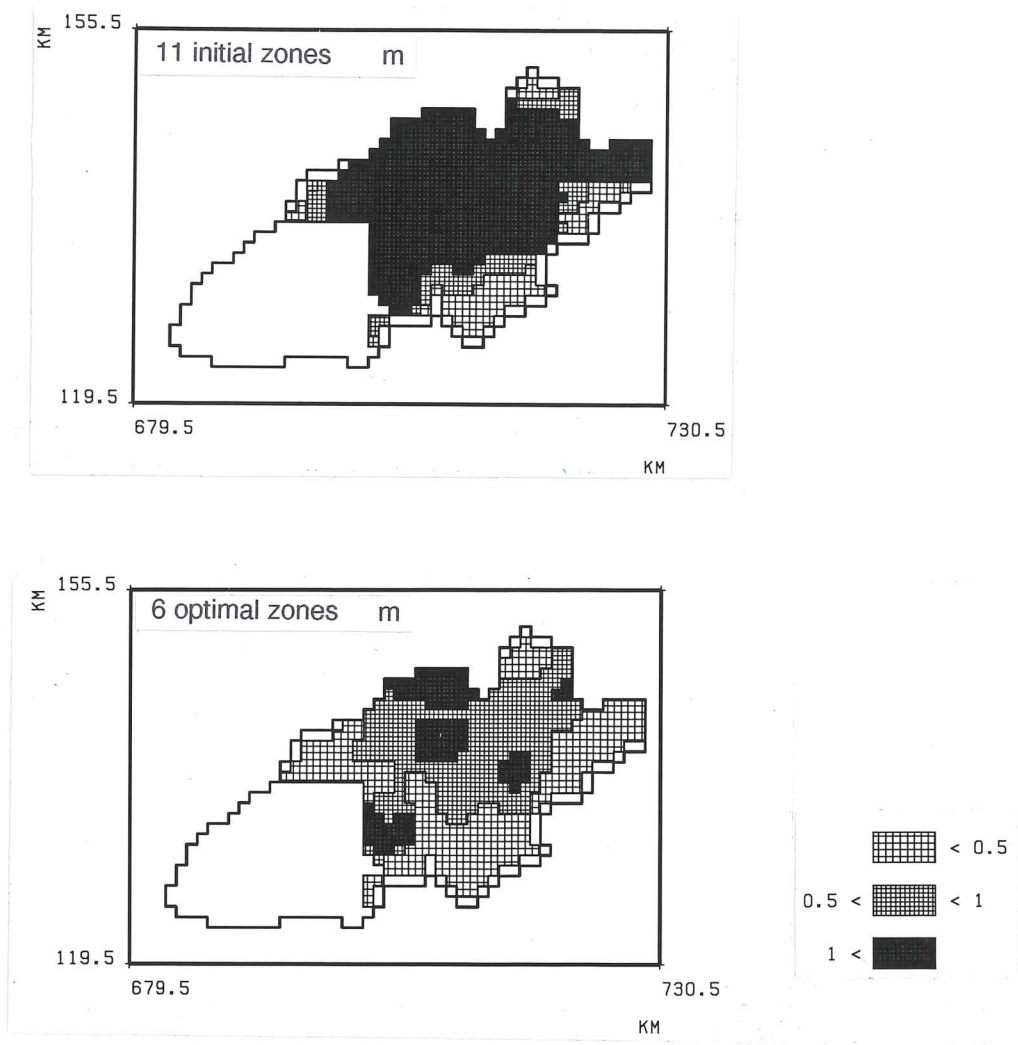


Fig. 6 - Thau aquifer : standard deviation of hydraulic heads simulation.

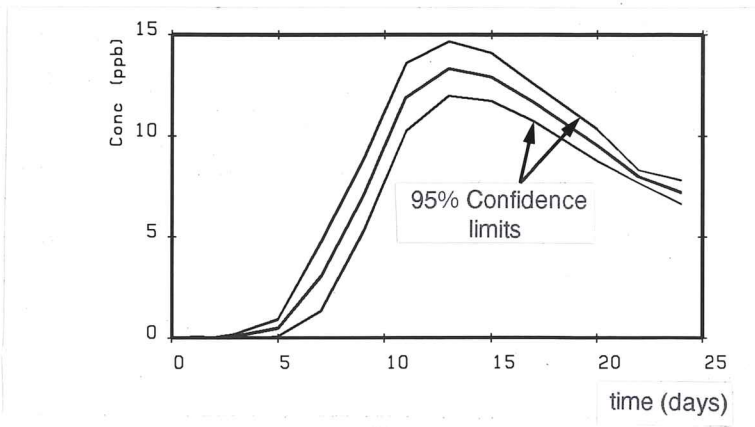


Fig. 7 - Finnsjon tracer test : concentration prediction corresponding to other injection and pumping rates.

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