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Deterministic and stochastic modelling for protection zone delineation

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- ***Deterministic approach***
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  - *- advection-macrodispersion*
  - *- advection-dispersion + multi tracer tests*
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- ***Stochastic approach***
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  - *- Synthetic case*
  - *- Stochastic generation of K-fields combined to inverse modelling*
  - *- Additional conditioning by geoelectrical resistivity data*
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Definitions

***Well capture zone** : … the set of points on the groundwater surface from which a tracer particle will reach the well*

→ *total catchment of the well*

***Time-related capture zones**: … isochrones (contour lines of equal travel time to the well)*

→ *only parts of the total catchment*

*In many regions: **protection zones** at the surface corresponding to particular isochrones in saturated zone*

→ *a time-related protection*

Protection zones ↔ time-related capture zones

- ***numerical computational methods are used to obtain a delimitation…***

- ***What are the conceptual choices ?***
  What are the needed data ?
  What are the uncertainties linked to the obtained delineation ?
  Deterministic or Stochastic approach ?

- ***… in heterogeneous geological formations, all direct and indirect data, respectively hard and soft data, must be used in an optimal way !***

Deterministic approach

Advection + Macrodispersion

- *different values of hydraulic conductivity (and possibly also for effective porosity)*
- *a macrodispersion term representing statistically the general contaminant behaviour around the advective mean position*
- *smaller scale heterogeneities are not introduced in detail*
- *'scale effect' is observed and difficulties to assess upscaled values*

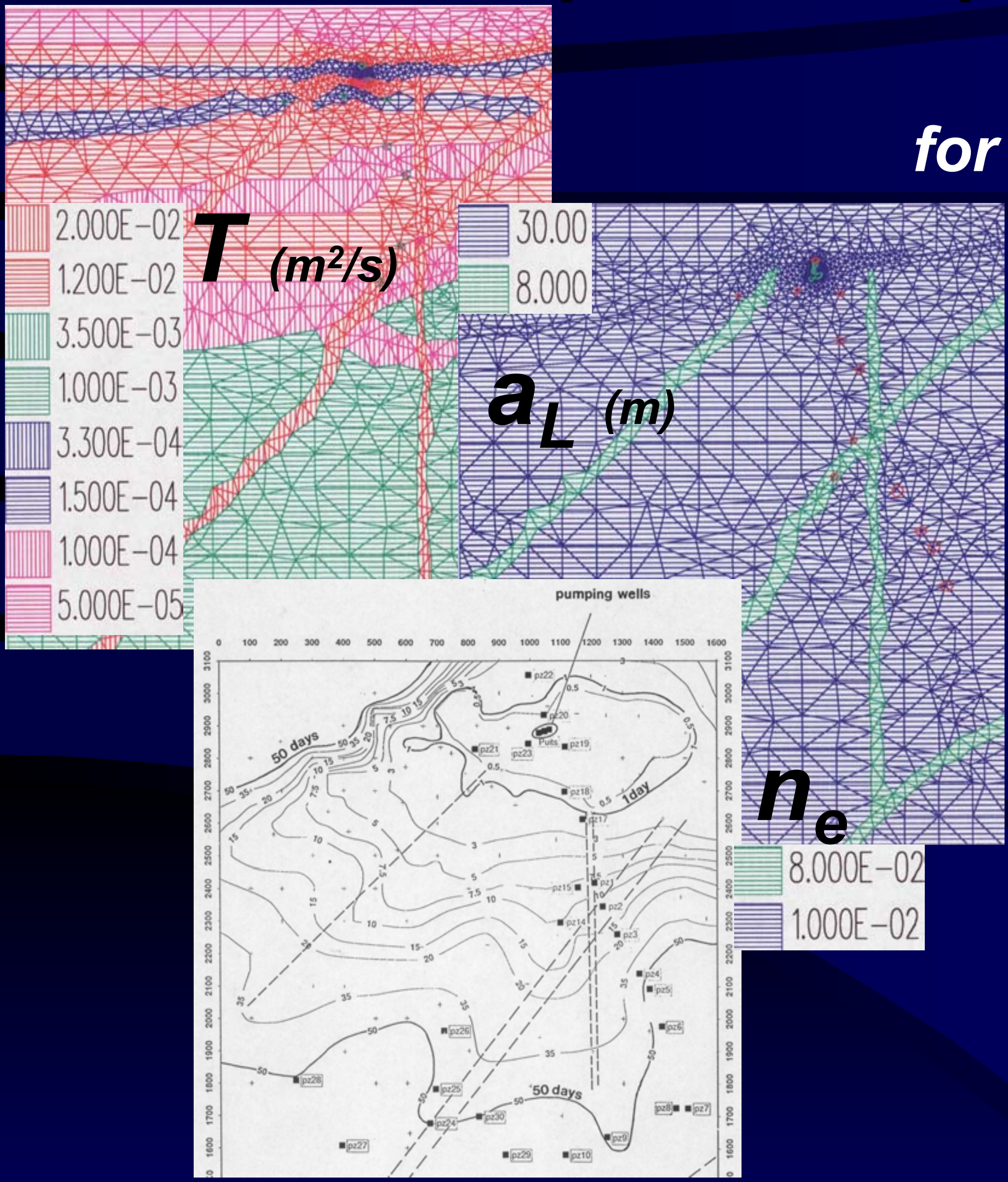
Advection + Dispersion

➡ *heterogeneous conditions for both the groundwater flow model and the transport model*

Example: a methodology proposed to water suppliers in Walloon Region of Belgium (Dassargues, 1994)

- *geology, geomorphology, basic hydrology*
- *geophysical prospecting*
- *piezometers and observation wells*
- *pumping tests in each borehole*
- *multi-tracer tests in pumping conditions*
- *first analytical interpretations*
- *building of a flow-transport model considering heterogeneity in the layers*
- *calibration for flow (on measured piezometric levels)*
- *calibration for transport (on the measured breakthrough curves)*
- *simulations and computations of the travel times for different injection points (including the dispersion)*

… extrapolation of parameters



for each geological unit:

- ***lithology***
- ***fissuration/ fracturation degree***

➡ ***values of*** - ***K***
- n_e
- a_L, a_T
- ***...***

➡ ***purely deterministic extrapolation based on 'hard data' and 'soft data'***

… challenges

- *tracers behaviours in different geological media (adsorption, ...)*
- *injection control and measurement of the real input function in the aquifer*
- *2D and 3D aspects of the tracer tests and modelling*
- *boundary conditions for groundwater flow and transport models*
- *multiple possible calibrations using 'trial and error' calibration or automatic calibration*
- *how the role of the geology (soft data) can be combined with a calibration objective function ?*
- *upscaling and spatial extrapolation of the parameters taking the spatial variability and specific heterogeneities into account*
- *uncertainty of the results…*
- *immobile water effect, ...*
- *legal aspects concerning - the 'first arrival' of tracer (contaminant) - the non-saturated zone*

Stochastic approach

General aims

- to obtain a quantification of the uncertainty of results;
- optimising the use of the available data;
- how to combine inverse modelling procedure with integration of soft-data;

Many different approaches !

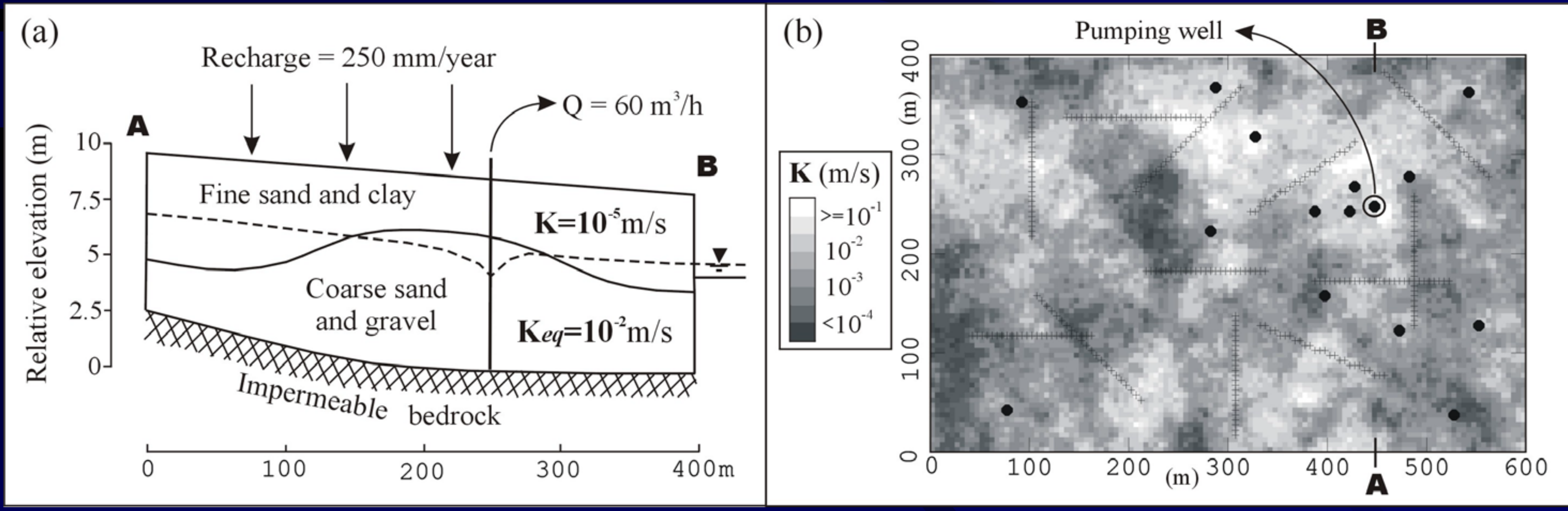
Our example of methodology:

➡ a stochastic approach integrating different sorts of data:

- K-data (hard data) by conditional stochastic simulations;
- h data (soft data) by inverse modelling;
- ρ data (soft data) by conditional stochastic co-simulations

Synthetic example

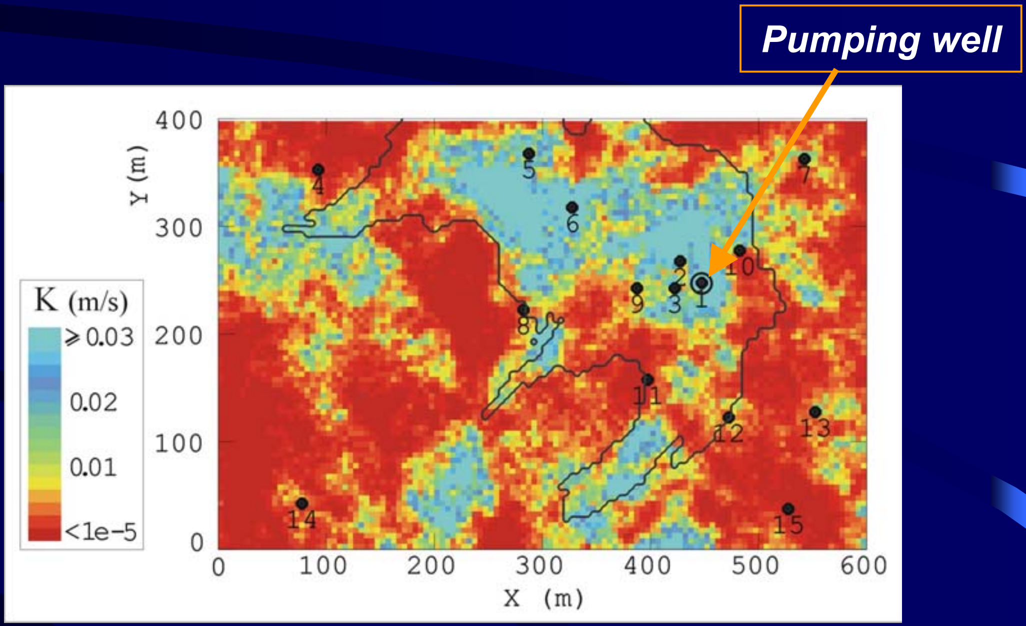
- *hypothetical groundwater flow domain with hydro-geological conditions similar to actual alluvial sites*
- *domain large enough to avoid boundary effects*
- *two layers:* *- fine sand and clay layer (K = 10^{-5} m/s)*
  - lower coarse sand and gravel layer
  for which a "true" hydraulic conductivity field representing the "reality" is created using a non-conditional simulation



using the Turning Band algorithm (Mantoglou & Wilson, 1982) with an isotropic, exponential correlation structure of log K (alluvial sediments of the Meuse River valley downwards to Liège, Belgium)

from a grid of 9600 cells: selection 15 K values providing the hard data set

- *pumping well (60 m^3/h)*
- *flow simulation providing the synthetic "measured“ heads at the 15 virtual piezometers (first set of soft data)*
- *considering advective transport time to the well,*

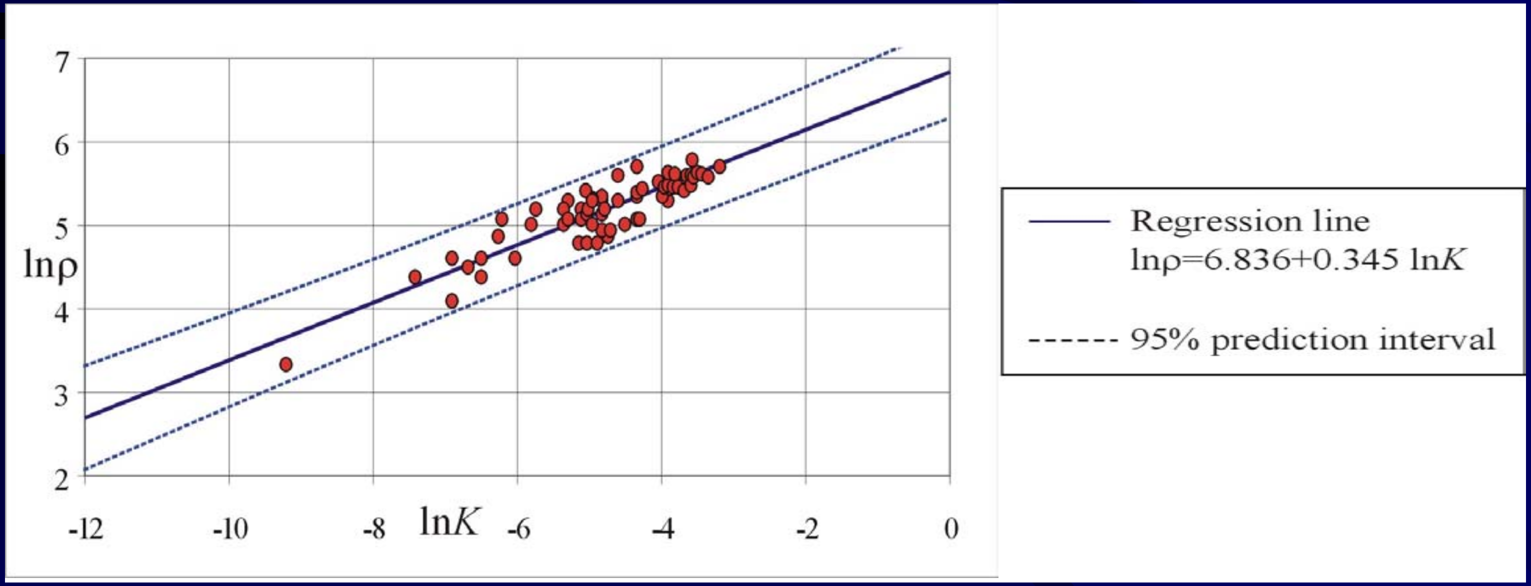


the "true" 20-day isochrone (associated with the concerned pumping rate and n_e = 0.05) resulting from the "true" hydraulic conductivity field → reference isochrone

- *a resistivity data set (second set of soft data) is created based on the observed correlation (r = 0.9) existing between electrical resistivity (ρ) and hydraulic conductivity (K) in the alluvial sediments of the Meuse River*

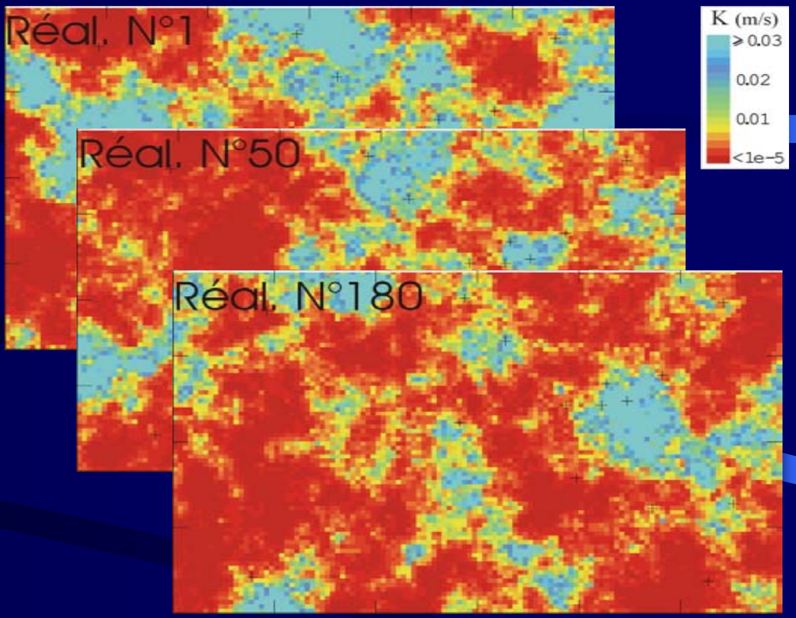
- *considering N(0,1) as a random draw within a standard normal distribution and* $\hat{\sigma}$ *the standard deviation of the regression residual,* → *300 resistivity values, distributed on 12 tomographic profiles*

$$\ln \rho = 6.836 + 0.345 \ln K + \hat{\sigma}\ N(0,1)$$



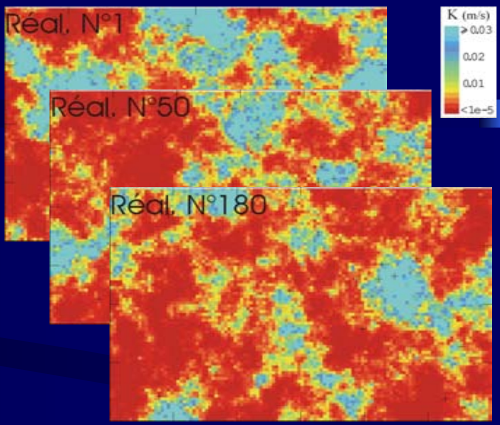
Stochastic conditional simulations

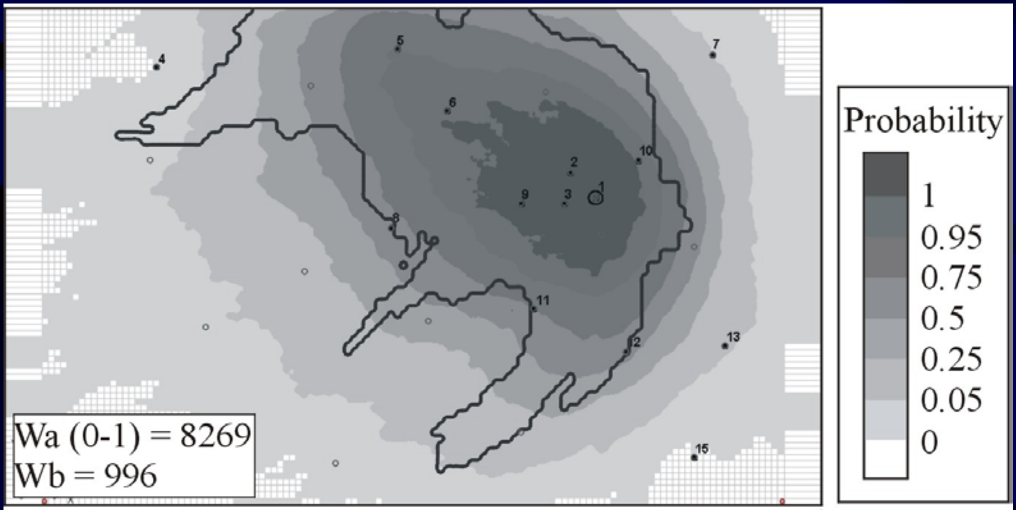
- *four hundred stochastic simulations of equally likely hydraulic conductivity fields*
- *subsequently conditioned on hydraulic conductivity measurements by a kriging technique*

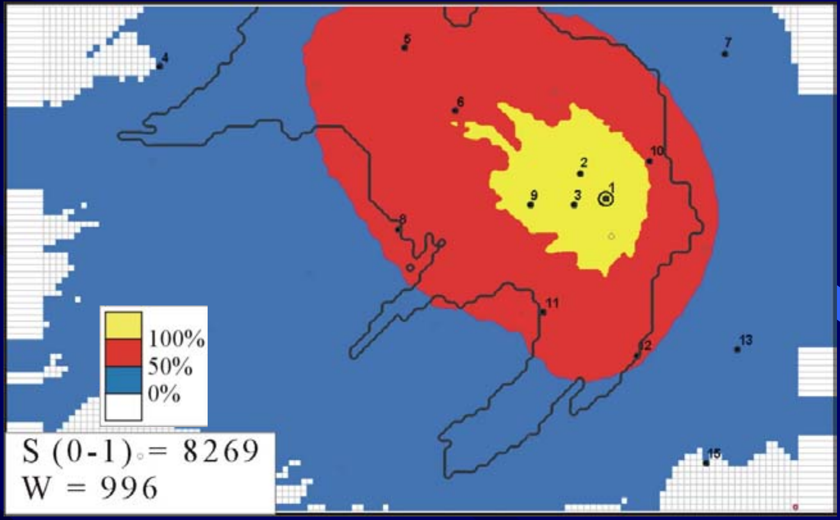


Conditional simulation	=	Non-cond. simulation = realisation	–	Kriging of each realisation	+	Kriging
		noise except in the measurement points				Exact estimator + smoothing

- *groundwater flow and a particle tracking process were computed for each realization*
- *ensemble of obtained capture zones*
- *treated statistically to infer the capture zone probability distribution (CaPD)*
- *CaPD gives the spatial distribution of the probability that a conservative tracer particle released at a particular location is captured by the well within a specified time span (van Leewen, 2000)*



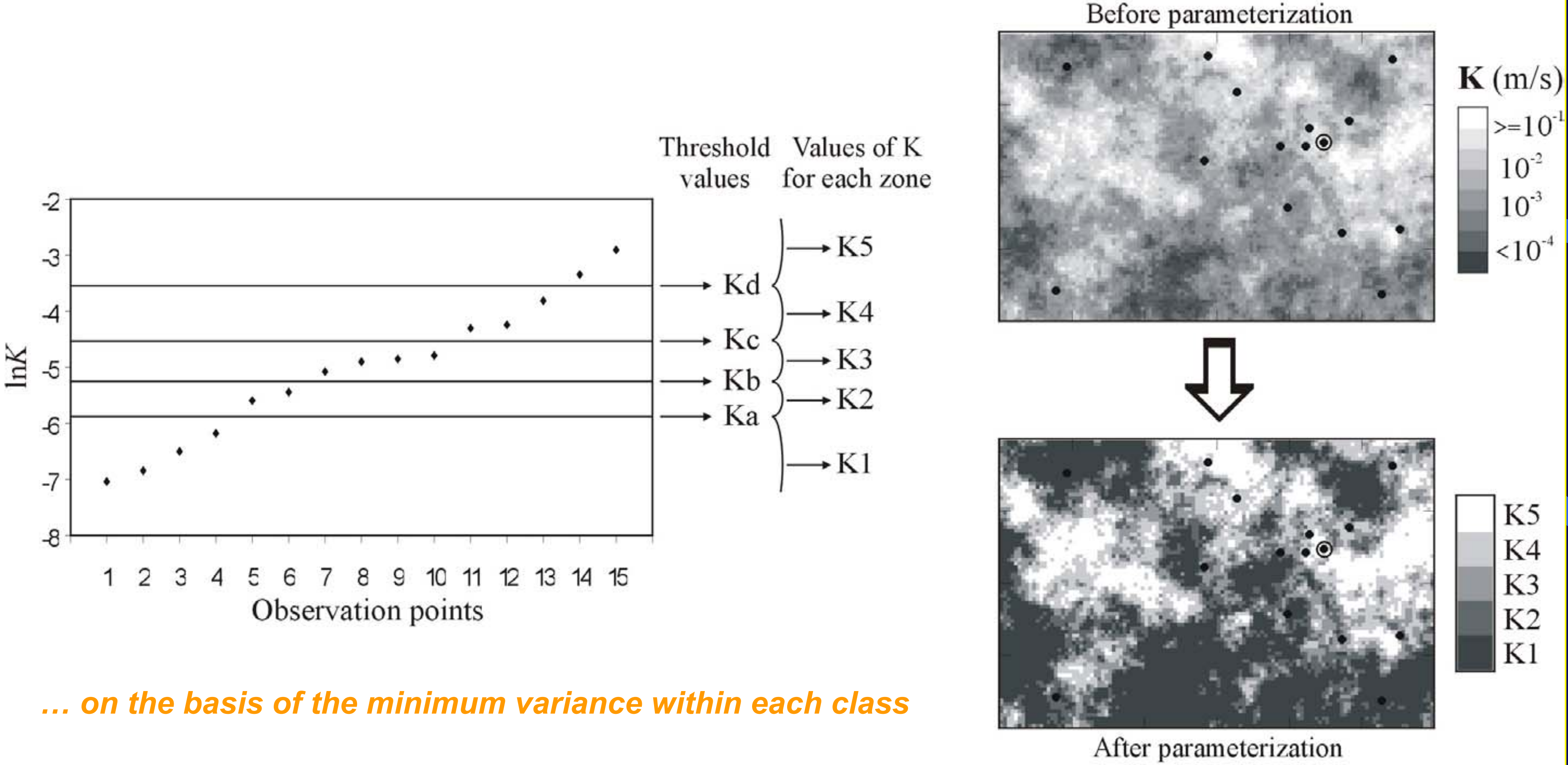




Wa : extent of the uncertainty zone for which the probability P of capture is 0<P<1
Wb : difference between reference isochrone and isoline 50% (probability of capture)

Additional conditioning by head measurements (first set of soft data)

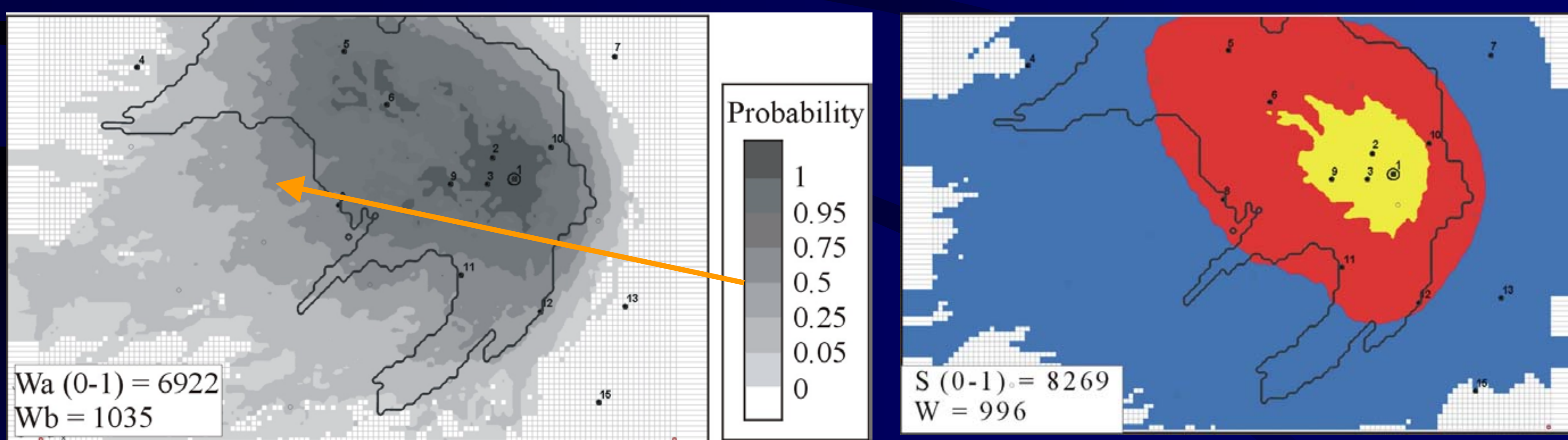
- *parameterization of each K-field*
- *thresholds values for dividing in five zones of uniform value (K_i, $i = 1,...,5$)*



… on the basis of the minimum variance within each class

for each parameterized K-field:

- ***a groundwater flow calibration on head measurements using PEST*** *(Doherty, 1994)*
- ***rejecting obtained (calibrated) realizations that did not respect ($K_i < K_{i+1}$), considering them as geologically erroneous***
- ***for each remaining realization, computation of the 20-day capture zone ➔ CaPD for the ensemble of possible capture zones***

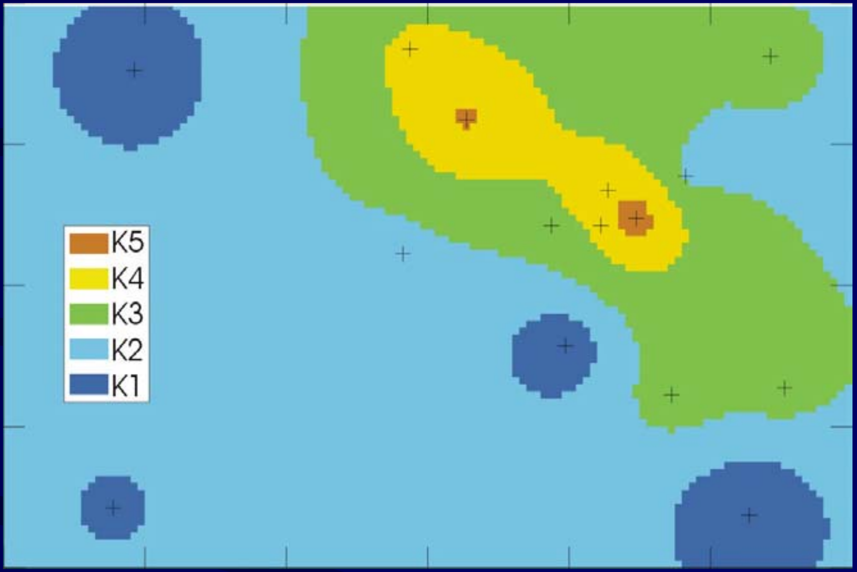


… reducing Wa *(uncertainty zone for which the probability P of capture is 0<P<1)*

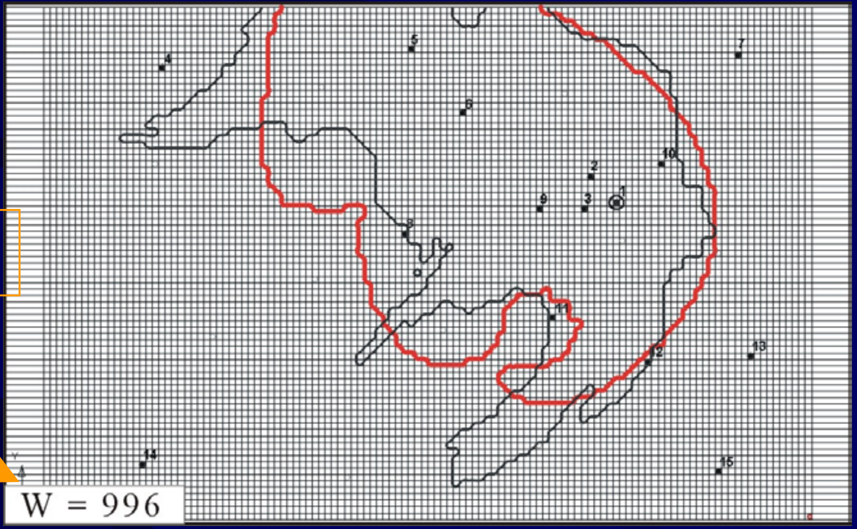
… not changing Wb (*difference between reference isochrone and isoline 50%)*

… if we were deterministic

- collecting the 15 measured K values and piezometric heads
- definitions of zones (on the basis of kriging and the threshold method)
- calibration of the groundwater flow model on the 15 measured h
- advective transport simulation
- 20 days isochrone line



difference (in 5m x 5m cells)



Additional conditioning by geoelectrical resistivity data (second set of soft data)

- integration of the geophysical data set by conditioning each stochastic simulation on both hydraulic conductivity measurements and resistivity values
- cokriging technique, providing stochastic conditional "co-simulations"
- four hundred K-fields conditioned on K values (hard data) and on ρ values (soft data)

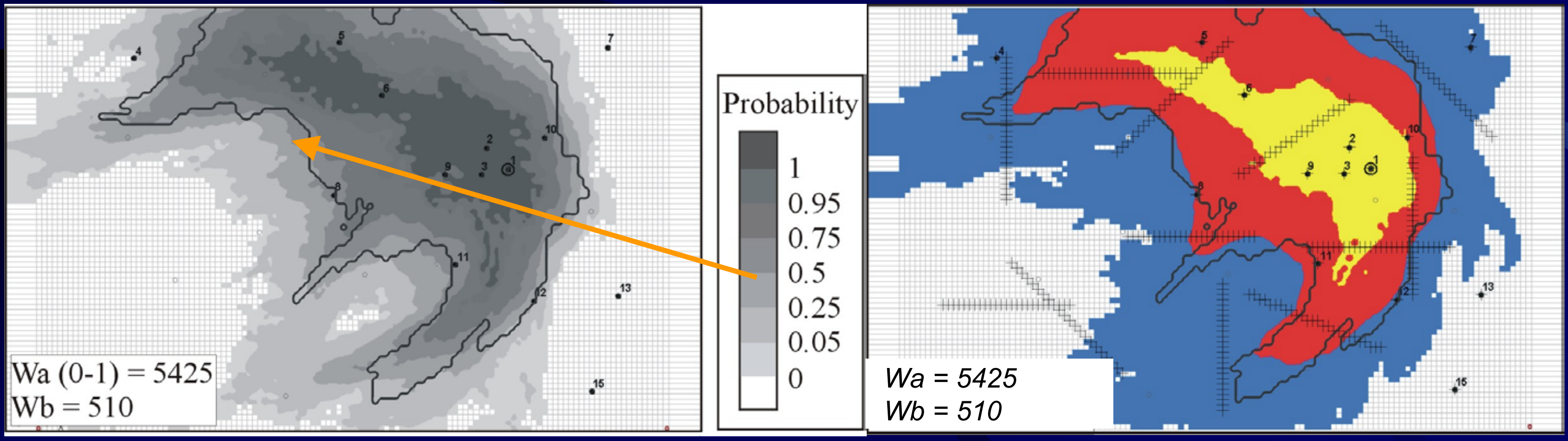
Conditional co-simulation	=	Non-cond. simulation = realisation	–	Cokriging of each realisation	+	Cokriging
		noise except in the measurement points				Exact estimator + smoothing

… as previously:

- parameterization of each K-field
- thresholds values for dividing in five zones of uniform value (K_i, $i = 1,\dots,5$)

… as previously, for each obtained K-field:

- inverse modelling using PEST (conditionning on h)
- rejecting realizations that did not respect ($K_i < K_{i+1}$)
- for each remaining realization, computation of the 20-day capture zone → CaPD for the ensemble of possible capture zones



Work being done …

Sensitivity analysis

- number of hard data (K)
- number of first soft data (measured h)
- number of second soft data (ρ)
- threshold method used for parameterization and values for dividing in zones
- relaxation of the rejection criterion

Application to a practical study case

- what are the practical difficulties ?

  CPU time ? local minima in inverse modelling ?
- number of K values and measured h : very limited

Conclusions / Perspectives

- stochastic approaches bring improvements
- it does not spare us the acquisition of measured data
- selection of 'best' locations for geophysical measurements
- all other issues concerning modelling and tracer tests interpretation remain
- further conditioning on tracer travel times, and on other soft data
- do we include dispersion ? to which extent ?
- are these methodologies applicable at another scale ?
- are these methodologies applicable in fissured media ?