Reducing the uncertainty of hydrogeological parameters by co-conditional stochastic simulation:

lessons from practical applications in aquifers and in low permeability layers

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Introduction

- ... "numerous theoretical papers have been published based on a stochastic description of aquifer heterogeneity (Neuman, 1982; Sudicky & Huyakorn, 1991; Yeh, 1992) but the central question of whether the stochastic method, which treats aquifer heterogeneity as a random field, is applicable to real aquifers under field conditions, has not been definitively answered"
  M.P. Anderson, 1995

- … the future of « dealing with heterogeneity » in hydrogeology depends largely on a conscious decision to better characterize, describe and model the geology of the sites…
  de Marsily *et al.*, 2005

- … from a practical point of view with two main classical questions of hydrogeology:
  - delineation of protections zones around pumping wells in aquifers;
  - waste disposal studies in low permeability layers

Outline

- Aquifers: capture zones delineation
  - Co-conditional stochastic method for delineation of time-related capture zone combined with an inverse modelling procedure
  - Application to a virtual (synthetic) study case
  - Application to a real case
  - Lessons
- Low permeability layers: solute fluxes and transfer times
  - Objectives
  - Application with K as hard data
  - Application with other transport parameters as hard data
  - Lessons
- Conclusions/perspectives from a practical point of view

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General context: groundwater protection

- Time-related capture zone (protection zone)

→ delineation based on the concept of travel time

= area around the well from which water is captured within a certain time t

→ based on the reliability of the hydrogeological models

→ depends strongly on our ability to describe the aquifer system properties (K, n_e, ...)

→ based on our knowledge of the geology (limited by the existing field data)

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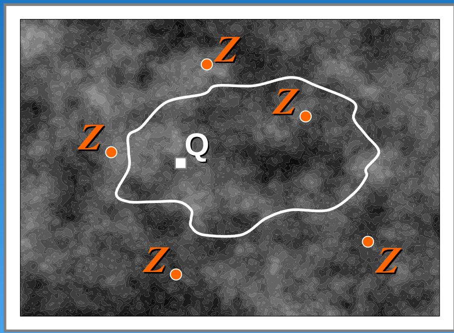
Heterogeneity

- Hydrogeological properties → heterogeneous

→ Irregular distribution of groundwater flow and solute transport

→ Few, ponctual and spread data



- Source of uncertainty → hydraulic conductivity *K*
- Particle tracking → following the path of imaginary water particules placed in a groundwater flow field

Hard data and soft data

Field data

↙ ↘

Direct measurements of *K*	Indirect measurements of *K*
Hard data	Soft data
(generally few)	(geological or hydrogeological informations, results provided from geophysical prospections, expert advice, …)

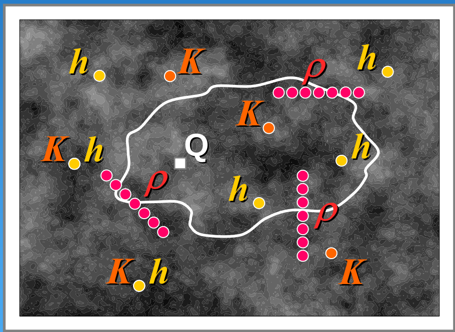
→ Reduce uncertainty on the predictions

↙ ↘

Piezometric heads h | Electrical resistivities ρ

Objectives

Propose a stochastic method to delineate protection zones, applicable to real study case



- ✓ quantification of the well capture zone uncertainty
- ✓ reduction of this uncertainty by integrating direct (hard data) and indirect (soft data) measures of K

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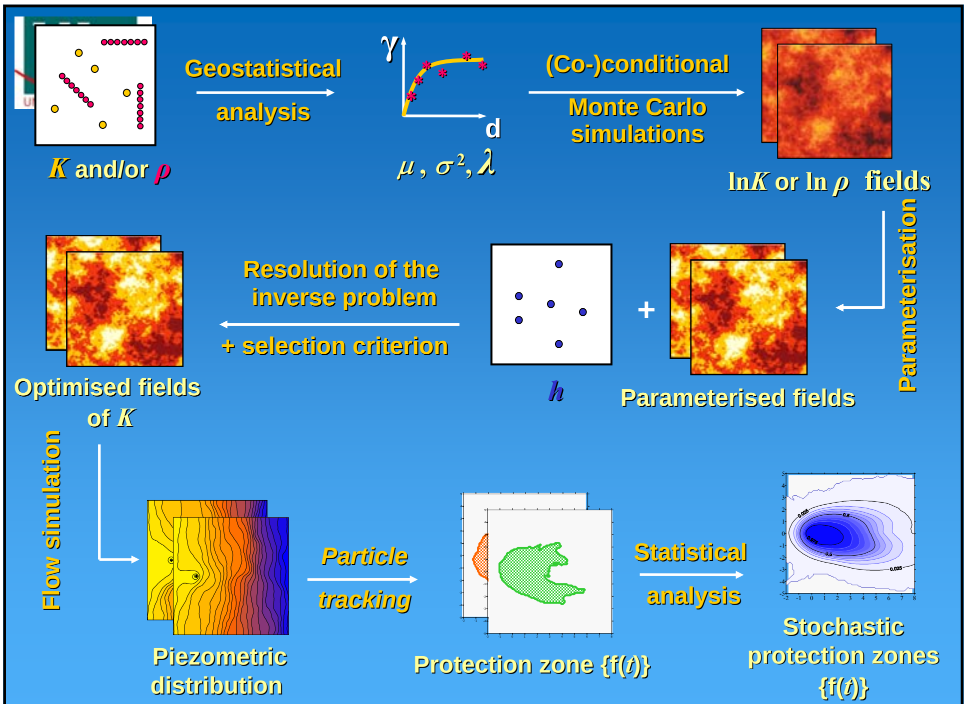

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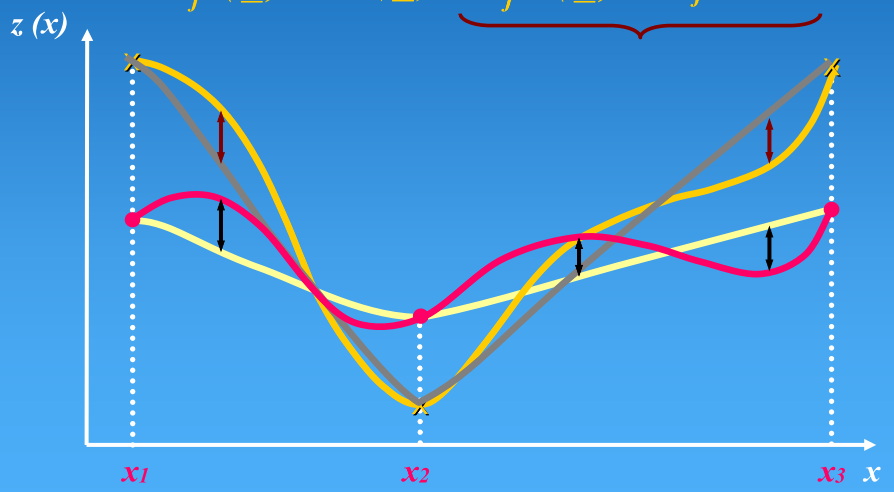
Conditional simulations

$$z_j^{CS}(\underline{x}) = z^*(\underline{x}) + z_j^{NCS}(\underline{x}) - z_j^{NCS*}(\underline{x})$$



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Conditional simulations

$$z_j^{CS}(\underline{x}) = z^*(\underline{x}) + z_j^{NCS}(\underline{x}) - z_j^{NCS*}(\underline{x})$$

Conditional Simulation (CS) = Kriging + Non-cond. simulation (NCS) – Kriging of the NCS

Turning Bands (Matheron, 1973 – Mantoglou & Wilson, 1982)

Kriging: 'Best Linear Unique Estimator' + smoothing

Non-cond. simulation (NCS) – Kriging of the NCS: 'Noise' (zero at the measurement points)

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Co-conditional simulations

$$z_j^{SC}(\underline{x}) = z^*(\underline{x}) + z_j^{SNC}(\underline{x}) - z_j^{SNC^*}(\underline{x})$$

Co-conditional simulation	=	Cokriging	+	Non cond. simulation NCS	–	Estimation by cokriging of the NCS

Many collected soft data measurements

→ better caracterisation of the spatial variability

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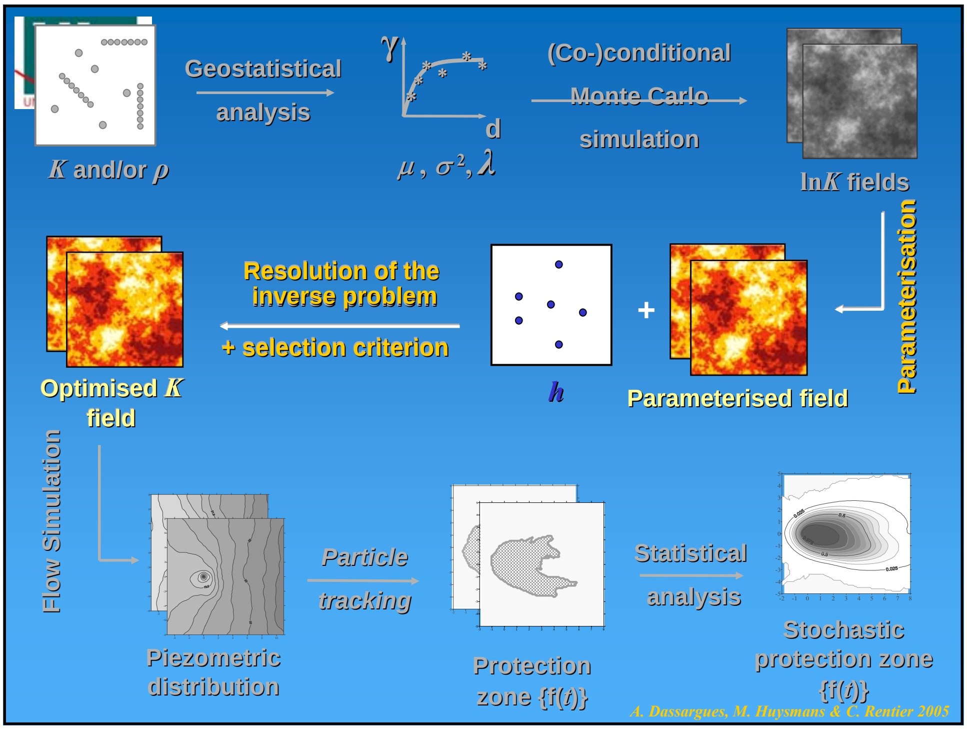
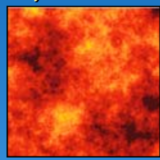


Conditioning on measured *h* through an inverse modelling procedure

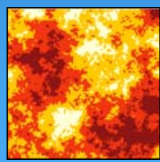
- … requires parameterisation (zonation in 'facies')
- How to perform that without loosing the geostatistical properties of the K fields ?



Actual variation range for $\ln K$

$-\infty \longleftrightarrow +\infty$

Zonation



$-\infty$ S1 S2 S3 S4 $+\infty$

C1 C2 C3 C4 C5

avec

$K_{C1}<K_{C2}<K_{C3}<K_{C4}<K_{C5}$

- thresholds values for dividing in 'facies' of uniform value (K_i, i = 1,…,5)

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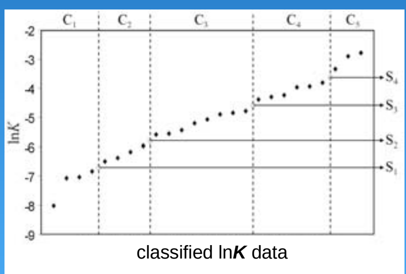
Which threshold values (S_i) ?

- Principle : minimum variance within each 'facies'

→ minimising function f



$$f = \sum_{i=1}^{N_c} \sum_{j=1}^{N_{di}} (\ln K_{ij} - \overline{\ln K_i})^2$$

$$\overline{\ln K_i} = \frac{1}{N_{di}} \sum_{j=1}^{N_{di}} \ln K_{ij} \quad , i = 1, N_c$$

- then the value of K_{Ci} = average value / facies
- serve as initial value in (not adjoining) zones of the facies
- optimised by the inverse procedure

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After the inverse procedure: selection criterion (order criterion)

- after optimisation of the K values in each ‘facies’, we add the selection criterion that the initial respective order must be respected : $K_{Ci} < K_{C(i+1)}$
  or relaxing:
  ➡ only one permutation

➡ eliminating realisations not respecting this criterion as « irrealistic fields for a geological point of view »

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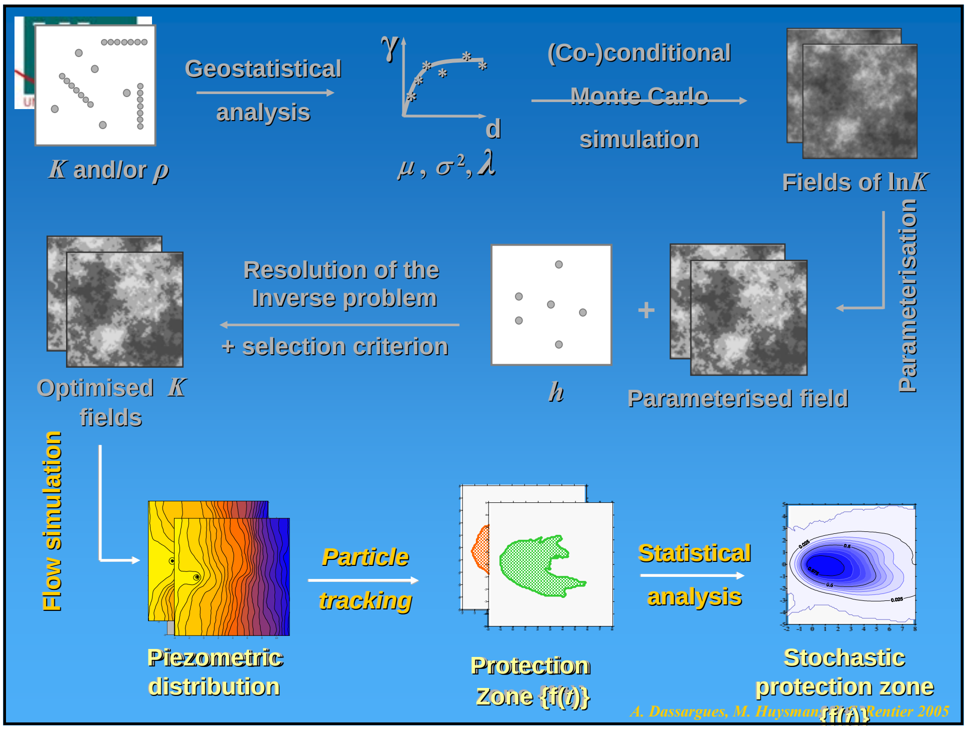


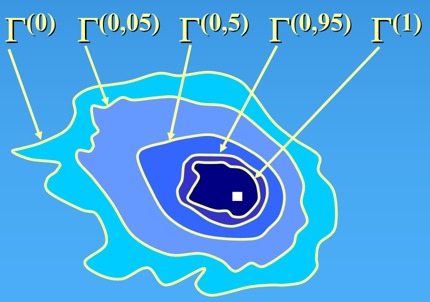
Statistical analysis

Capture zone probability distribution

$$[CAP(\underline{x},t)] = \frac{1}{n} \sum_{k=1}^{n} (I(\underline{x},t))_k$$

= probability that a tracer particle released at a particular location is captured by the well within a specified time

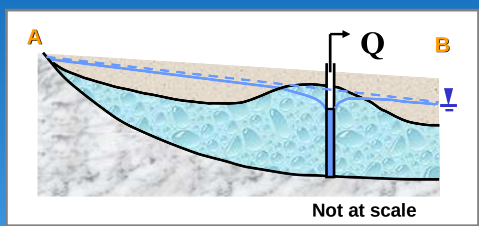
The isolines $\Gamma^{(i)}$ connect the locations in the *CAP* with the same probability $p(CAP(x,t)) = i$

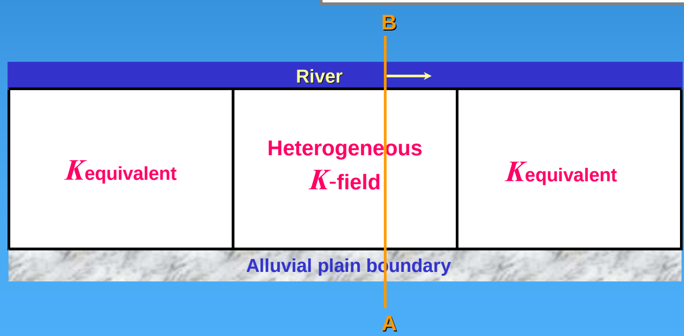


Synthetic study case

Groundwater model representing « a reference situation »

very similar to alluvial aquifer conditions



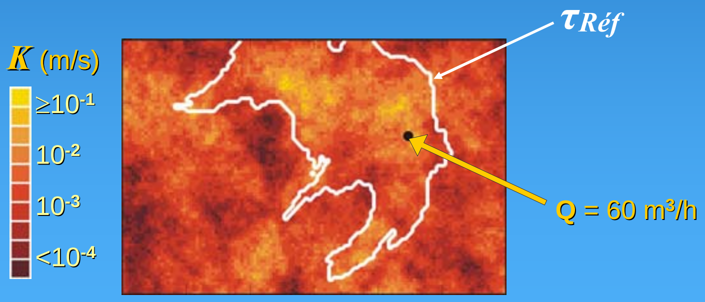


Construction of a reference capture zone

One non-conditional ***K***–field generation: reference medium

➡ Reference protection zone f(*t*)
(by direct groundwater flow simulation and particle tracking)

➡ Create sets of ***K***, ***h*** and ***ρ***



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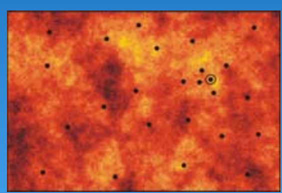
Creating realistic 'measured data sets'

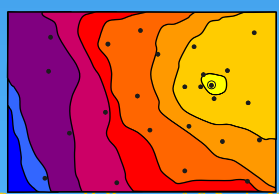
- Creating a (***K***) hydraulic conductivity data set

  ➡ in few 'measurement points': value from the ***K*** field



- Creating a (***h***) piezometric heads data set

  ➡ in few 'measurement points': value from the reference flow field



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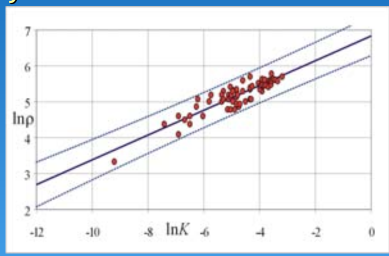
Creating realistic 'measured data sets' (following)

- Creating a (ρ) geoelectrical resistivity data set

Data measured and collected in many sites of the alluvial sediments of the River Meuse



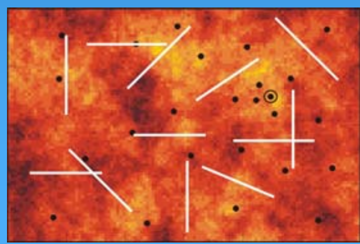
→ correlation between $\ln K$ and $\ln \rho$

→ artificial generation of a ρ data set from the reference K field

considering N(0,1) as a random draw within a standard normal distribution and $\hat{\sigma}$ the standard deviation of the regression residual,

$$\ln\rho_i = b_0 + b_1 \ln K_i + \sigma . N_i(0,1)$$

300 resistivity values, distributed on 12 tomographic profiles



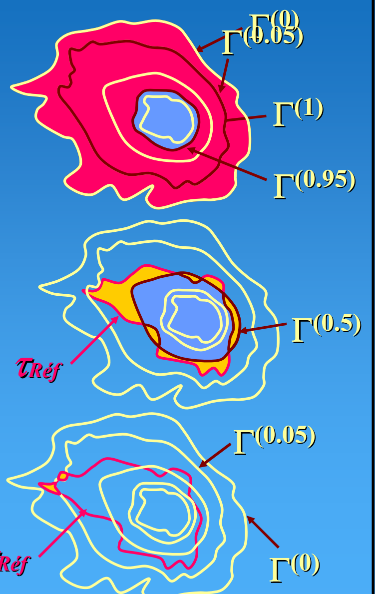
Application to the synthetic study case

	0 K	15 K	25 K
0 ρ	[$CAP(x,t)$]	[$CAP(x,t)$| K_{15}, h_{15}] [$CAP(x,t)$| K_{15}, h_{25}]	[$CAP(x,t)$| K_{25}, h_{15}] [$CAP(x,t)$| K_{25}, h_{25}]
150 ρ	[$CAP(x,t)$| h_{15}, ρ_{150}] [$CAP(x,t)$| h_{25}, ρ_{150}]	[$CAP(x,t)$| K_{15}, h_{15}, ρ_{150}]	[$CAP(x,t)$| K_{25}, h_{25}, ρ_{150}]
300 ρ	[$CAP(x,t)$| h_{15}, ρ_{300}] [$CAP(x,t)$| h_{25}, ρ_{300}]	[$CAP(x,t)$| K_{15}, h_{15}, ρ_{300}]	[$CAP(x,t)$| K_{25}, h_{25}, ρ_{300}]

t = 1, 5, 10, 20 days

Performance quantification
(after van Leeuwen & *al.*, 2000)

- w_{a1} and w_{a2} = a measure of the surface between $\Gamma^{(0)}$ and $\Gamma^{(1)}$; and between $\Gamma^{(0.05)}$ and $\Gamma^{(0.95)}$
- w_b = deviation of $\Gamma^{(0.5)}$ with regards to $\tau_{Réf}$
- w_{s1} and w_{s2} = how far $\tau_{Réf}$ is well included in the zone $\Gamma^{(0)}$ and $\Gamma^{(0,05)}$



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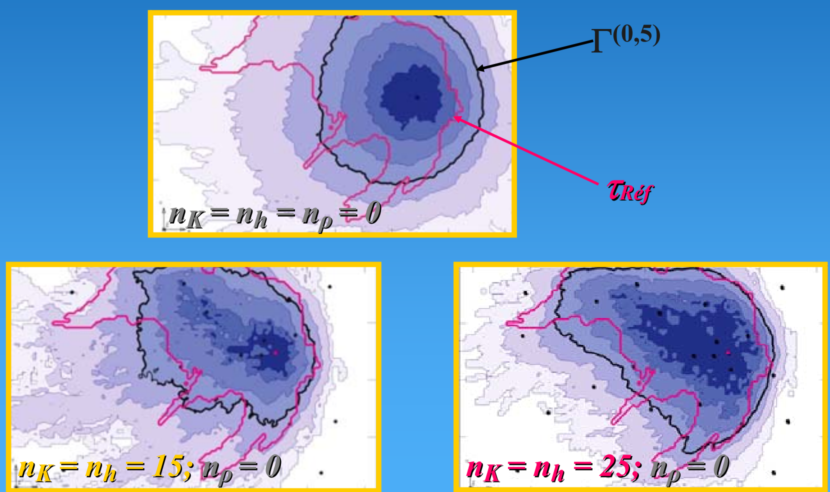
For each realisation, computation of the 20-day capture zone ⟶ CaPD



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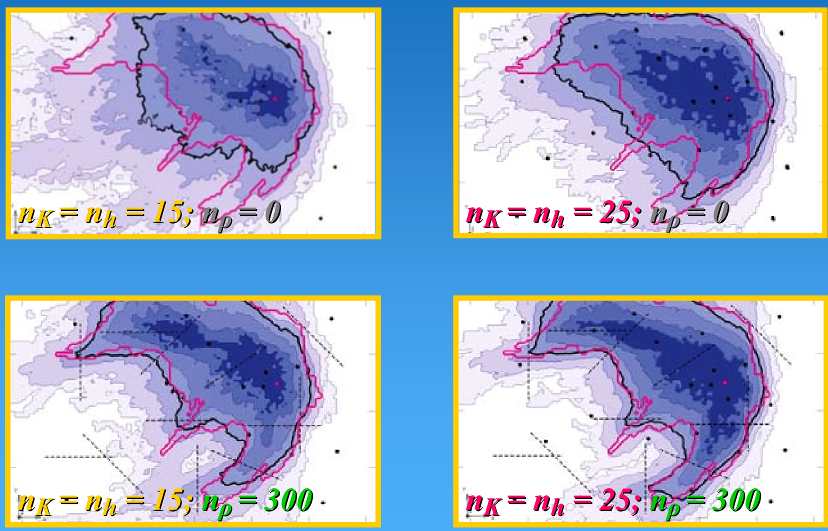
… strong effect of the co-conditioning



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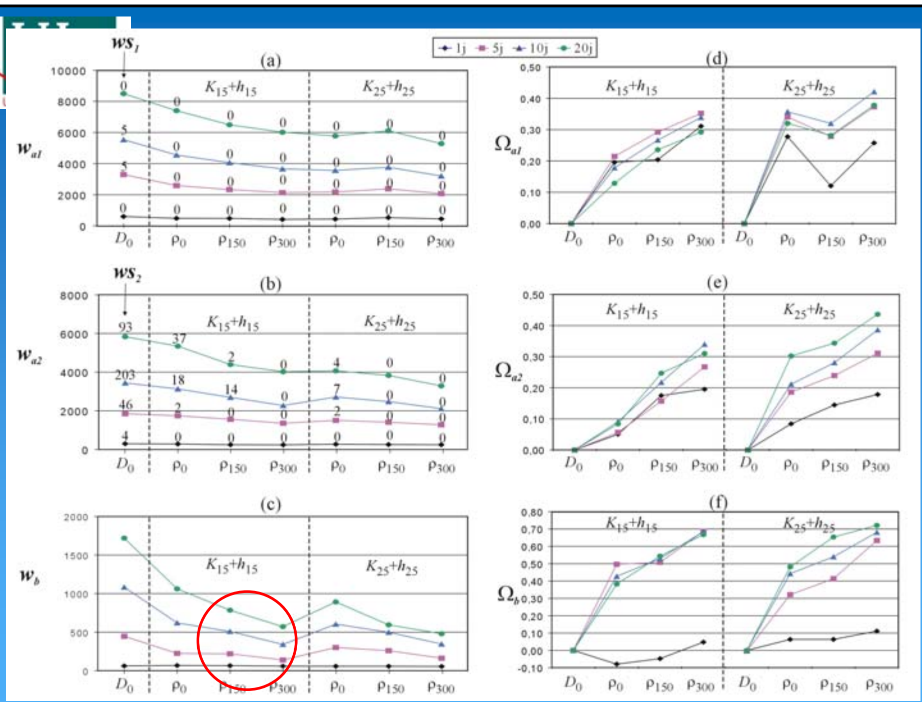

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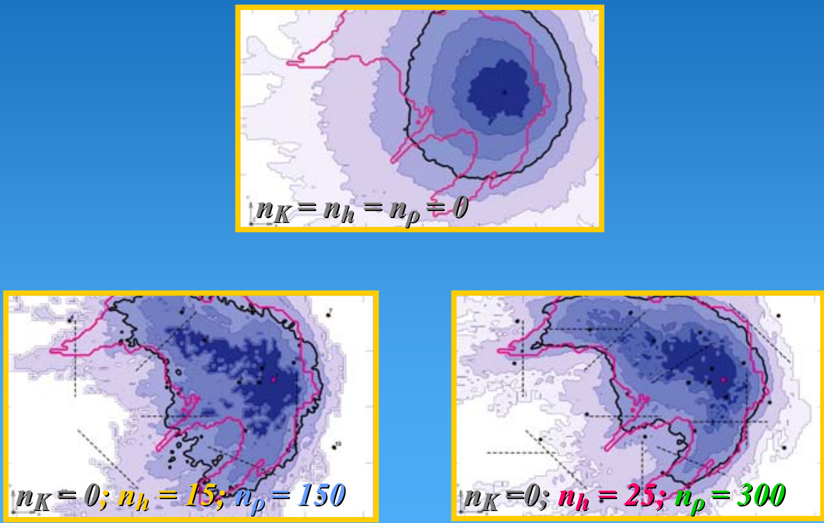
Synthetic case: summary



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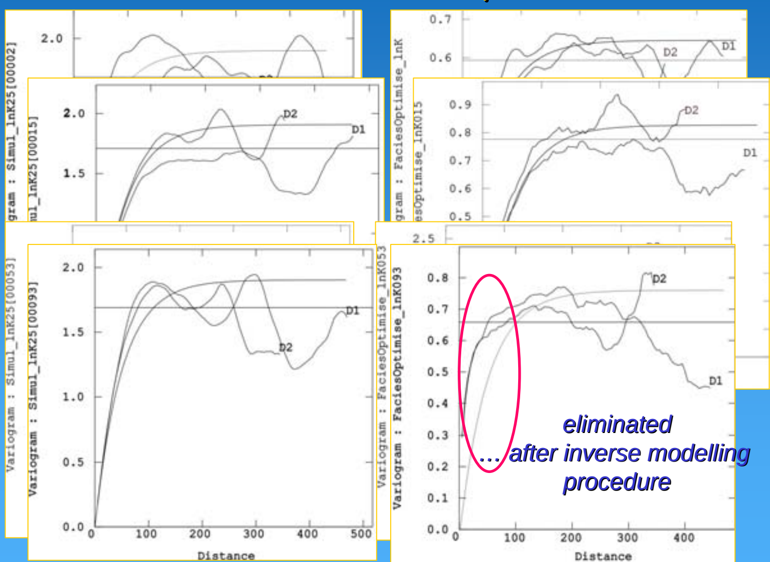
Effect of the zonation in facies and selection on the spatial structure ?



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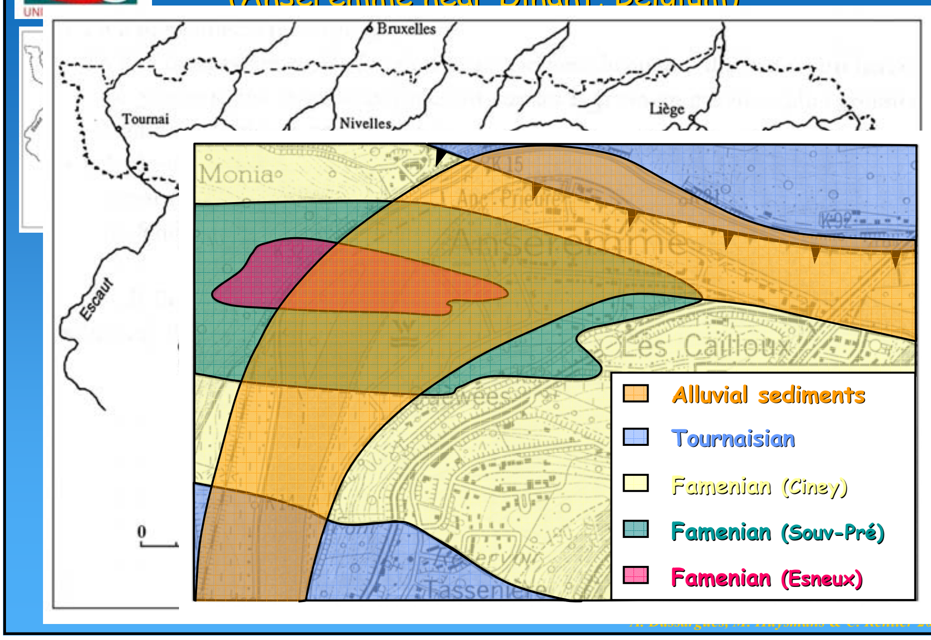
Application to a real case
(Anseremme near Dinant, Belgium)



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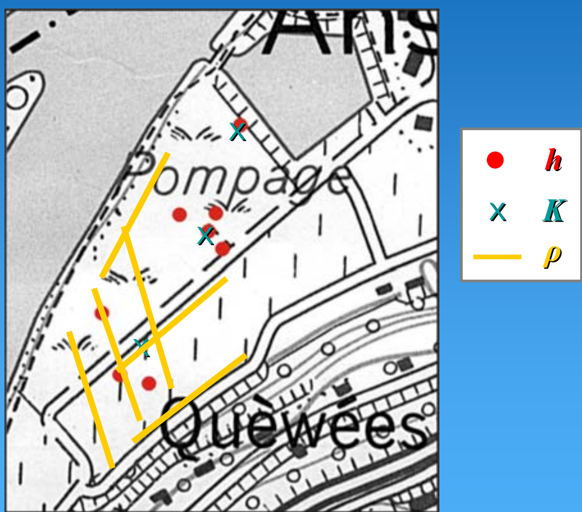

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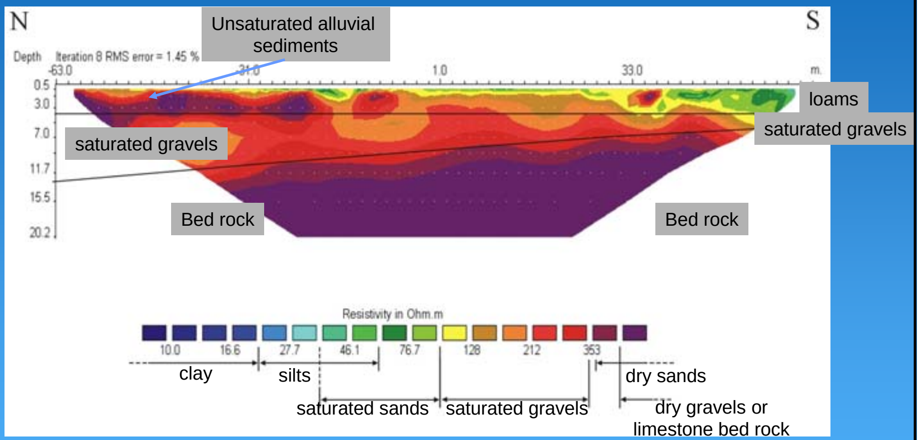

Equivalent value of ρ obtained in the gravel layer (alluvial sediment)

$$\frac{e_{tot}}{\rho} = \sum_{i=1}^{n} \frac{e_i}{\rho_i}$$

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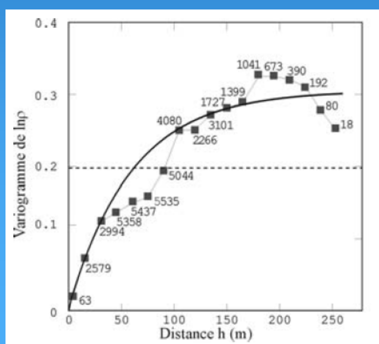
Application to a real case
(Anseremme near Dinant, Belgium)

- conditioning on lnρ (293 data points)
- inverse modelling on h (8 data points)
- verifiying the coherence of the obtained K fields with regards to the 3 data points of measured K



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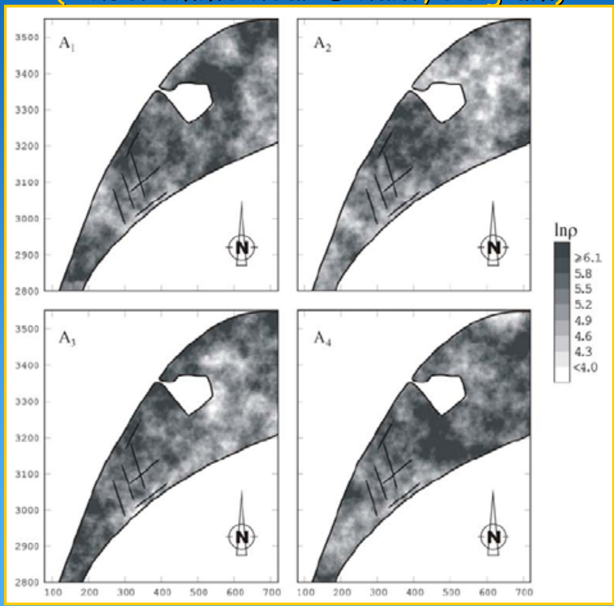
Application to a real case
(Anseremme near Dinant, Belgium)



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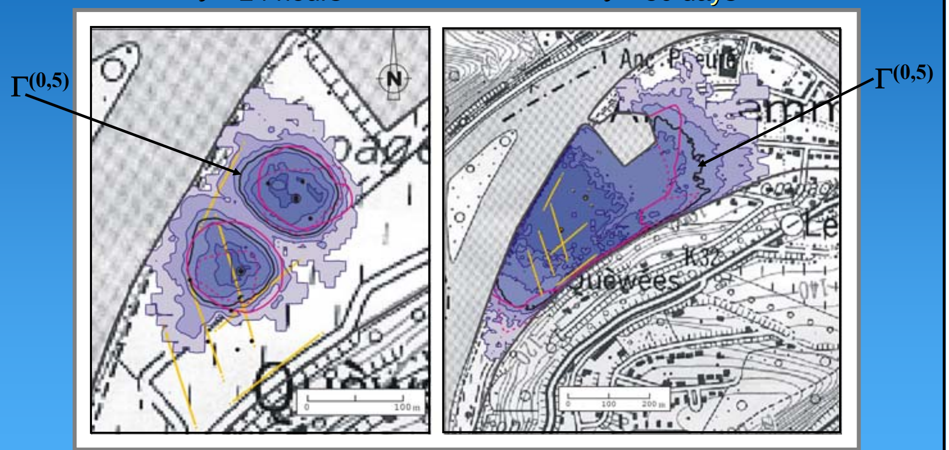
Application to a real case
(Anseremme near Dinant, Belgium)

t = 24 hours $\qquad$ t = 50 days



τ 3D deterministic model

τ 2D deterministic model

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Lessons

- stochastic co-conditional approaches bring improvements
- it does not spare us the acquisition of measured data
- selection of 'best' locations for geophysical measurements
- if piezometric heads are used for inverse modelling
  - ➡ parameterisation / zonation in 'facies'
  - ➡ thresholds values / selection criterion
  - ➡ statistics on remaining realisations
  - ➡ if selection criterion not too bad

    geostatistical structure seems to be preserved
- the 'facies' zones can be disjoint … possible links to be found with more 'genetic' based geological analysis

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Co-conditional stochastic simulations in low permeability layers

- Aim /objectives:

  impact of the heterogeneity on the vertical solute transport through a very low permeability layer

  ➡ transfer times

  ➡ quantification of the solute fluxes
- Case study of the Boom clay:

  radioactive waste disposal under study
- Vertical heterogeneity of K_v correlated with secondary data:
  - resistivity values
  - gamma-ray
  - grain size (d_{40})
  - lithostratigraphic column (descriptive data) through indicators calculated by a 'Formation Micro Imager' (clay =1; sandy clay =2; clayey sand = 3; sand = 4)

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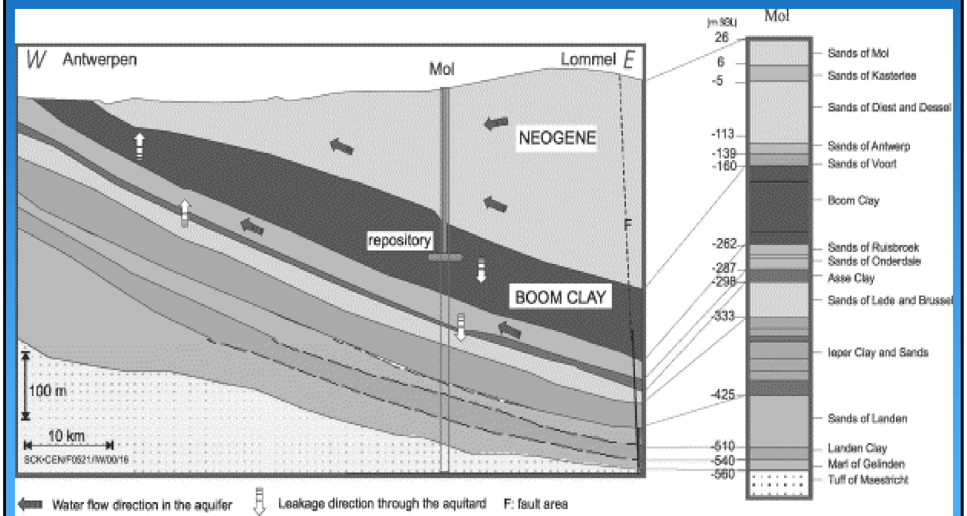
Co-conditional stochastic simulations in low permeability layers



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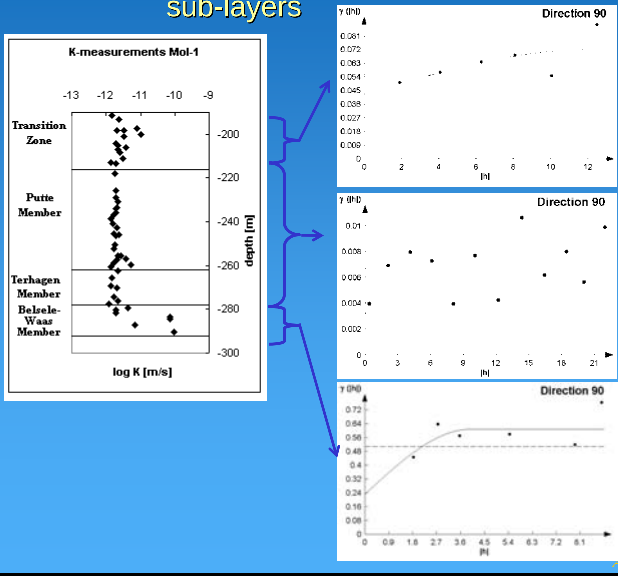
Low permeability layers: data sets

- Spatial structure of (K_v) in each of the three horizontal sub-layers



Variograms in the three distinguished zones

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Low permeability layers: data sets

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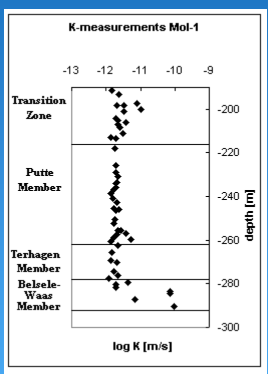
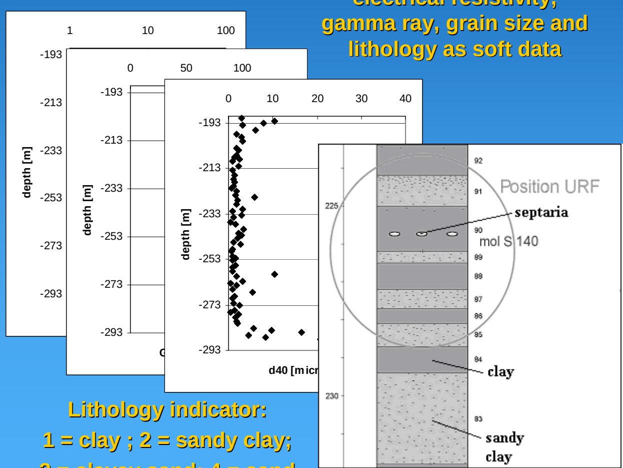


Measurements of electrical resistivity, gamma ray, grain size and lithology as soft data



Lithology indicator:
1 = clay ; 2 = sandy clay;
3 = clayey sand; 4 = sand

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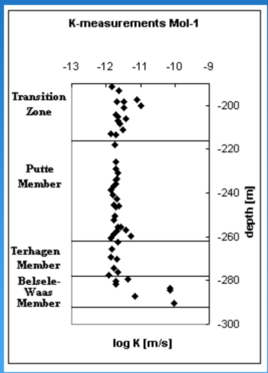
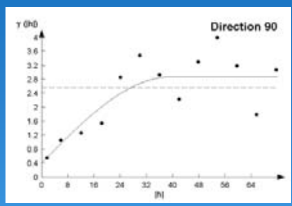
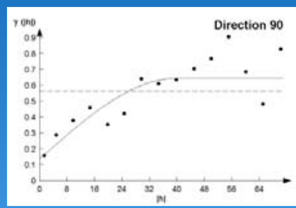
Co-kriging and Co-conditional simulations

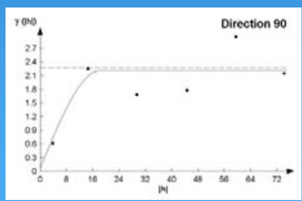




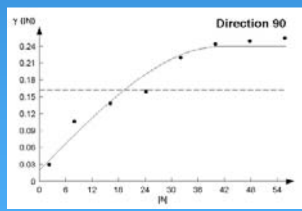
Cross-variogram logK_v - –GR



Cross-variogram logK_v - resistivity



Cross-variogram logK_v – d_{40}



Cross-variogram logK_v – lithology

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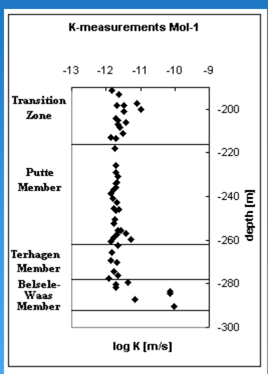
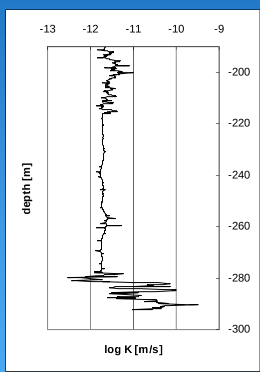
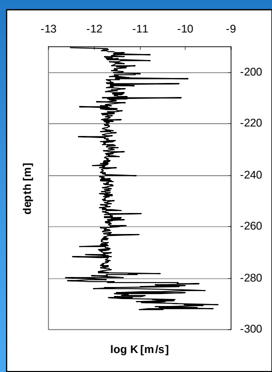
Co-kriging and Co-conditional simulations





Cokriging logK_v with resistivity, gamma ray, grain size and lithology



Co-conditional simulation of logK_v using resistivity, gamma ray, grain size and lithology as soft data

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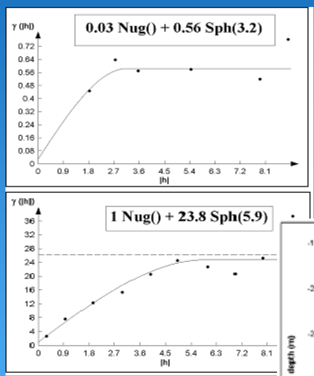
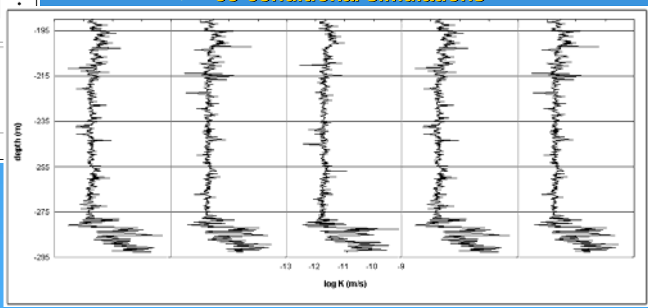
Co-conditional simulations

Variogram of logK_v in the deepest zone of the formation



Cross-variogram of resistivity and gamma-ray in the deepest zone of the formation

5 among 100 simulations of the K_v
using sequential simulation with histogram reproduction (Oz *et al.*, 2003), replacing kriging by a co-kriging :
→ co-conditional simulations



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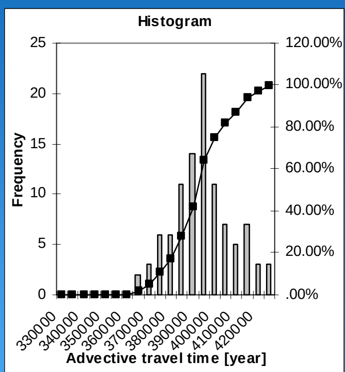
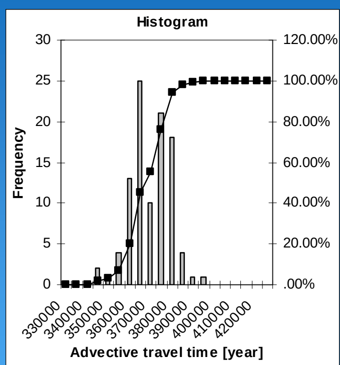
Modelling advective travel time



... co-conditioned on soft data



... conditioned only on hard data

... including the soft data increases the mean advective travel time and increases the standard deviation (larger variance) ...
because it is introducing a higher variability of the simulated hydraulic conductivity values

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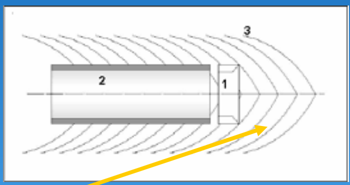
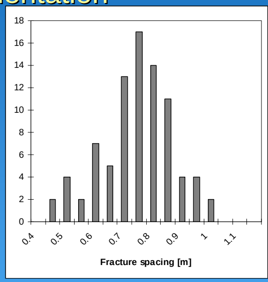
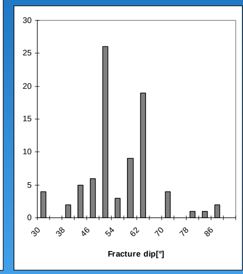
Adding the effect of exacavation induced fractures

- Fractures geometry and properties: extent, aperture, spacing, dip, orientation



induced shear planes





$$K_f = \frac{\rho g (2b)^2}{12\mu}$$

Aperture: random number between 0 and 50 µm

Orientation: strike perpendicular to the gallery axis

Use of FRAC3DVS

(Therrien & Sudicky, 1996; Therrien et al., 2003)

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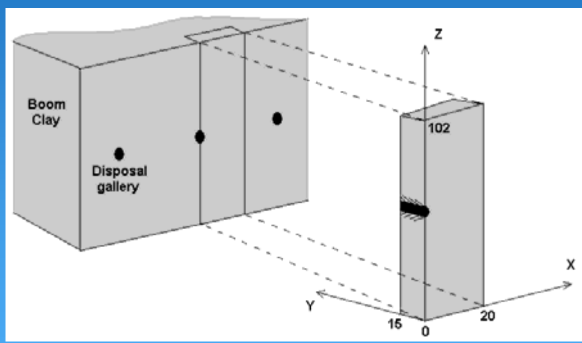
Fluxes results for 3 radionuclides (Advection + Diffusion + Decay)

- Se-79, I-129, Tc-99 (most important in terms of dose rates) (Mallants et al.,1999; details on the source conditions in Huysmans & Dassargues, 2005)



- Heterogeneity taken into account only for K

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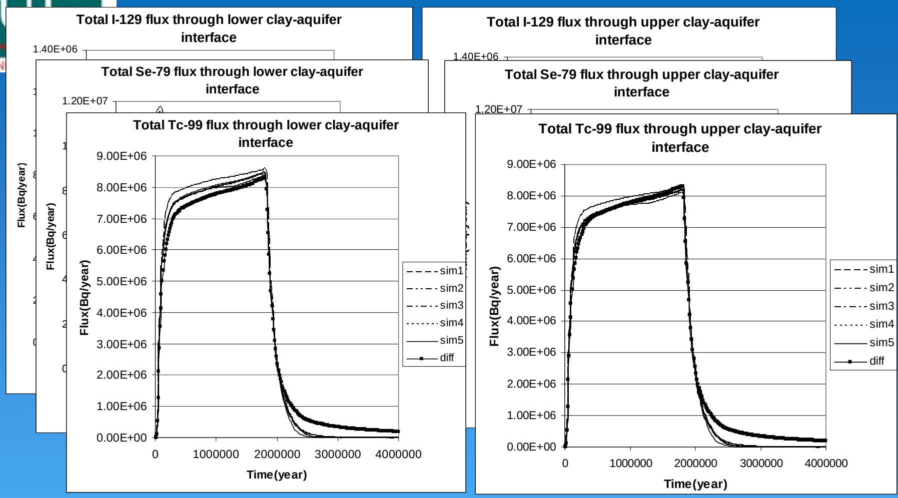

- an average difference of about 5% between the fluxes of the heterogeneous and the homogeneous model
- maximum value of the difference is 10%
- indicates that transport by advection only has a small importance in this model

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… and diffusion ?

$$Pe = \frac{V_D x}{n D_e}$$

- Peclet number for low permeability layers:

  where V_D (m/s) = Darcy's velocity,
  x (m) distance,
  n (-) = diffusion accessible porosity,
  D_e (m²/s) = effective diffusion coefficient. :

- diffusion expected to be dominant:

$$F = -nD_e gradC$$

➡ heterogeneity of the diffusion accessible porosity ?

➡ heterogeneity of the effective diffusion coefficient ?

➡ about 25 % smaller computed fluxes:

the heterogeneity of the diffusion parameters proved to have a much larger effect than the heterogeneity of K_v

… for more details: cfr the paper given by Marijke Huysmans !

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Conclusions: … from a practical point of view

- advantages of including available geological / geophysical / hydrogeological data
- optimizing soft data measurements is required …
- through conditioning, field measurements are taken as criteria of physical plausibility … in addition to the pure spatial correlation as captured by variograms
- assumption that geology generates ‘sediment facies’
- genetic/genesis models modelling rock formation processes should help more and more !
- when zones corresponding to ‘facies’ are defined, … how to deal with a calibration ?
    * keeping the geometry of the facies: changes in parameters values and find criteria for selection
    * adjustment of the geometry: ‘gradual deformation’ (Hu et al., 2001)

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Thanks !

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- René Therrien (U. Laval) and Rob McLaren (U. Waterloo)

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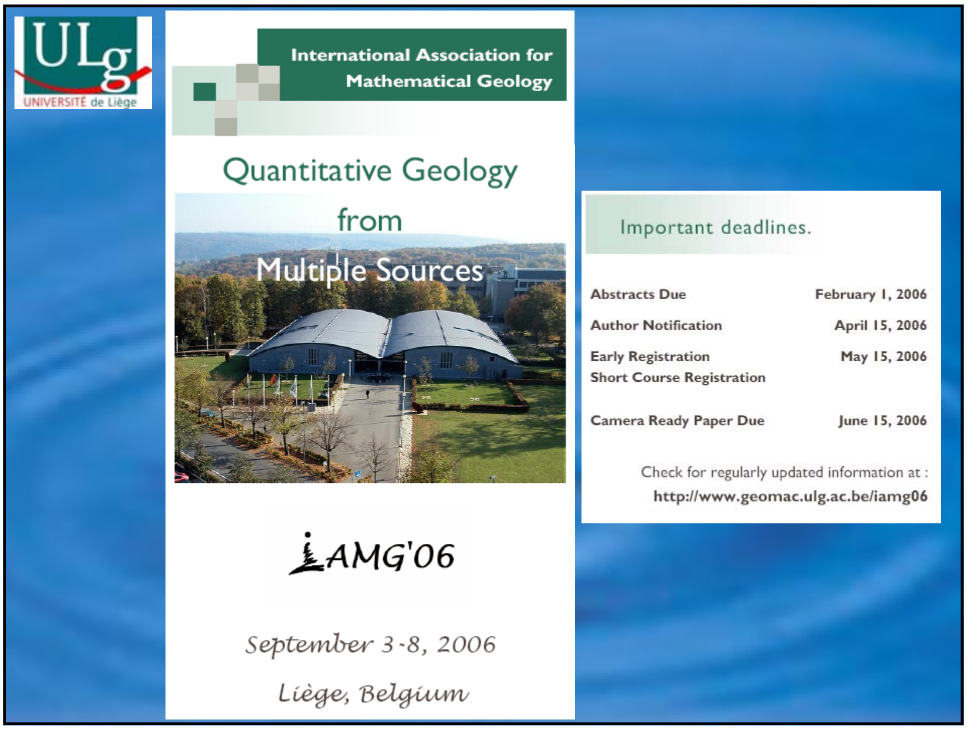
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