Deterministic and stochastic modelling for protection zone delineation

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Definitions / General scope

Deterministic approach
- pure advection
- advection-macrodispersion
- advection-dispersion + multi tracer tests
- challenges

Stochastic approach
- Background
- Synthetic case
- Stochastic generation of K-fields combined to inverse modelling
- Additional conditioning by geoelectrical resistivity data
- Discussion of results

Conclusions / Perspectives
**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 \((K = 10^{-5} \text{ m/s})\)
  - 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 m³/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 \((\rho)\) 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 the standard deviation of the regression residual, 300 resistivity values, distributed on 12 tomographic profiles 

\[
\ln \rho = 6.836 + 0.345 \ln K + \tilde{\sigma} \quad N(0,1)
\]
Stochastic conditional simulations

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

\[
\text{Conditional simulation} = \text{Non-cond. simulation} - \text{Kriging of each realisation} + \text{Kriging}
\]

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 \( \text{CaPD} \) 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 $\rho$ 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 ($K_i$, $i = 1,...,5$)

... as previously, for each obtained K-field:

- inverse modelling using PEST (conditioning 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 ($\rho$)
- 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?