Characterising the vadose zone hydraulic properties by inverse modeling

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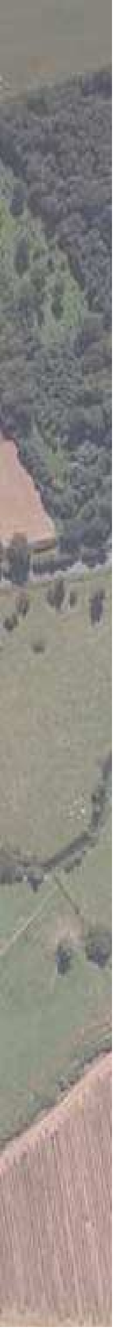

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Introduction

Rationale of the study

Modelling the fate and transport of pesticides in the vadose zone, supporting higher tier assessments, necessitates the characterisation of the sub-soil hydraulic properties.

Inverse modelling may be a way of obtaining the required hydraulic properties, thereby exploiting observed time series of sub-soil moisture transport.

Classical problems of inverse modelling

- Ill-posed
- Uniqueness
- Robustness

Strategies to remediate inversion problems

- Adapt the transport experiments to improve the parameter informativiness
  - Develop alternative system perturbations
  - Increase the spatio-temporal resolution of the measurements
- Adapt the inversion procedures
  - Consider alternative inversion routines (combined local serach and global search method)
  - Consider alternative object functions

Experimental set-up

Undisturbed soil monolith

Equipment per monolith

In

10	TDR probes	Humidity, EC
4	tensimeters	Moisture tension
4	CTN	Temperature
4	Suction lysimeters	Water quality

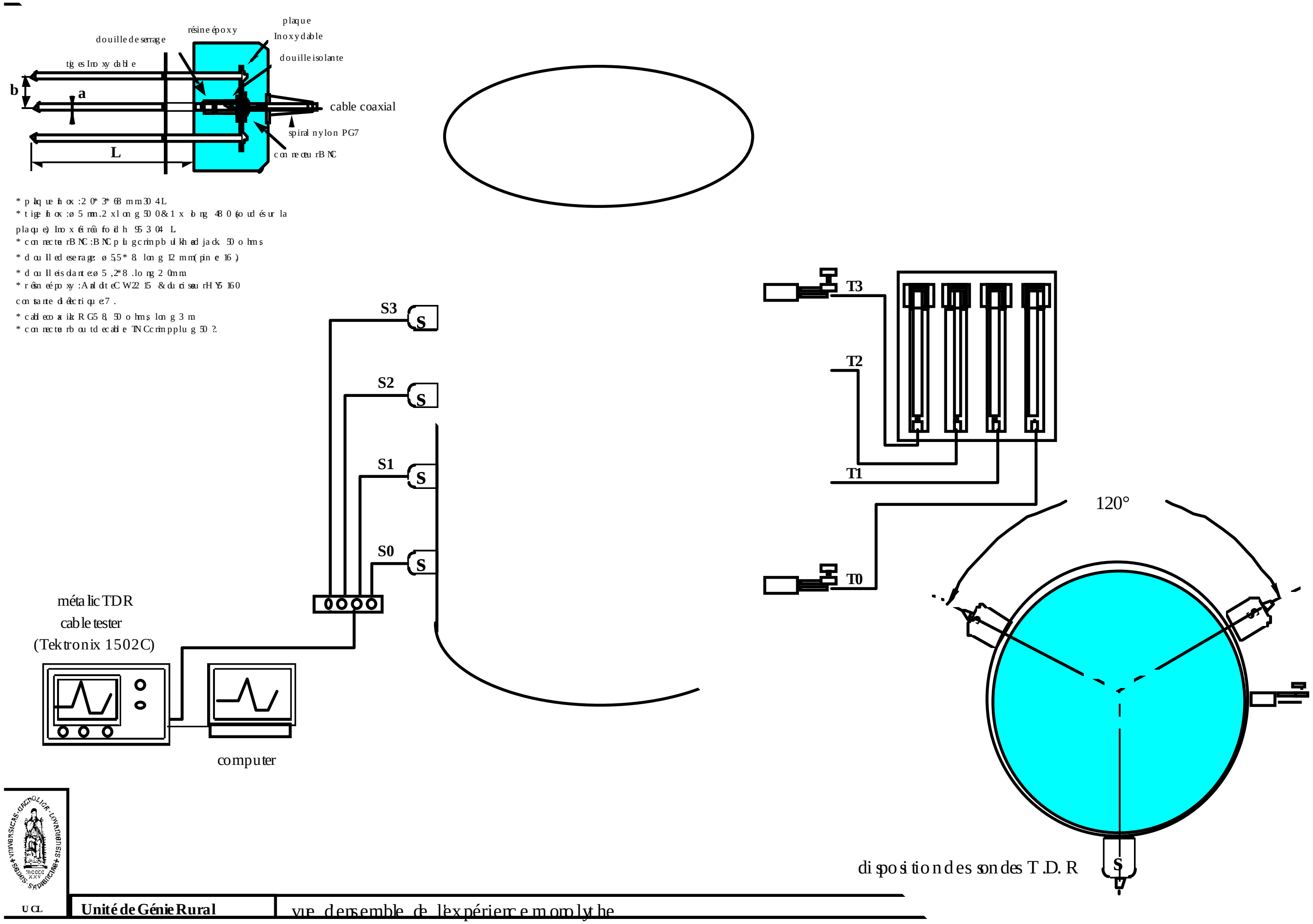
Top

Controlled water/solute flux or pressure head

Bottom

Controlled water/solute flux or pressure head

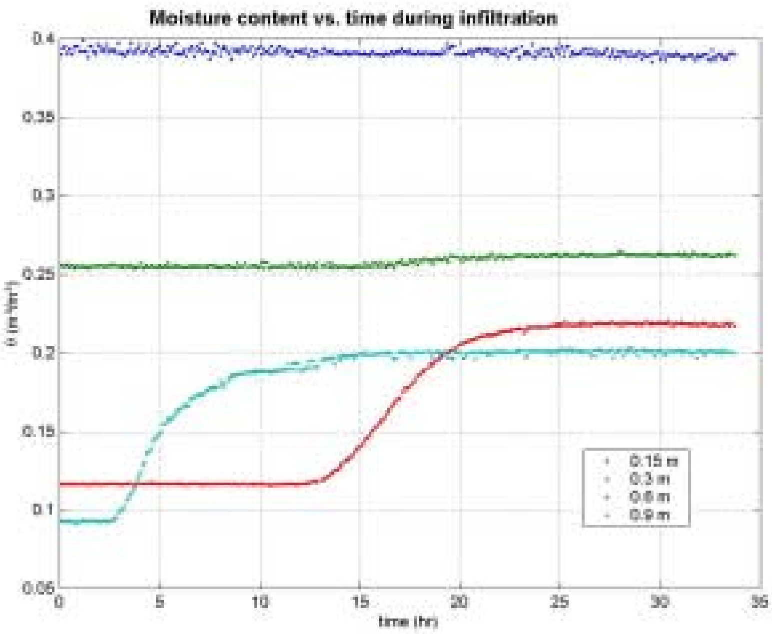
Experimental scheme

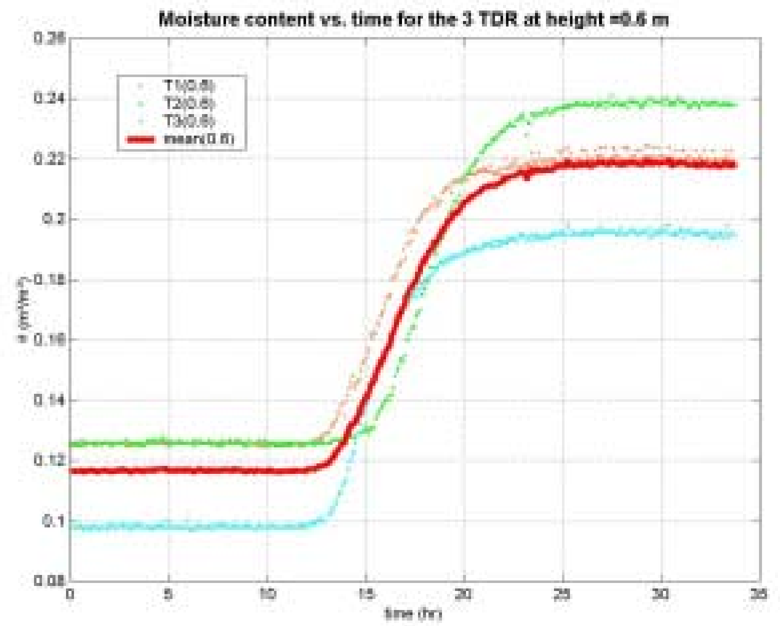


Experimental conditions

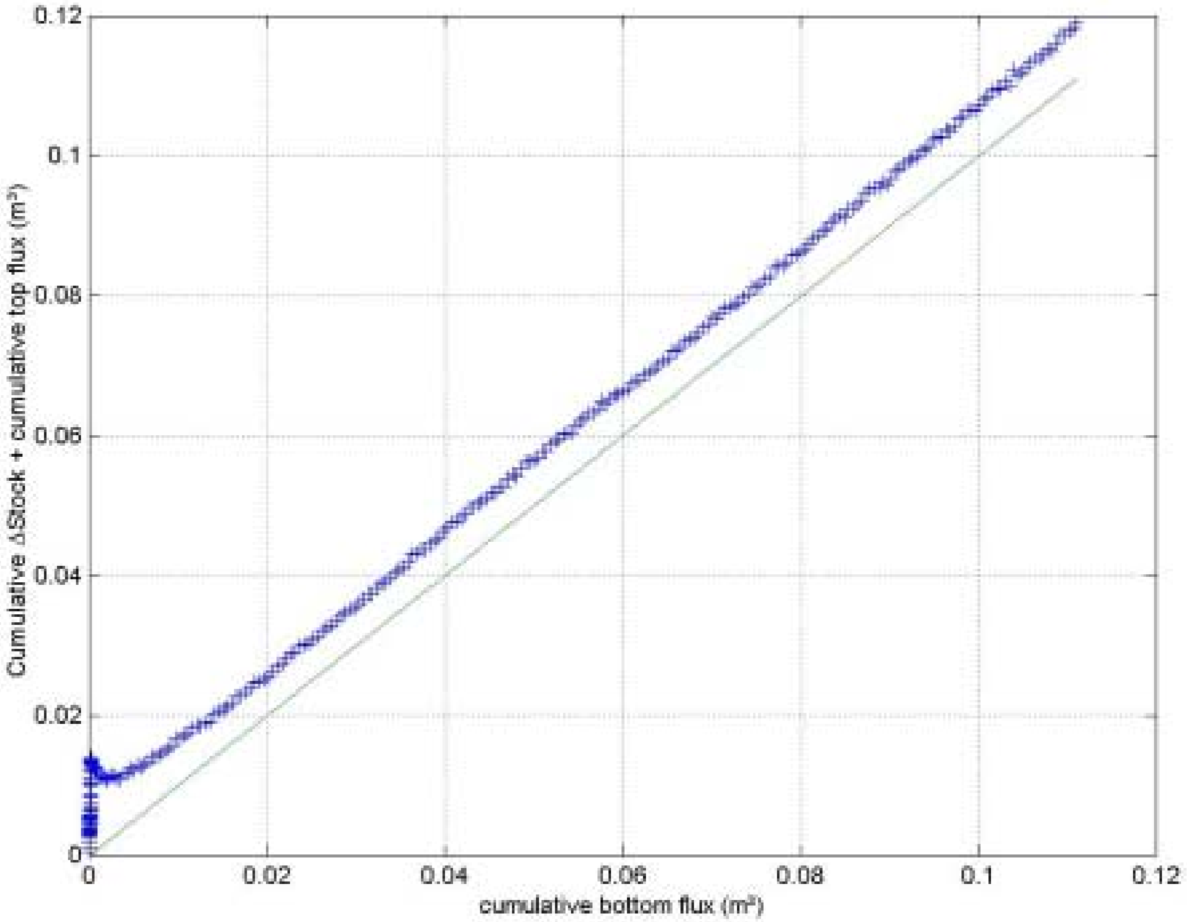
• Type of experiment:	Infiltration
• Time of the experiment:	2000 minutes
• Imposed infiltration flux:	0.0039168 m/hr
• Measurement parameters	
• Volumetric moisture	10 positions 1 per 10 min.
• Water tension	4 positions 1 per day
• Top flux	Cumulative
• Bottom flux	

Available data





Water balance



Inverse modelling

Direct model

$$\frac{\partial\theta}{\partial t} = C(h)\frac{\partial h}{\partial t} = \frac{\partial}{\partial z}\left[K(h)\left(\frac{\partial h}{\partial z} + 1\right)\right]$$

$$Se(h) = \frac{\theta - \theta_r}{\theta_s - \theta_r} = \frac{1}{\left(1 + (\alpha|h|)^{1-1/m}\right)^m}$$

$$k(Se) = ks.Se^{\lambda}.\left(1 - \left(1 - Se^{1/m}\right)^m\right)^2$$

Inverse modelling procedure

- Local optimisation: *Levenberg-Marquardt, Simplex*
- Combined global and local optimisation: *Multilevel co-ordinate search (Huyer and Neumaier, 1998)*
  - For level < level_max
    - Split box procedure along one single co-ordinate search
    - Assign (asymmetric) base points at each box: BP
    - Calculate object function at each base point: O(BP)
  - For level = level_max
    - Calculate local minimized object function: tri-point quadratic model O(BP ’)
- Advantage
  - Combined global and local search
  - Converges if function is continue in the neighbourhood of global minimizer
  - Outperforms with other global optimizer if n < 4

Object functions

$$O(P) = \frac{1}{n.\sigma_\theta^2} \sum_{i=1}^{n} \left(\theta_m(ti) - \theta_0(ti, P) \right)$$

$$O(P) = \frac{1}{n.\sigma_\theta^2} \sum_{i=1}^{n} \left(\overline{K}(ti) - Se(ti, P) \right)$$

$$O(P) = \frac{1}{n.\sigma_\theta^2} \sum_{i=1}^{n} \left(\frac{\partial}{\partial t} \left(\overline{K}(ti) \right) - \frac{\partial}{\partial t} Se(ti, P) \right)$$

Inverse modeling : van Genuchten parameters

. Fixed parameters :

$\theta r = 0.075$

$\theta r = 0.390$

$\lambda = 0.5$

. Estimeted parameters :

α in the range :	[0.015	0.020]	(1/cm)
n in the range :	[6.0	12.0]	
Ksat in the range :	[0.01	0.15]	(cm/min)

Inverse modeling : inversion methods

. Plotting of the objective function

$$OF(\mathbf{P}) = \frac{1}{n\sigma_\theta^2} \sum_{i=1}^{n} \left(\theta m(ti) - \theta o(ti,\mathbf{P})\right)^2$$

. Global minimization

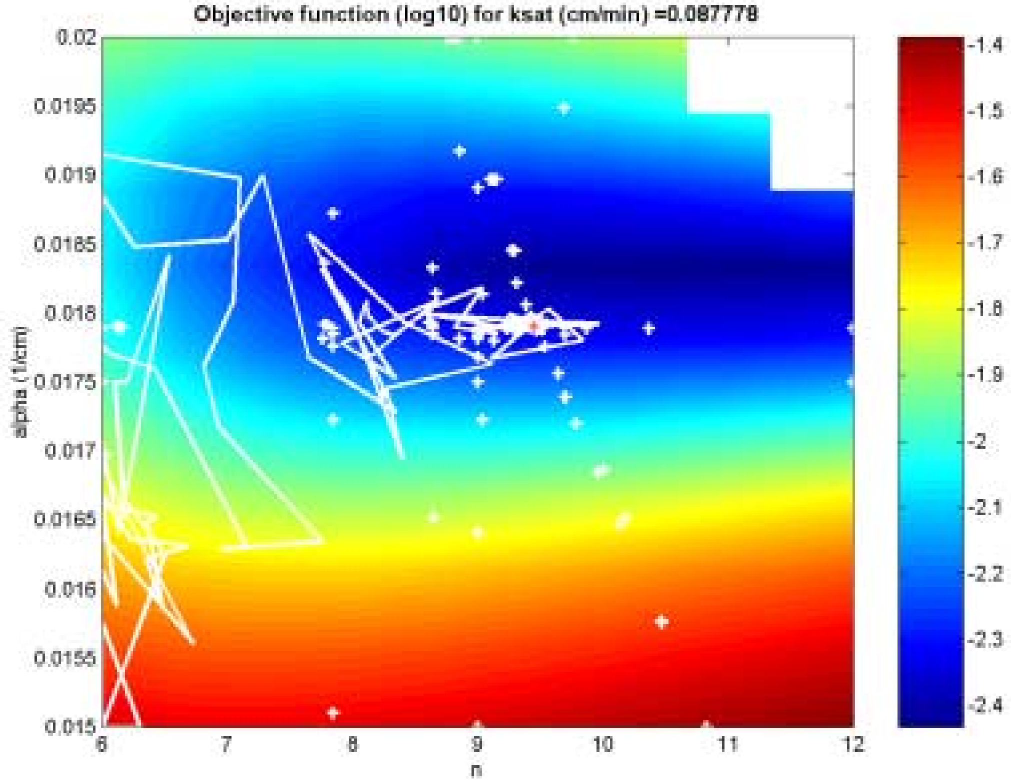
Global optimization by multilevel coordinate search

(Waltraud Huyer and Arnold Neumaier)

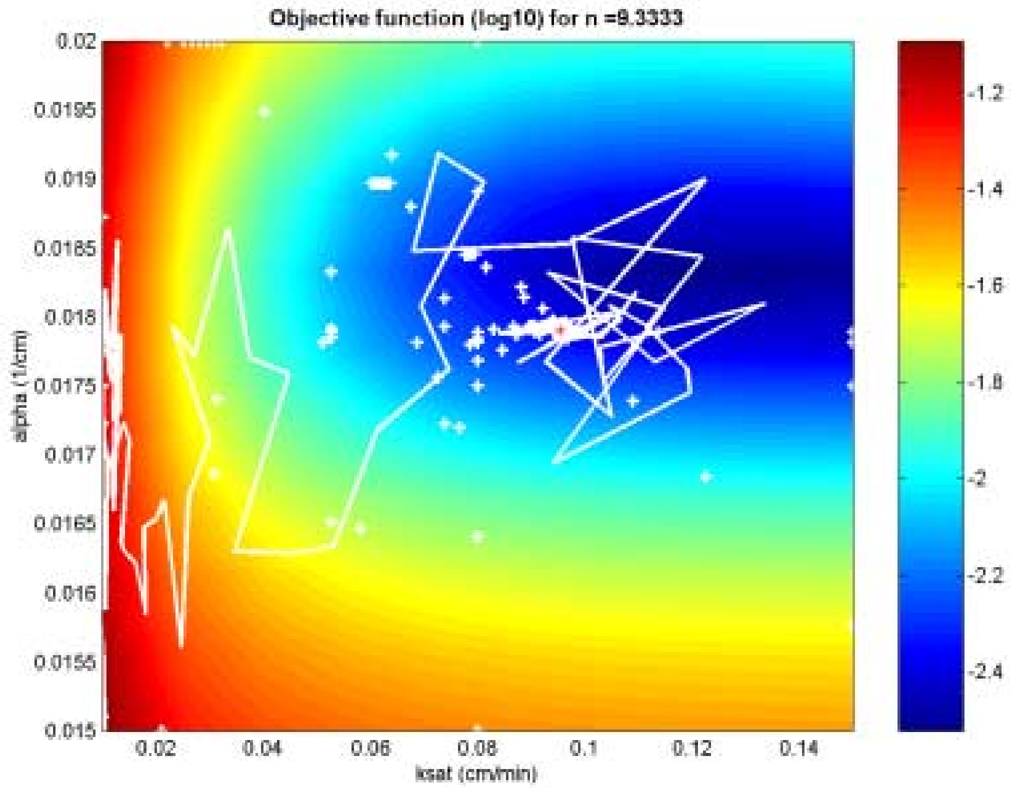
. Local minimization

Multidimensional unconstrained nonlinear minimization (Nelder-Mead)

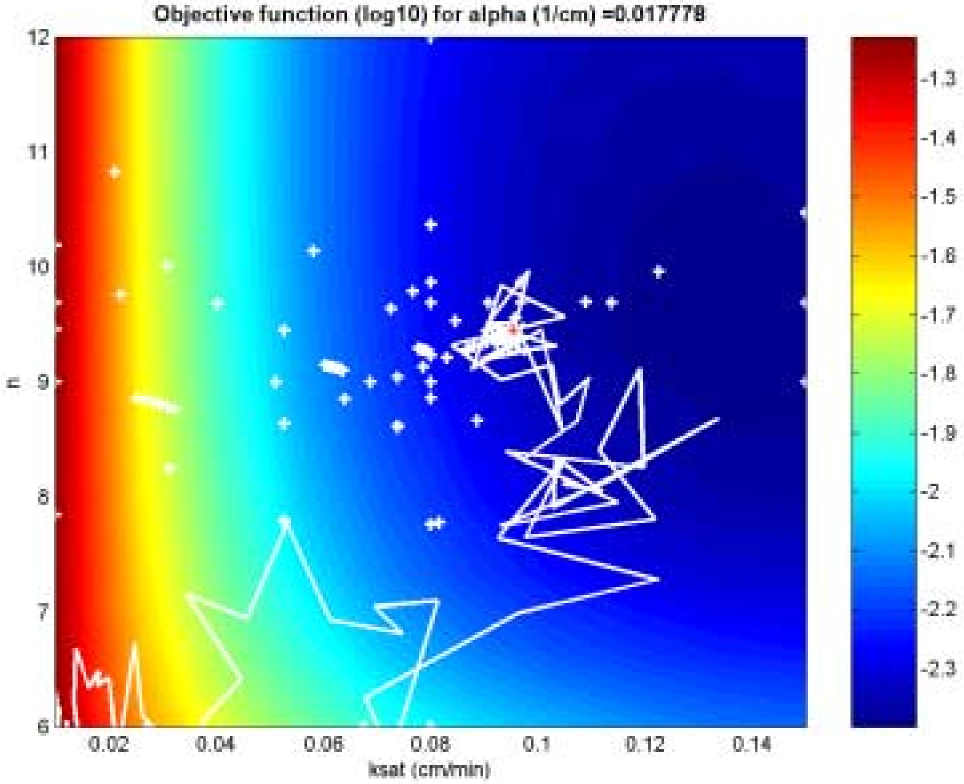
Inverse modeling : response surfaces



Inverse modeling : response surfaces



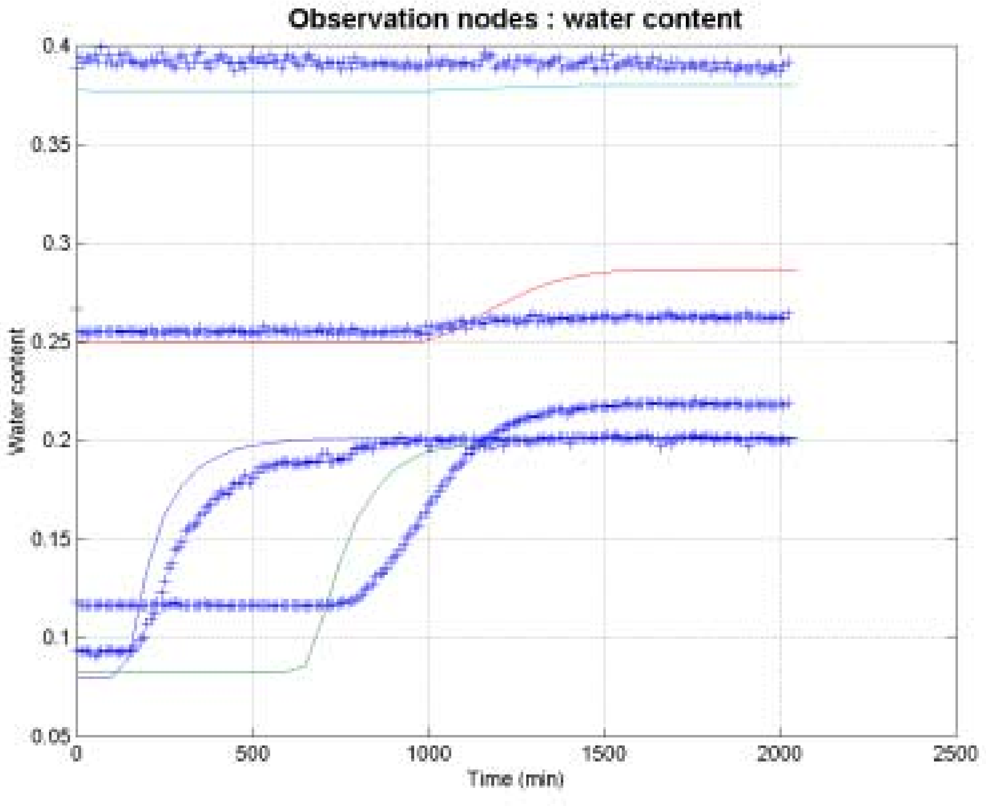
Inverse modeling : response surfaces



Inverse modeling : estimated parameters

Estimation method	*α (1/cm)*	*n*	*Ksat (cm/min)*
Direct measurement	0.0181	4.44	0.11
Plotting OF	0.0183	10.0	0.134
mcs	0.0179	9.4418	0.0956
Nelder-Mead	0.0179	9.4488	0.0951

Inverse modeling :
comparison optimized - observed



Inverse modeling : discussion

. The OF seems to present only one global minimum

. α forms a sink, but n and Ksat form small valleys

. Local method gives the same result as global method

. It appears that the other parameters of van Genuchten could be optimized too

Some conclusions

- Soil monoliths are operational for studying local scale transport phenomena within the vadose zone of the Brusselean aquifer
- Transport experiments on undisturbed soil monoliths deliver experimental data with the appropriate temporal resolution for identifying local scale transport parameters by inverse modelling procedures. However, improvements of the spatial resolution is still needed
- The numerical solution of the Richards equation in an *MATLAB* environment is a flexible tool for analysing soil flow and transport experiments
- A local search (*Levenberg-Marquardt*, *Simplex*) and global search (*Multilevel Coordinate Search*) model has successfully been coupled to the numerical solution of the Richards equation, which allows to identify the local scale unsaturated hydraulic properties of the Brusselean vadose zone.

Some perspectives

- Increase the number of parameters to be identified by the global search methods (tortuosity parameters!)
- Analyse the stability of the parameter sets (uncertainty propagation analysis!)
- Improve the stability of the parameter sets by adopting alternative formulations of the object functions, thereby reducing errors induced by problematic calibration formula 's (e.g. the site specific TDR calibration for moisture content profiling)
- Apply the method to other transport experiments (solute transport experiments, nitrate transport experiments, pesticide transport experiments)