Modeling a heat tracer test in alluvial sediments using Monte Carlo: On the importance of the prior

Richard Hoffmann[1,2], Alain Dassargues[1], Pascal Goderniaux[2] & Thomas Hermans[3]

[1]Hydrogeology & Environmental Geology, Urban and Environmental Engineering, University of Liege
[2]Geology and Applied Geology, Polytech Mons, University of Mons
[3]Department of Geology, Ghent University, Gent, Belgium

Corresponding Author: Richard.Hoffmann@uliege.be

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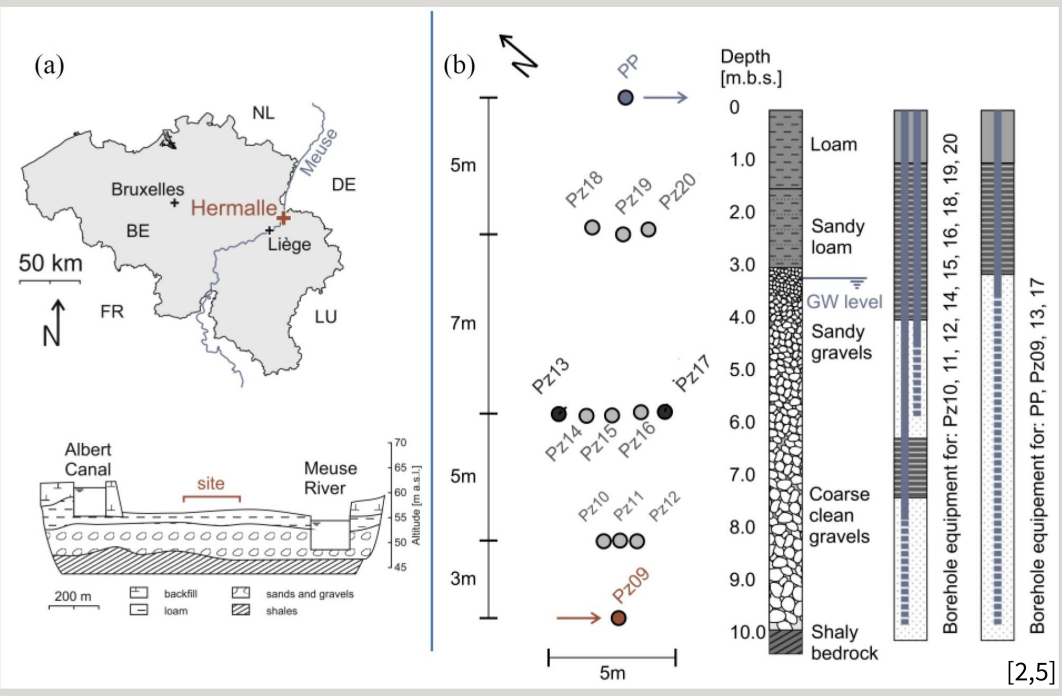
Motivation

Deterministic model calibrations in hydrogeology are useful for understanding the influence of parameters on the considered variables, e.g. how an optimized hydraulic conductivity field influences the groundwater velocity. One main issue of a deterministic solution is generally a too smoothed derived parameter distribution leading to unrealistic predictions with underestimated uncertainty. Thus, transport predictions with reference data confirming an optimized parameter distribution (i.e. "calibrated model") must be questioned and replaced by considering a realistic heterogeneity. Random generated models (i.e. prior) using e.g. Monte Carlo simulations can be considered as multiple hypotheses. A hypothesis may be rejected, when the generated models (prior) do not confirm the reference data, i.e. the simulations are not informative enough (falsification step [1]).

Material and Methods

1. The reference data set is a heat tracer experiment in alluvial sediments (Belgium). Hot water (39 °C) was jointly injected with napthionate (24 h), recovered in a pumping well at a 20 m distance and observed in 3 panels (3, 8, 15 m downgradient) [2].
2. A deterministic calibration of the experiment on temperature data, using jointly HydroGeoSphere and PEST [3], hardly describes the experimental observations.
3. Instead, 250 realizations using Monte Carlo in combination with sequential Gaussian simulation for the K-distributions define the prior (hypotheses). For the K-distribution two scenarios are used:
   (1) a random K-distribution with unknown mean, variance and spatial correlation and
   (2) the same approach but with a downwards increasing vertical trend for the K-distribution, to mimic the observed increasing grain of the sediment with depth.
4. Then, a distance-based sensitivity analysis (DGSA [4]) using accepted hypotheses (prior / simulations) gives key information about parameters most influencing the model outcomes and quantifies the relationship between input and model response uncertainty. DGSA analyzes both, global parameters (porosity, etc.) and local high dimensional parameters characterizing the spatial heterogeneity (e.g. K-field generated with sequential Gaussian simulation):
   (1) The distance between model outcomes is calculated and projected in a low dimensional space.
   (2) A cluster groups simulations with a comparable distance to the reference data.
   (3) The parameter cumulative distribution function within k clusters is compared to the reference distribution to deduce the sensitivity. Local parameters are considered through their principal components replacing multiple statistical variables with a limited, smaller and approximated amount of linear combinations.



[2,5]

Parameter	Simulation range U	Unit	Fixed parameter+	Value	Unit
$Log(K_{mean})$	A: [−3.5 −2]	$m\ s^{-1}$	Longitudinal dispersivity (upper / lower part)	1.5/3	m
	B: Trend [−4 −2] + [−3.5 −2.5]	$m\ s^{-1}$	Transversal dispersivity (upper / lower part)	0.15/0.3	m
Variance K	[1 100]	$m\ s^{-1}$	Solid thermal conductivity (apparent)	1.37*	$W\ m^{-1}\ K^{-1}$
Porosity	[0.05 0.12]	1	Fluid thermal conductivity	0.59	$W\ m^{-1}\ K^{-1}$
X	[1 to 8]	m	Solid specific heat capacity	1,000	$J\ kg^{-1}\ K^{-1}$
Y=Z	[0.1 0.5]	m	Water specific heat capacity	4,189	$J\ kg^{-1}\ K^{-1}$
Azimuth	[0 pi]	1	Specific Storage	10^{-4}	m^{-1}
Gradient at prescribed head BC	[0.01 0.1]	%	Bulk density	1,950	$kg\ m^3$

+The fixed values are taken from Klepikova et al. (2016).
*The solid thermal conductivity estimated at 1.43 $W\ m^{-1}\ K^{-1}$ is replaced by an apparent value for simulation (see section: Deterministic porous media model).
[ ] Sampled from a random uniform distribution.

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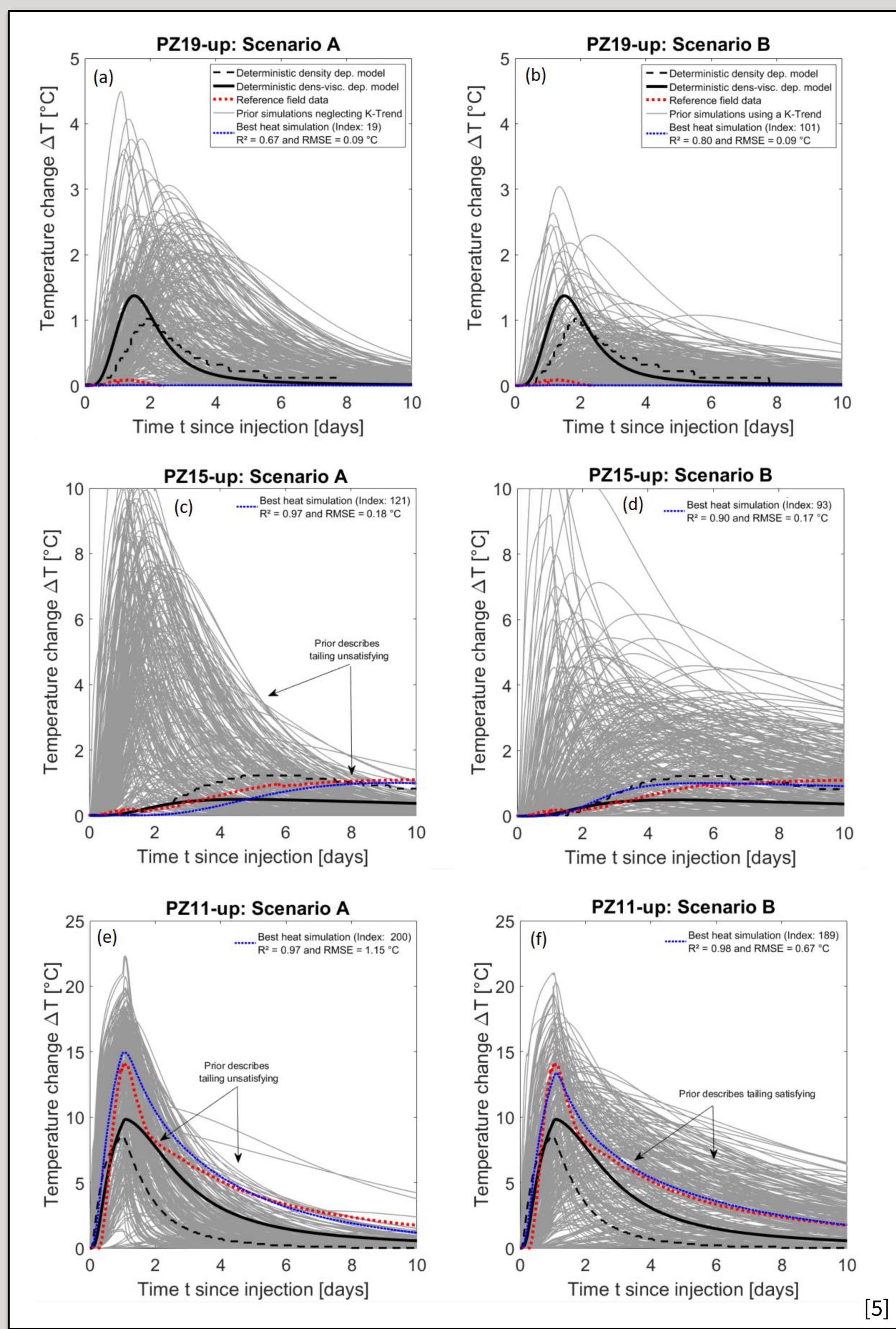
Results



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Prior Uncertainty investigation:

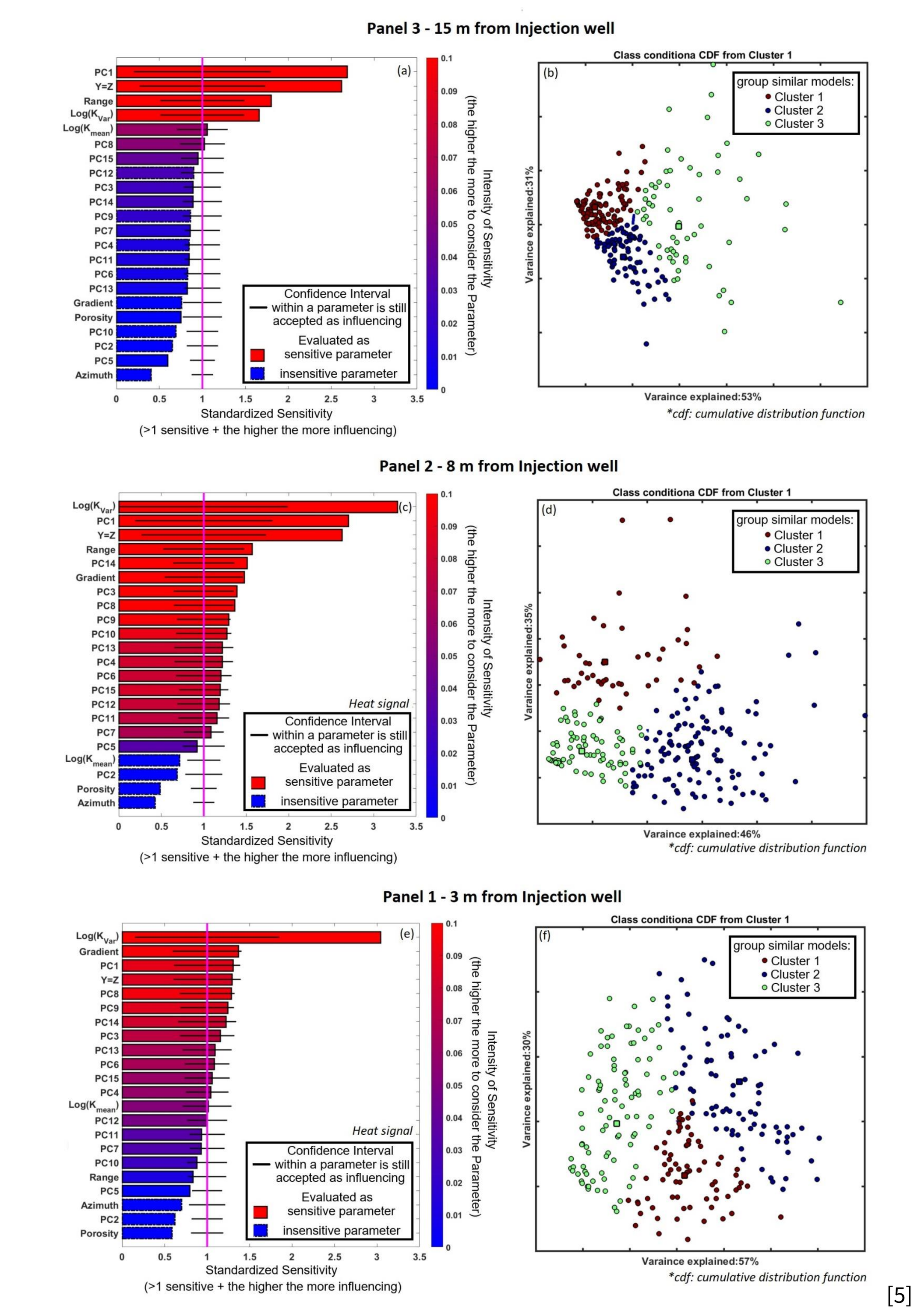
- *Scenario 1 (without vertical K-trend):* the prior range (250 simulations) surrounds the reference data (i.e. heat breakthrough curves) for most of the experiment, but not for the tailing.
- *Scenario 2* (with the vertical K-trend): improves the simulation of the breakthrough tailings for panel 1 and 2. In panel 3 (15 m downgradient), simulations for the lower aquifer part show significant lower peaks than measured.

=> *Scenario 1* is falsified (rejected), because the prior (250 models) do not confirm the reference data.

=> *Scenario 2* is not-falsified till panel 2 (8 m downgradient).

Distance based sensitivity Analysis:

- Scenario 2 is used for global sensitivity analysis
- At panel 1 and 2 the spatial K-distribution and its variance are the most sensitive parameters.
- When heterogeneity is considered, heat seems to be less sensitive to global advective parameters like porosity. This may be indicating the complementary tracer behavior.
- The principal components describing local spatial heterogeneity are sensitive using the heat signal, but still heat tends to remain more dominated by conduction.



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Discussion

A Considering all the efforts done to calibrate a deterministic model on the complex heat tracer data, always a too smooth K distribution biases the interpretation. Avoiding the deterministic approximations (e.g. K-zones) by using stochastic models, allows the relaxation of those approximations and heterogeneity can be considered realistically.

B Scenario 2, considering a downwards increasing K-Trend in the random generated K-distribution, addresses the heterogeneity of the test site more realistically than all previous unsatisfying deterministic attempts. In this study stochastic models can reproduce specific behaviors of breakthrough curves significantly better.

C The global sensitivity analysis confirms, that future efforts needed for panel 3, should focus on identification of heterogeneous patterns in the aquifer and their subsequent introduction in the model. A prior uncertainty investigation using Monte-Carlo in conjunction with a global distance-based sensitive analysis is very promising for hydrogeology.

Conclusion + Outlook

As a perspective, the use of a direct predictive framework (e.g. Bayesian Evidential Learning), avoiding the commonly used calibration procedure, promises robust decisions made by more realistic quantifications of the uncertainty caused by heterogeneity. Thus, for robust transport decisions using any stochastic Bayesian inversion, an adequate prior description in conjunction with a global sensitivity analysis considering uncertainty is a prerequisite.

Acknowledgements

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