The usefulness of CPTs for deterministic, spatially heterogeneous, large-scale aquitard parameterisation

B. ROGIERS[1,2], D. MALLANTS[3], O. BATELAAN[2,4], M. GEDEON[1], M. HUYSMANS[2] & A. DASSARGUES[2,5]

1 Institute for Environment, Health and Safety, Belgian Nuclear Research Centre (SCK•CEN), Boeretang 200, BE-2400 Mol, Belgium
brogiers@sckcen.be

2 Dept. of Earth and Environmental Sciences, KU Leuven, Celestijnenlaan 200e – bus 2410, BE-3001 Heverlee, Belgium

3 Groundwater Hydrology Program, CSIRO Land and Water, Waite Road – Gate 4, Glen Osmond SA 5064, Australia

4 Dept. of Hydrology and Hydraulic Engineering, Vrije Universiteit Brussel, Pleinlaan 2, BE-1050 Brussels, Belgium

5 Dept. of Architecture, Geology, Environment and Civil Engineering (ArGEnCo), Université de Liège, B.52/3 Sart-Tilman, BE-4000 Liège, Belgium

Abstract Aquitards can be effectively parameterised and incorporated in a groundwater flow model by using standard cone penetration tests (CPTs). Several conceptually different realizations of an aquitard's hydraulic conductivity field were evaluated based on: (i) conventional methods of soil behaviour type classification, (ii) recent relationships from the literature, and (iii) novel site-specific relations with hydraulic conductivity. We show that use of most of these CPT-based hydraulic conductivity estimations in groundwater flow modelling effectively enhance model performance based on absolute head values and gradients across the aquitard. Conceptual models that considered a spatially heterogeneous hydraulic conductivity for the aquitard performed better than the reference case with a uniform aquitard hydraulic conductivity. However, the hydraulic conductivity of thin heavy clay lenses, characteristic of the aquitard present in our study area, cannot be captured using these continuum approaches. The latter leads to a bias in the direct hydraulic conductivity predictions; an alternative is to invoke inverse modelling with the heterogeneous parameter fields. To address this issue, the concept of the boundary energy associated with the CPT signal is also introduced for characterising the presence of heavy clay lenses. Overall, the CPT-based concepts provide more accurate, robust, and high-resolution data-based parameterisation of the studied aquitard.

Key words groundwater modelling; hydraulic conductivity; soil behaviour types; cone resistance; friction ratio; geostatistics; inverse optimisation; upscaling; cone penetration tests; model performance

INTRODUCTION

Several studies have investigated the correlations between geotechnical data (e.g. cone penetration tests or CPTs, see Fig. 1) and hydrogeological parameters such as hydraulic conductivity K (e.g. Anagnostopoulos *et al*., 2003; Tillmann *et al*., 2008; Robertson 2010; Van Der Wal *et al*., 2010). Typically, such geotechnical data has a high vertical resolution and is therefore suited for studying small-scale variability in the subsurface. This is important, since it has been shown that even sub-metre scale heterogeneity can have an important influence on transport of matter in aquifers (e.g. Mallants *et al*., 2000; Huysmans & Dassargues 2009; Ronayne *et al*., 2010).

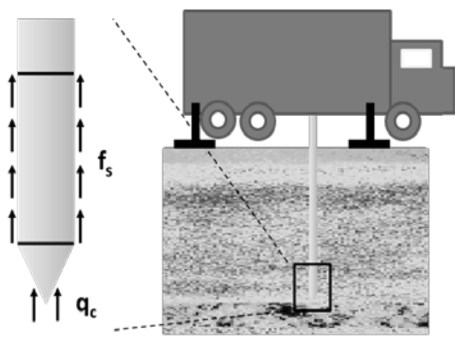

Fig. 1 Standard cone penetration testing parameters: cone resistance q_c, and sleeve friction f_s.

Efforts in using geotechnical data for conditioning hydrogeological models are very limited (besides stratigraphical mapping), though gathering of such information is usually much easier and cheaper than doing expensive drilling campaigns. A case was published by Flach *et al*. (2005) who studied an environmental waste site of 8 km^2 where 139 CPTUs (CPTs with piezometer data) were performed, instead of conventional borehole techniques. They categorized the CPTU parameters into high, medium and low conductivity classes, and upscaled it to the flow model resolution using a geostatistical approach; this resulted in increased groundwater model performance.

This paper investigates the use of several different interpretative approaches to generate hydrogeological parameterisations of an aquitard, thereby honouring small-scale heterogeneity. For this purpose we use only standard CPT data (cone resistance q_c and sleeve friction f_s, see Fig. 1) and the relationship with borehole core analyses. The resulting changes in the performance of an optimised groundwater flow model are discussed for the different heterogeneous parameterisations. Recommendations are made for including small-scale heterogeneity in hydrogeologic properties in a stochastic modelling approach.

METHODS

Site characterisation

A detailed hydrogeological characterisation to depths of 40–50 m has been carried out in 2008–2009 for a sub-basin of the Kleine Nete catchment in the region of Mol/Dessel, Belgium (Beerten *et al*., 2010). This site characterisation complements earlier campaigns that did not address spatial variability in hydraulic properties. A large amount of quantitative and semi-quantitative information has now been collected, including borehole logs, CPTs (more than 200 down to depths of 40 m), approximately 340 *K* measurements on undisturbed cores, etc. (see Fig. 2). The hydrostratigraphy of the site is simplified in the following way: an upper aquifer with an average thickness ranging from 25 to 35 m, which consists of Quaternary, Mol and Kasterlee Sands, a very heterogeneous 5–10 m thick aquitard that is known as the Kasterlee Clay, and a lower aquifer with a thickness of about 150 m, consisting of the Diest, Dessel, Berchem and Voort Sands, with a less permeable top of a few metres at the interface with the aquitard (see Fig. 3). For a more detailed description, the reader is referred to Beerten *et al*. (2010). Since the heterogeneous aquitard is an important factor determining the hydrogeological system, its quantification in terms of hydraulic conductivity is the subject of the present study.

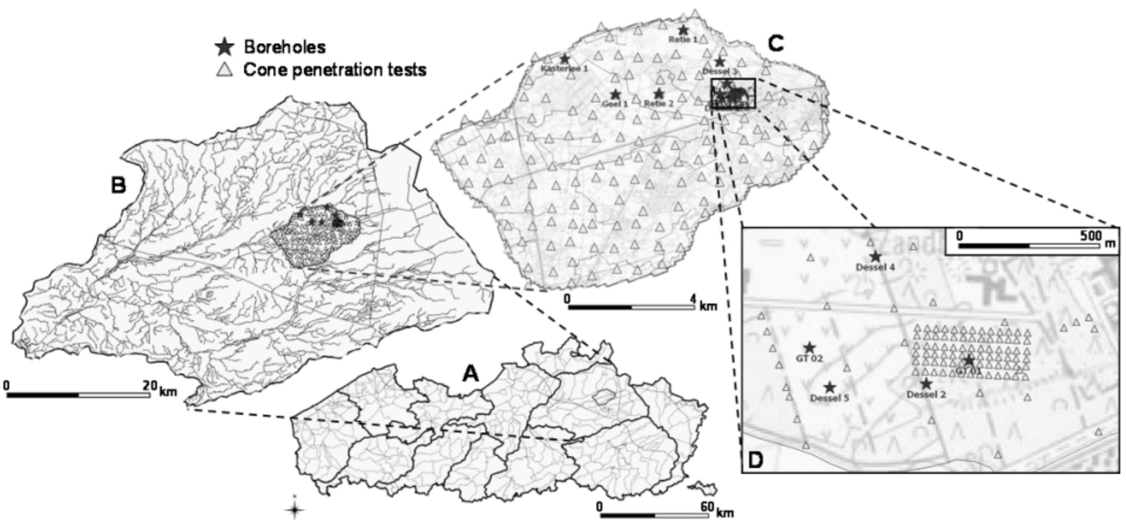

Fig. 2 Geographical situation of the study area and site investigations, including different cored boreholes and several cone penetration test campaigns. A: Flanders, B: Nete basin, C: local groundwater model extent, and D: future waste disposal site.

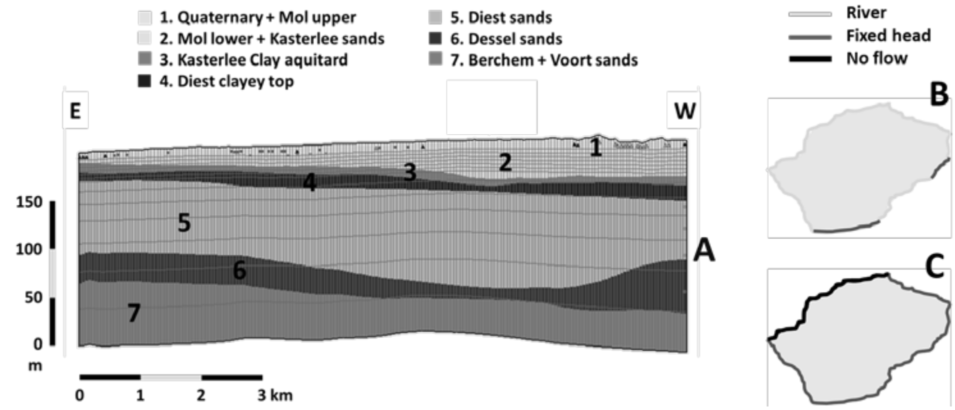

Fig. 3 A: Hydrostratigraphy and numerical model grid of an EW profile through the study area. B: Upper model layer boundary conditions. C: Lower aquifer boundary conditions (Diest clayey top and below).

Model performance reference case

The groundwater model used in this paper was developed by Gedeon *et al.* (2011) in MODFLOW (Harbaugh, 2005). The upper model layer and lower aquifer boundary conditions are illustrated in Fig. 3. Three approaches to the parameterisation of the aquitard were initially proposed. These include a uniform hydraulic conductivity value across the model domain, manually delineated zones based in part on the aquitard thickness, and an initial CPT-based estimate derived from the clayey, silty and sandy soil behaviour type percentages (see e.g. Robertson *et al.*, 1986). The concept of a uniform aquitard hydraulic conductivity is used as the reference case in this study. More details on the groundwater model concept, boundary conditions, and parameter values can be found in Gedeon *et al.* (2011) and Rogiers *et al.* (2010a).

Alternative aquitard parameterisations

Nine different approaches to convert the CPT data into a hydrogeological parameterisation of the aquitard, based on literature methods and several previous studies, were tested. The aquitard thickness is used as relative information in the first parameterisation to derive aquitard scale effective conductivities. Next, the most widely used soil behaviour type (SBT) classification by Robertson *et al.* (1986) and a recent update of it (Robertson, 2010) are further considered, as well as a site-specific SBT classification approach using model-based clustering (Rogiers *et al.*, 2011). To assign K values to each of the discrete SBT classes, geometric mean K values were determined from borehole core analysis, for which CPT data were also available (see Table 1).

In addition to the discrete K estimates from Table 1, continuous K estimates were obtained from the linear model of Robertson (2010). A second linear model was derived from site-specific data on the cone resistance, friction ratio and hydraulic conductivity ($\log_{10}(K) = -7.36 + 1.77 \log_{10}(q_{c,n}) + 1.18 \log_{10}(f_{r,n})$, with $q_{c,n}$ and $f_{r,n}$ the normalised cone resistance and friction ratio). In yet another approach continuous K values were obtained by interpolation in the CPT data space (Rogiers *et al.*, 2010b,c). A final continuous K estimate is obtained by a regression with the lognormal transformed K data, and a back transform to obtain K values.

Table 1 Overview of discrete CPT data classifications and corresponding K values.

Soil behaviour type classification	Class number and mean $\log_{10}(K)$ from borehole core analysis (m/s)
Robertson 2010	2: –6.1; 3: –6.3; 4: –5.1; 5: –4.7
Robertson *et al.*, 1986	3: –7.0; 4: –7.7; 5: –6.9; 6: –6.5; 7: –5.1; 8: –5.2; 9: –5.1; 11: –5.8; 12: –5.0
Rogiers *et al.*, 2011	1: –5.5; 2: –4.8; 3: –5.4; 4: –4.9; 5: –7.0; 6: –5.4; 7: –5.5; 8: –6.0; 9: –4.4

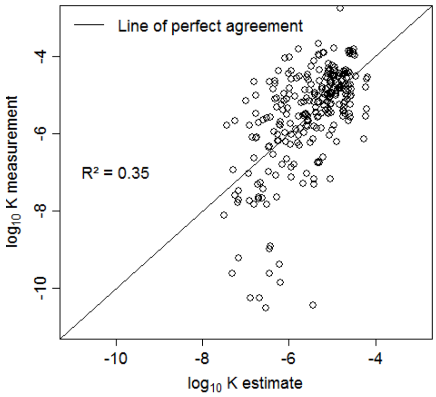

Fig. 24 Linear site-specific *K* estimates *vs* measured values.

The results of the linear site-specific estimate are plotted in Fig. 4 to illustrate the limitations of these models. A relationship is clearly present in the 10^{-8}–10^{-4} m/s range, but the lowest values associated with thin, heavy clay lenses, are all overestimated in this model, as well as in the other approaches.

To overcome the problem of poorly predictable *K* values for heavy clay lenses, the cone resistance boundary energy (also called bending energy; see Costa & Cesar, 2001) was also included as a covariate for deriving soil classes. The approach is that of Bhattacharya & Solomatine (2005) where a CPT log-shape characteristic is incorporated allowing for use of expert knowledge as part of a machine learning CPT classification. Large excursions of this parameter are believed to correspond to distinct thin features, which possibly relate to the presence of heavy clay lenses. These excursions are coupled to the respective mean of the clay lens *K* distribution ($10^{-9.75}$ m/s), while the background signal is attributed a mean value of 10^{-6} m/s. An overview of these different *K* estimates is given in Fig. 5 for a single CPT.

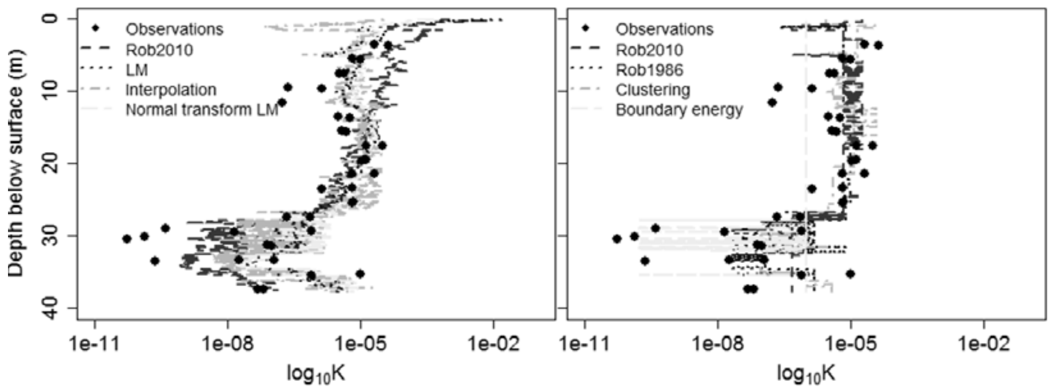

Fig. 5 Overview of considered continuous (left), and discrete (right) *K* estimates for a single CPT-borehole pair. (Rob2010: Robertson 2010; Rob1986: Robertson 1986; LM: linear model; Interpolation: *K* interpolation in CPT space; Clustering: model-based clustering into SBTs.)

Upscaling and interpolation

Simple vertical upscaling and horizontal interpolation transforming discrete CPT investigation points to a full parameter field was performed for incorporation into a groundwater flow model. Harmonic means are calculated from the CPT data (every data point represents a vertical thickness of 2 cm) within the aquitard domain to obtain a single value for every CPT. These values are then interpolated in the horizontal plain with isotropic 2D ordinary kriging.

Inverse optimisation

Inverse optimisation of hydrogeological parameters with UCODE (Poeter *et al*., 2005) was performed. To allow for calibration of the obtained hydraulic conductivity estimates, as well as converting relative information like the aquitard thickness to *K* values, a factor *b* and bias *a* were included after standardisation of the parameter fields resulting from the upscaling and interpolation. The following three parameters were thus optimised in all cases: the standardised spatially heterogeneous logarithmic vertical conductivity field factor *b*, the bias *a*, and the overall upper aquifer *K* (one single *K* value is optimised for the entire upper aquifer), from which the sub-units are derived, and *idem* for the lower aquifer conductivity. The aquitard logarithmic vertical hydraulic conductivity in each model grid is hence calculated as *a* + *b** (the standardised heterogeneous parameter field). For the model performance measure, the sum of squared errors for 86 head observations and 21 derived vertical head differences across the aquitard were used, with 10 times more weight given to each head difference observation, since these are the most sensitive to the aquitard parameterisation.

RESULTS

The different approaches that were used are summarised in Table 2, together with the sum of squared errors (SSE) obtained after the model run, expressed in percentage relative to the reference case SSE. The corresponding aquitard parameter fields are shown in Fig. 6. All concepts performed better than the uniform reference case. The aquitard thickness and cone resistance boundary energy (concept 2 and 5) did not increase the model performance much (92% and 96% of the reference case SSE).

For the SBT classifications, the model-based clustering of CPT data (concept 6) shows the best performance (44% of the reference case SSE). Both classifications of Robertson (concept 3 and 4) perform worse. The one from 2010 seems to be much more robust, with a performance of 65% of the reference case SSE, instead of 99% for the 1986 version.

However, the continuous estimates perform best, with a relative SSE of 35%, 40% and 42% for the normal transformed linear *K* estimate, the untransformed estimate, and the Robertson 2010 estimate, respectively. The interpolation of *K* in the CPT data space did not contribute much to the model performance (92% of the reference case SSE).

All concepts with a SSE of less than 50% of the reference case SSE show a similar spatial pattern in the aquitard vertical *K* field. This indicates the presence of a large-scale channel-like structure within the Kasterlee Clay unit, with preferential deposition of fine material.

Table 2 Definition of the different heterogeneous aquitard parameterisation approaches, and the sum of squared errors (SSE) in percentage relative to the reference case, as a model performance measure.

Nr	Definition	CPT parameters used for *K* parameterisation	Rel. SSE
1	Uniform value; reference case	None	100%
2	Aquitard thickness	Aquitard thickness	92%
3	Robertson 2010 SBTs	SBT classes + corresponding geometric *K* means	65%
4	Robertson 1986 SBTs	SBT classes + corresponding geometric *K* means	99%
5	Cone resistance boundary energy	Cone resistance log shape characteristic	96%
6	Model-based clustering SBTs	SBT classes + corresponding geometric *K* means	44%
7	Robertson 2010 *K* estimate	Soil behaviour type index	42%
8	Site-specific linear *K* estimate	Normalised cone resistance and friction ratio	40%
9	Site-specific interpolated *K* estimate	Normalised cone resistance and friction ratio	92%
10	Site-specific linear normal transform *K* estimate	Normalised cone resistance and friction ratio	35%

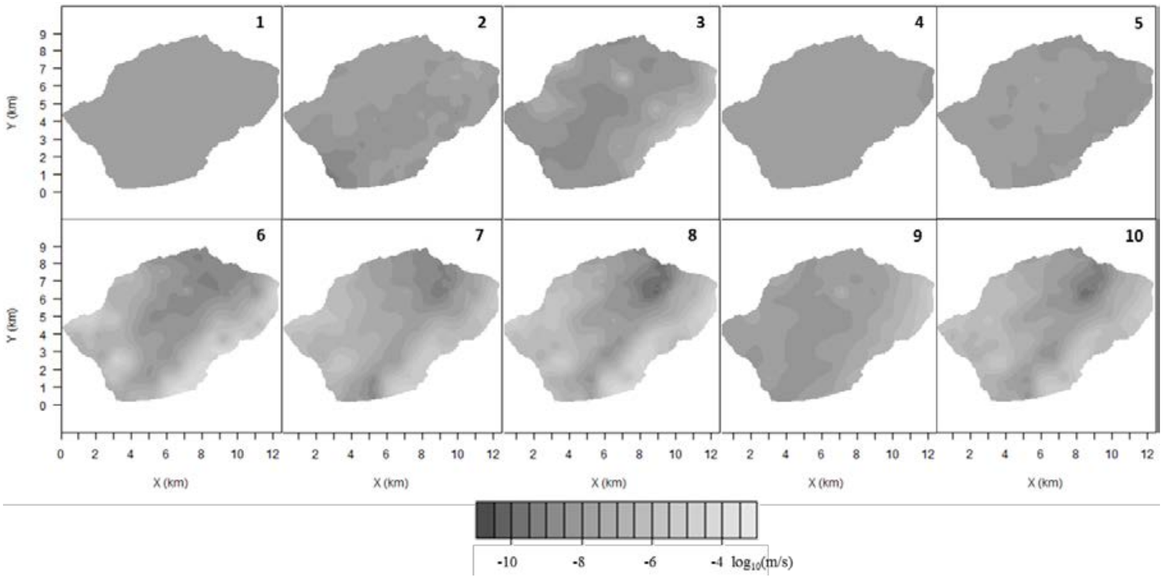

Fig. 6 Different standardised log-transformed vertical K fields for the Kasterlee Clay aquitard, created following the approaches listed in Table 2.

CONCLUSIONS

Large-scale deterministic groundwater flow modelling can benefit considerably from detailed spatial sampling, which allows for incorporating deterministic large-scale heterogeneous parameter fields. This study demonstrates that standard CPT data is useful for the parameterisation of the hydraulic conductivity of an aquitard.

The model-based clustering of the CPT parameters and coupling with the site-specific K data proved to yield more information on the aquitard large-scale K variation than existing SBT classifications from the literature. Continuous estimates of K, based on the CPT data, led to even better model performance. The linear site-specific estimate, with normal-transformed K data, performed especially well. It is therefore recommended to use this type of approach for smaller-scale modelling. These results clearly show the benefit of using a site-specific approach rather than existing classification diagrams or K estimates from literature.

The cone resistance boundary energy concept did not improve the model performance significantly. This indicates that it does not provide much information on a large scale, but does not exclude that it might indicate the presence of thin clay lenses at the small scale.

For a smaller scale approach, geostatistical simulation would be required in 3D. For the discrete classification, indicator simulation could be applied, with two K parameters per SBT class, using the borehole dataset for the prior distributions. For the continuous K estimates, co-simulation would be the best option.

Due to the inability to capture the clay lenses with the CPT data, additional work on the borehole cores is needed to derive a way to include these important features in the small-scale stochastic model. Moreover, the current lithostratigraphical subdivision is too coarse to apply at the small scale. A local variography and moving neighbourhood approach should be applied to exclude possible conceptual model errors concerning layer geometry and non-stationarity.

Acknowledgements The authors are grateful to ONDRAF/NIRAS, the Belgian Agency for Radioactive Waste and Enriched Fissile Materials, for providing the data. Findings and conclusions in this paper are those of the authors and do not necessarily represent the official position of ONDRAF/NIRAS.

REFERENCES

Anagnostopoulos, A., Koukis, G., Sabatakakis, N. & Tsiambaos, G. (2003) Empirical correlations of soil parameters based on Cone Penetration Tests (CPT) for Greek soils. *Geotechnical and Geological Engineering* 21(4), 377–387.

Bhattacharya, B., & Solomatine, D. P. (2005) Machine learning in soil classification. *Proceedings of International Joint Conference on Neural Networks* 19, 2694–2699.

Beerten, K., Wemaere, I., Gedeon, M., Labat, S., Rogiers, B., Mallants, D., Salah, S. & Leterme, B. (2010) Geological, hydrogeological and hydrological data for the Dessel disposal site. Project near surface disposal of category A waste at Dessel. *STB-SIE(HYD) - Version 1, NIROND-TR 2009-05 E,* 261.

Costa, L. & Cesar, R. (2001) *Shape Analysis and Classification: Theory and Practice*. CRC Press, Boca Raton, Florida.

Flach, G. P., Harris, M. K., Smits, A. D. & Syms, F. H. (2005) Modeling aquifer heterogeneity using cone penetration testing data and stochastic upscaling methods. *Environ. Geosci.* 12(1), 1–15.

Gedeon, M., Mallants, D., Vandersteen, K. & Rogiers, B. (2011) Hydrogeological modelling of the Dessel site. Overview report. *NIROND-TR 2008-15 E V2.*

Harbaugh, A. W. (2005) MODFLOW-2005, The US Geological Survey modular ground-water model—the Ground-Water Flow Process: *US Geological Survey Techniques and Methods* 6-A16, USGS, 2005.

Huysmans, M. & Dassargues, A. (2009) Application of multiple-point geostatistics on modelling groundwater flow and transport in a cross-bedded aquifer (Belgium). *Hydrogeol. J.* 17(8), 1901–1911.

Mallants, D., Espino, A., Van Hoorick, M., Feyen, J., Vandenberghe, N. & Loy, W. (2000) Dispersivity estimates from a tracer experiment in a sandy aquifer. *Ground Water* 38(2), 304–310.

Poeter, E. P., Hill, M. C., Banta, E. R., Mehl, S. & Christensen, S. (2005) UCODE_2005 and six other computer codes for universal sensitivity analysis, calibration, and uncertainty evaluation. *US Geological Survey Techniques and Methods* 6-A11, 283p.

Robertson. P. K., Campanella, R. G., Gillespie, D. & Greig, J. (1986) Use of piezometer cone data. In: *In-Situ'86 use of In-Situ Testing in Geotechnical Engineering*, GSP 6 , ASCE, Reston, VA, Specialty Publication, SM 92, pp 1263–1280.

Robertson, P. K. (2010) Estimating in-situ soil permeability from CPT & CPTu. In: *CPT'10, Proceedings of the 2nd International Symposium on Cone Penetration Testing*.

Rogiers, B., Schiltz, M., Beerten, K., Gedeon, M., Mallants, D., Batelaan, O., Dassargues, A. & Huysmans, M. (2010a) Groundwater model parameter identification using a combination of cone-penetration tests and borehole data. In: *IAHR International Groundwater Symposium*. Valencia.

Rogiers, B., Mallants, D., Batelaan, O., Gedeon, M., Huysmans, M. & Dassargues, A. (2010b) Geostatistical analysis of primary and secondary data in a sandy aquifer at Mol/Dessel, Belgium. In: *8th International Conference on Geostatistics for Environmental Applications, geoENV 2010* (Gent, 13–15 September 2010).

Rogiers, B., Mallants, D., Batelaan, O., Gedeon, M., Huysmans, M. & Dassargues, A. (2010c) Caractérisation de l'hétérogénéité de la conductivité hydraulique à saturation au moyen d'essais de pénétration au cône. 35 èmes journées scientifiques du Groupe Francophone d'Humidimétrie et des TraNsferts en Milieux Poreux: Transferts en milieux poreux: Hétérogénéité des processus et des propriétés, GFHN 2010, Louvain-la-Neuve, 23–25 November 2010.

Rogiers, B., Mallants, D., Batelaan, O., Gedeon, M., Huysmans, M. & Dassargues, A. (2011) Site-specific soil classification from cone penetration tests and borehole data: a multivariate statistical analysis. In: *NovCare 2011* (Cape Cod, 9–11 May 2011).

Ronayne, M. J., Gorelick, S. M. & Zheng, C. (2010) Geological modeling of submeter scale heterogeneity and its influence on tracer transport in a fluvial aquifer. *Water Resour. Res.* 46(10), 1–9.

Tillmann, A., Englert, A., Nyari, Z., Fejes, I., Vanderborght, J. & Vereecken, H. (2008) Characterization of subsoil heterogeneity, estimation of grain size distribution and hydraulic conductivity at the Krauthausen test site using Cone Penetration Test. *J. Contaminant Hydrol.* 95(1–2), 57–75.

Van Der Wal, T., Goedemoed, S. & Peuchen, J. (2010) Bias reduction on CPT-based correlations. In: *CPT'10, Proceedings of the 2nd International Symposium on Cone Penetration Testing,* 2–26, 7.