MRS2015 / 6th International Workshop on Magnetic Resonance

On determining uncertainties of MRS estimated transmissivities

Troels Norvin Vilhelmsen
Dep. of Geoscience,
Aarhus University
Høegh-Guldbergs Gade 2
DK8000, Aarhus C
Troels.norvin@geo.au.dk

Steen Christensen
Dep. of Geoscience,
Aarhus University
Høegh-Guldbergs Gade 2
DK8000, Aarhus C
sc@geo.au.dk

Esben Auken
Dep. of Geoscience,
Aarhus University
Høegh-Guldbergs Gade 2
DK8000, Aarhus C
Esben.auken@geo.au.dk

SUMMARY

This paper demonstrates a method to determine uncertainties of MRS derived transmissivity estimates. The method uses linear approximations to compute uncertainties of parameter estimates obtained from joint inversion of TEM and MRS data. To ensure the validity of the linear approximation we compare the uncertainties to those obtained from a full nonlinear analysis of the same datasets.

It is documented that the uncertainties obtained from the nonlinear analysis are slightly higher than those obtained from the linear analysis, but the results are comparable in general.

The outcome of this analysis facilitates the incorporation of MRS estimated transmissivities into groundwater flow models in an objective manner by using the uncertainty estimates to define weights given to the MRS based transmissivity estimates.

Key words: MRS, Transmissivity, Hydrological modelling, Uncertainty analysis

INTRODUCTION

The most important purpose of the magnetic resonance sounding method (MRS) is for the estimation of hydraulic conductivities or transmissivities as a part of a hydrological field campaign. Examples of this are numerous, with two recent papers by Baroncini-Turricchia et al., 2014 and Vouillamoz et al., 2014. In hydrological modelling, transmissivity is a key parameter since it governs the flow of groundwater in the subsurface. It is therefore of high importance to estimate transmissivity and to quantify its spatial variability. Normally transmissivities are estimated as a part of the inversion of the groundwater model by adjusting them to minimize discrepancies between field observations and modelled equivalents. Often these datasets comprise averaged hydraulic heads (steady state heads), stream flows, and/or time series of hydraulic head and stream flow measurements. Furthermore, if reliable transmissivity estimates can be obtained by other means then these can be used in the groundwater model calibration (in geophysical terms this is called inversion) as additional observations or prior knowledge. However, in order to determine the weight given to transmissivity estimates in the hydrological model calibration and subsequent uncertainty analysis the estimation of uncertainties of the prior information is of key importance. Without having estimates of uncertainty, the subsequent analysis may be biased e.g. by giving high confidence to uncertain data.

Several studies have quantified the uncertainty of MRS estimated transmissivities (T_{MRS}) (e.g. Boucher et al., 2009; Chalikakis et al., 2008; Legchenko et al., 2004) but the methodology used to quantify uncertainty is often not well described; it is often just said that the uncertainty of parameters and the data is taken into account (e.g. Legchenko et al., 2004 and Boucher et al., 2009).

In the following we propose an objective linearized methodology to quantify the uncertainty of T_{MRS}. This methodology takes into account the noise level of the MRS sounding, the uncertainties of the derived parameters, the uncertainty of the transmissivities used for correlation (T_{HYD}), and the uncertainty of the estimated correlation-parameter between T_{MRS} and T_{HYD}. Uncertainties determined by the linearized method are evaluated by comparing them to uncertainties determined by a nonlinear method.

METHODS

Under the assumption of fast diffusion the permeability (k) of the subsurface can be determined from a MRS experiment as (Dlubac et al., 2014)

$$k = b * w^m * [T_2]^n$$

where b is a correlation factor, w is the water content or effective porosity, $T_2$is the transversal relaxation time, and m and n are constants often set to 1 and 2, respectively. This equation is commonly referred to as the Schlumberger-Doll research equation. It can often be assumed that the viscosity and density of the groundwater are constant, and the hydraulic conductivity can thereby be calculated from the permeability by a simple linear transformation. Moreover, assuming that the effects of magnetic field inhomogeneities are negligible, the hydraulic conductivity can be estimated as

$$K_{MRS} = C_p * w * (T_2^*)^2$$

where T_2^* is the relaxation rate observed for the free induction decay (FID), and C_p is a constant often determined by correlation to T_{HYD}. T_{HYD} is the aquifer transmissivity determined from either slug-tests or aquifer tests. For a given aquifer with a well-defined thickness T_{MRS} (transmissivity determined from MRS) can be determined by

$$T_{MRS} = C_p * w * (T_2^*)^2 * lt$$

where lt is the thickness of the aquifer.

By taking the log transform of the previous equation the following expression is obtained

$$\log(T_{MRS}) = \log(C_p) + \log(w) + 2 * \log(T_2^*) + \log(lt)$$

Using basic probability theory the combined uncertainty related to the MRS derived parameters (three last terms of the equation) can be determined as

$$\begin{aligned} var[\log(w) + 2 * \log(T_2^*) + \log(lt)] &= var[\log(w)] + 4 * var[\log(T_2^*)] \\ &+ var[\log(lt)] + 4 \\ &* cov[\log(w), \log(T_2^*)] + 4 \\ &* cov[\log(T_2^*), \log(lt)] + 2 \\ &* cov[\log(w), \log(lt)] \end{aligned}$$

where $var[x]$ is the variance of x and $cov[x, y]$ is the covariance between x and y. By assuming that the errors on $[\log(w) + 2 * \log(T_2^*) + \log(lt)]$ and the errors of $[\log(C_p)]$ are independent the variance of $\log(T_{MRS})$ can be determined as

$$\begin{aligned} var[\log(T_{MRS})] = var[\log(C_p)] \\ + var[\log(w) + 2 * \log(T_2^*) + \log(lt)] \end{aligned}$$

$\log(C_p)$ and $var[\log(C_p)]$ can be determined from weighted linear regression between $[\log(w) + 2 * \log(T_2^*) + \log(lt)]$ and $\log(T_{HYD})$, where the weights are determined from $var[\log(w) + 2 * \log(T_2^*) + \log(lt)] + var[\log(T_{AQ})]$ for each MRS sounding. This methodology secures that MRS soundings and Transmissivity estimates with uncertain parameters are down-weighted when determining the C_p and that the uncertainty of C_p is taken into account when determining T_{MRS}.

As shown above, determination of $var[T_{MRS}]$ requires determination of the variance of the parameters pertaining to the MRS model as well as the covariance between these. These can be determined either from the linear analysis obtained from the MRS inversion or through full nonlinear analysis of the parameter-space.

In the present study, we have performed both a linear and a nonlinear analysis to evaluate the performance of the linear approximation.

Both the inversion (used for the linear analysis) and the nonlinear analysis were made using PEST (Doherty, 2010) which is a model independent inversion software. AarhusInv (Auken et al., 2014) was applied to simulate MRS and the transient electromagnetic soundings (TEM) forward responses. The nonlinear analysis was performed using Null-Space Monte Carlo (NSMC) (Tonkin and Doherty, 2009). Compared to the original implementation of NSMC, the Null-Space of the parameter combinations was selected sufficiently large to include parts of the solution space. This secures that nonlinear contributions to parameter uncertainty are considered by the analysis. A complete description of NSMC is beyond the scope of this abstract and the reader is referred to Tonkin and Doherty (2009).

FIELD CASE AND RESULTS

Demonstration of the presented methodology is done using a dataset collected near Ristrup Well field located north-west of the town of Aarhus, Denmark (see Figure 1)

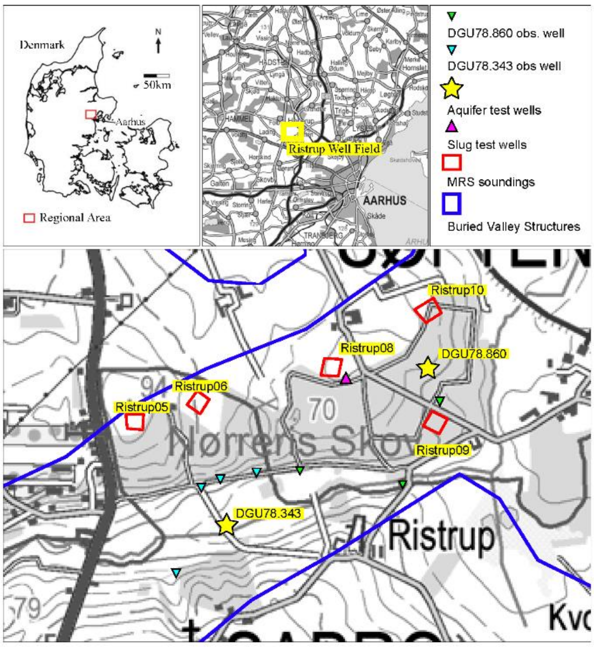

Figure 1: Field site with location of hydraulic data and MRS soundings

The dataset comprises 5 MRS soundings, 5 TEM soundings, 2 long-duration aquifer tests and 2 slug tests. One of the aquifer tests includes both drawdown and recovery data. Both of these were included in the analysis. At the site of the slug-test both an upper and a lower aquifer was present. Both of these aquifers were included in the analysis. In order to determine the C_p correlation factor, each MRS sounding was correlated to the transmissivity estimated from the aquifer test or slug test closest to the sounding.

To illustrate the difference between the linear and the nonlinear analysis, Figure 2 shows inversion results from MRS sounding “Ristrup09”. The model is set up with 5 layers for the TEM sounding and 4 layers for the MRS sounding. The gray lines on the figure are the equivalent models from the NSMC analysis and they illustrate the uncertainty of the parameter estimates as well as parameter correlations. The second feature to notice from the figure is that the optimal model from the linear analysis and the average model from the nonlinear analysis are comparable. Thirdly, it is apparent that the parameters for the upper part of the system cannot be determined (gray lines), whereas the parameters of the aquifer (layer 3) can be determined.

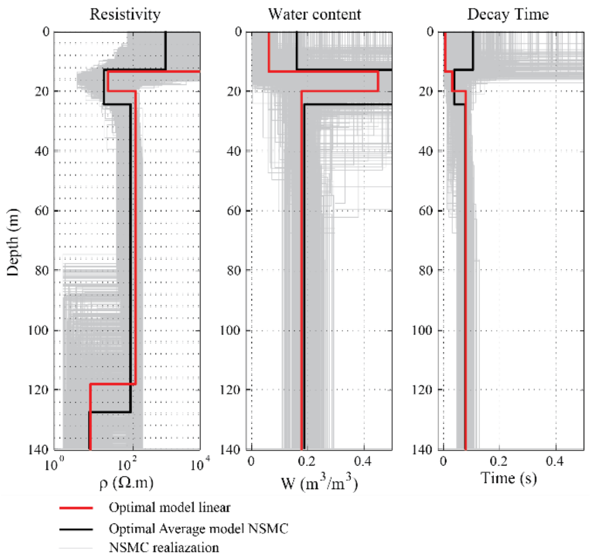

Figure 2: Analysis results Ristrup09. Comparison between linear and nonlinear NSMC analysis.

An analysis similar to the one shown in Figure 2 was performed for all MRS soundings, and the results were correlated to the transmissivities estimated from aquifer tests and slug-tests.

By applying the methodologies presented previously, T_{MRS} estimates were calculated and their uncertainties were quantified by calculating $var[\log(T_{MRS})]$. This was done for both the linear and the nonlinear analysis. The results are presented in Figure 3.

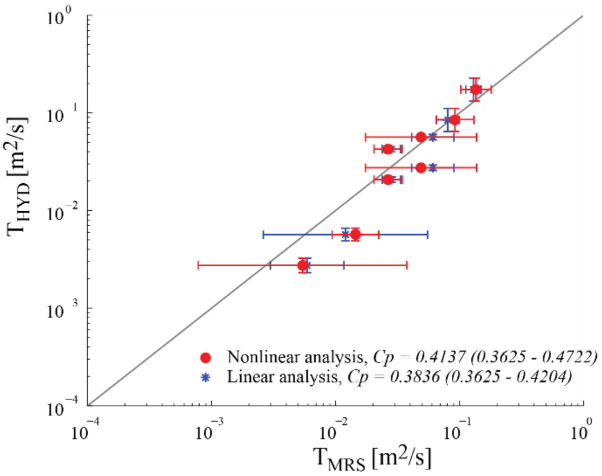

Figure 3: T_{MRS} estimates with uncertainties. Uncertainties for T_{HYD} have been determined from the linear analysis of the hydrological data. Cp values used to determine T_{MRS} for the linear and the non-linear analysis are shown with 95% confidence intervals

The results in Figure 3 show that the uncertainty estimates obtained by the nonlinear analysis in general are larger than those obtained by the linear analysis. It is also noticed that the uncertainty of T_{MRS} varies significantly between soundings. This variation is due to parameter uncertainties in the joint MRS-TEM inversion, where especially soundings with high noise levels and deep or multiple aquifers have high uncertainty.

CONCLUSIONS

This study demonstrates a methodology using linear approximations of parameter uncertainties to estimate uncertainties in transmissivity estimates obtained from MRS. The results are compared to those obtained from a nonlinear analysis. In general, the uncertainties obtained using the linear and the nonlinear methods are comparable.

The estimated uncertainties depend on both the uncertainties of both the parameters of the MRS models as well as the hydrological data. For the MRS parameters the noise depend on factors such as noise levels and depth to target aquifer or presence of multiple aquifers that both tend to reduce the signal obtained from the deep aquifers. We also determined the Cp factor using weighted least squares. Using this methodology MRS soundings with uncertain parameters and uncertain hydrological data are down weighted in the regression.

The estimated uncertainties can be used to determine weights to put on MRS-based transmissivity estimates when such estimates are used as data or prior information in hydrological model inversion.

ACKNOWLEDGMENTS

The Authors would like to acknowledge Ahmad Behroozmand from Stanford University for assisting in processing, evaluating the MRS noise levels and in setting up the input files. We would also like to thank Jakob Juul Larsen from Aarhus University for assisting in the signal processing.

The first author is funded by the ‘HyGEM – integrating geophysics, geology, and hydrology for improved groundwater and environmental management’ project The project is financed by the Danish Council of Strategic Research.

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