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# A feasibility study on the estimation of water retention parameters from surface nuclear magnetic resonance measurements in the vadose zone

## Introduction

➢Demand for non-invasive characterization of soil hydraulic properties

➢Idea: soil-physical parameterization of the capillary fringe (Costabel and Yaramanci, 2011) using surface nuclear magnetic resonance (SNMR)

➢Study: accuracy and resolution limits of parameter estimation using common water retention (WR) models:

•Brooks and Corey (1964):

$$\Theta_{CFP}(z) = \begin{cases} \Theta_R + (\Theta_S - \Theta_R)\left|\frac{h_0}{h}\right|^{\lambda} & (|h_0| < |h|) \\ \Theta_S & (|h_0| \geq |h|) \end{cases}$$

•Van Genuchten (1980)

$$\Theta_{CFP}(z) = \begin{cases} \Theta_R + (\Theta_S - \Theta_R)\frac{1}{(1+|\frac{h}{h_0}|^n)^m} & (h < 0) \\ \Theta_S & (h \geq 0) \end{cases}$$

•Kosugi (1996)

$$\Theta_{CFP}(z) = \begin{cases} \Theta_R + (\Theta_S - \Theta_R)\frac{1}{2}erfc\left(\frac{ln\left(\frac{h}{h_0}\right)}{\sqrt{2}\sigma}\right) & (h < 0) \\ \Theta_S & (h \geq 0) \end{cases}$$

## SNMR measurements in the vadose zone

➢Cable loop at the surface, loop diameter from 5 to 20m (Fig. 1)

➢Low excitation power, pulse moments $q$ from 0.01 to 1 As

➢NMR response from shallow depth, i.e., from the unsaturated zone (Fig. 2)

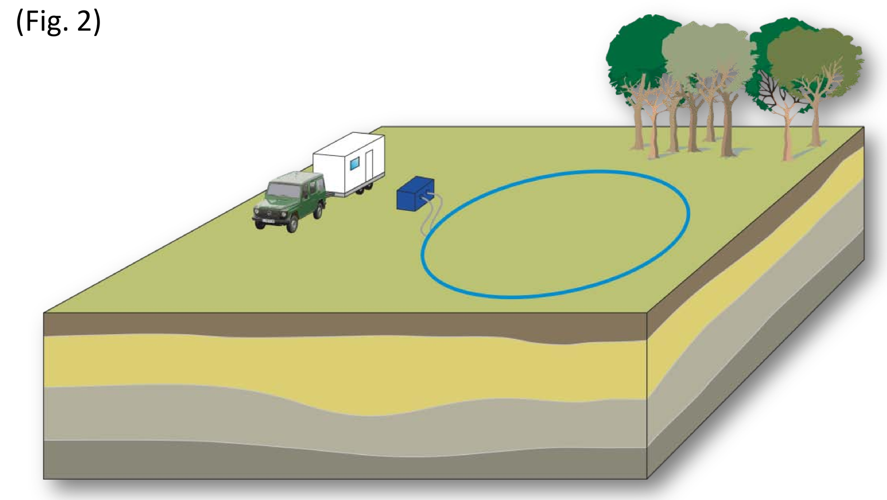

**Figure 1:** Measurement setup in the field.

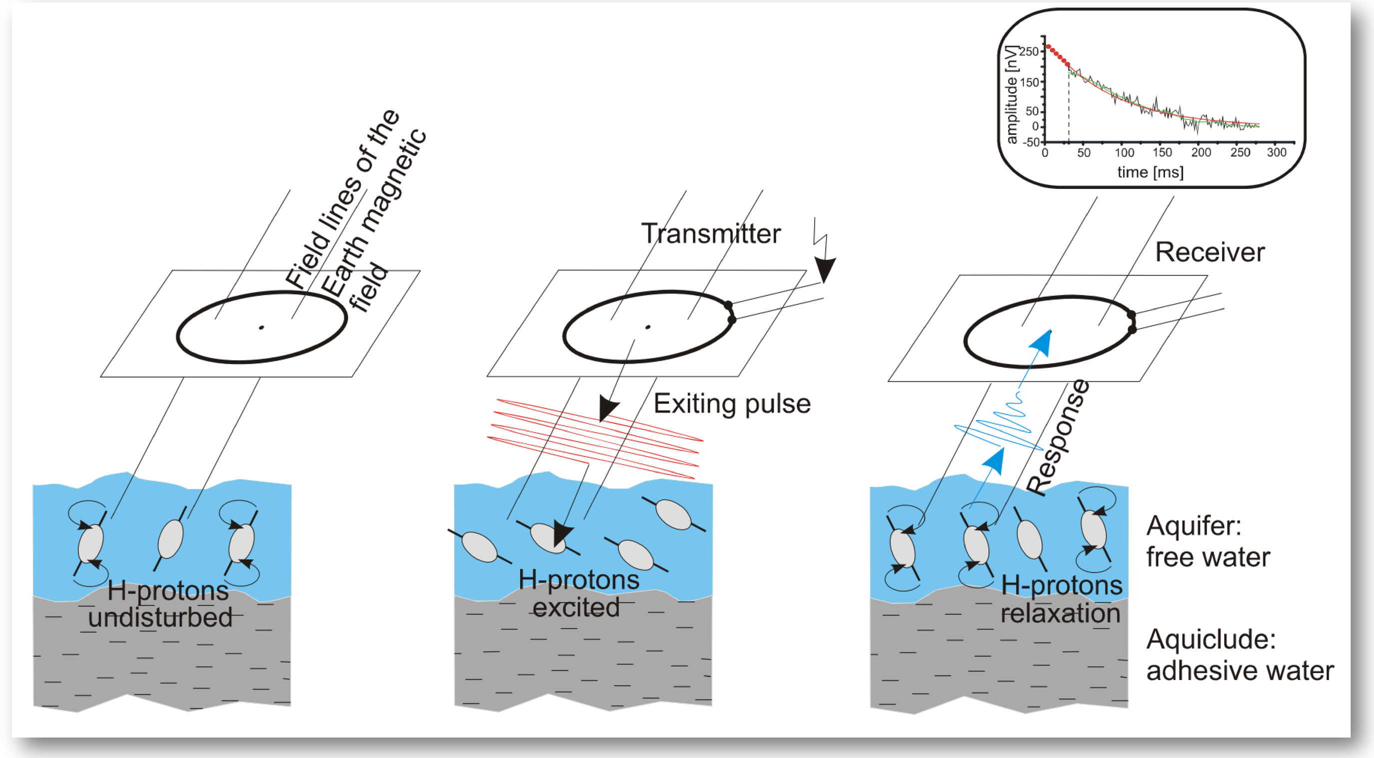


**Figure 2:** SNMR principle, excitation of and response signal from H-protons in the water molecules.

➢Continuous measurements with increasing excitation power $q$ leads to a 1D scan of the vertical water content distribution

➢The SNMR sounding curve $E_0(q)$ represents the signal amplitude depending on $q$, each point on $E_0(q)$ corresponds to a certain sensitivity range in the subsurface (the kernel function $\kappa_{1D}(q,z)$, Fig. 3).

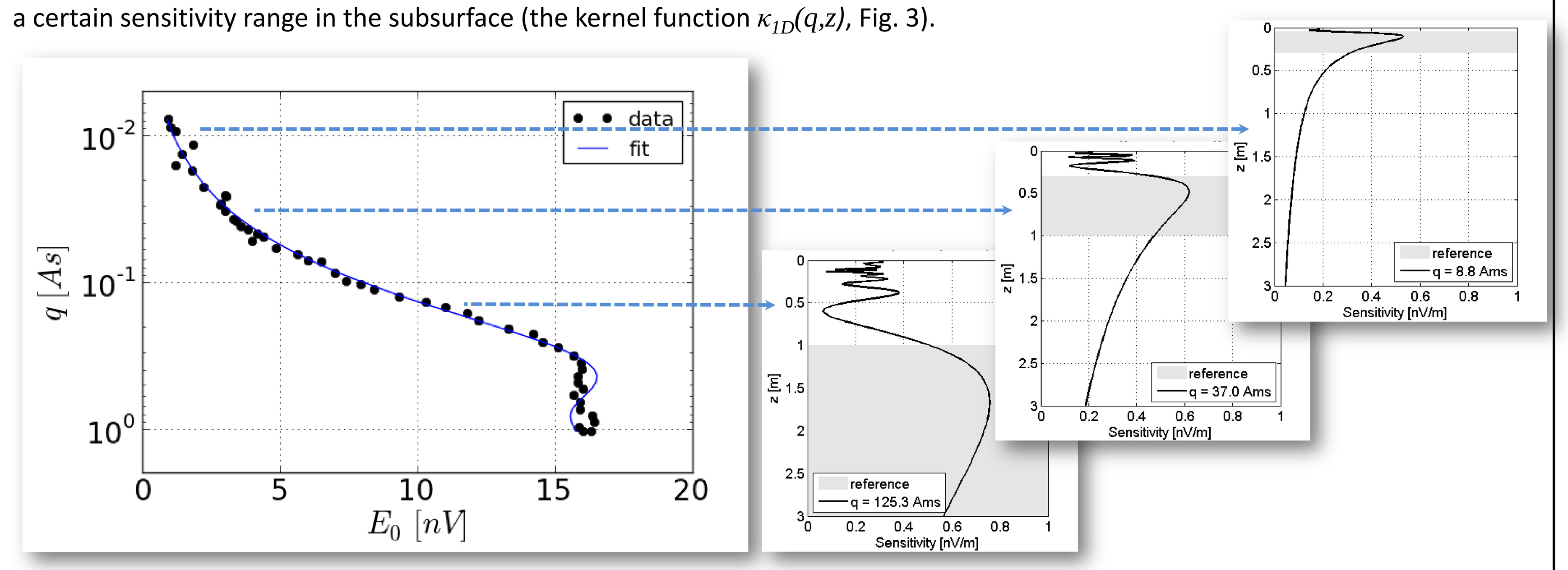


**Figure 3:** SNMR sounding curve $E_0(q)$ and corresponding sensitivity functions $\kappa_{1D}(q,z)$.

## Direct inversion for water retention parameters by SNMR

➢SNMR signal amplitude $E_0(q)$ proportional to water volume in the excited depth range, i.e., inversion of $E_0(q)$ yields 1D water content distribution:

$$E_0(q) = \int_z \kappa_{1D}(q,z)\Theta_{CFP}(z)dz$$

➢Reformulation of the forward problem by parameterizing the water content distribution in the capillary fringe $\theta_{CFP}$ (parameterization by WR model $f(h)$):

$$\Theta_{CFP}(z) = \begin{cases} \Theta_R + (\Theta_S - \Theta_R)f(h) & (z < z_{table} \text{ with } h = z - z_{table}) \\ \Theta_S & (z \geq z_{table}) \end{cases}$$

➢Inversion with GIMLI (Günther and Rücker, 2009):
•Marquardt-Levenberg algorithm,
•$\theta_R$ is set to 0, $z_{table}$ is given
•WR parameters are kept within realistic ranges using logarithmic barriers
•square roots of covariance matrix diagonal are considered as uncertainty intervals, analysis of resolution matrices

## Synthetic data

➢Model: water table $z_{table}$ at 3.0m, WR parameters for sandy soil

➢SNMR measurements with 11.3m circle loop, varying noise levels and varying numbers of $q$ (Fig. 4 to 6)

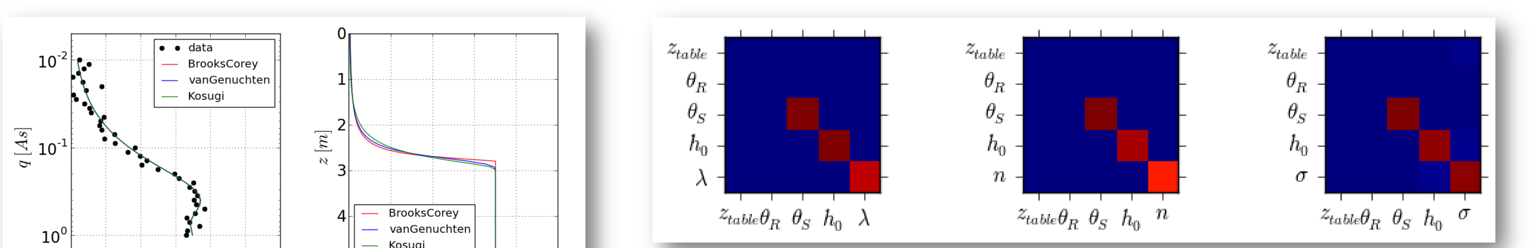

**Figure 4:** Simulated SNMR measurement with 1 nV noise and 40 pulse moments.

| Parameter | MRS (Brooks & Corey) | MRS (van Genuchten) | MRS (Kosugi) | Model |
|---|---|---|---|---|
| $\Theta_S$ [%] | 35.1 ± 0.1 | 35.1 ± 0.1 | 35.1 ± 0.1 | 35 |
| $h_0$ [m] | 0.22 ± 0.02 | 0.28 ± 0.3 | 0.32 ± 0.16 | 0.25 |
| Distribution index | 1.9 ± 0.3 | 3.2 ± 0.4 | 0.8 ± 0.1 | 2.0 3.0 1.0 |

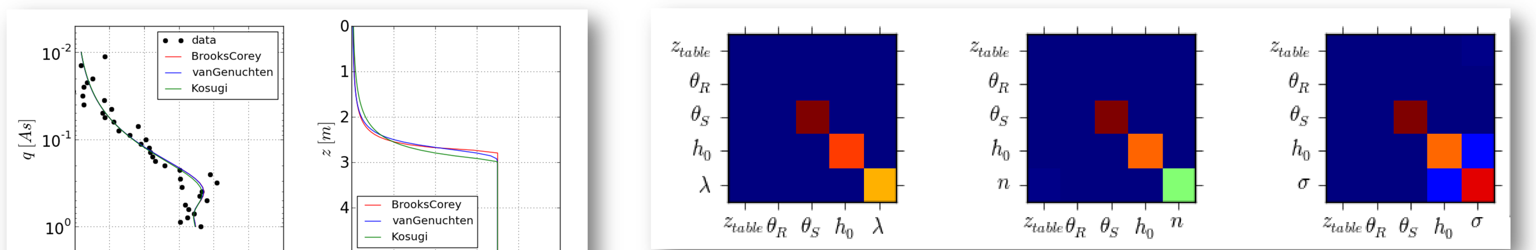

**Figure 5:** Simulated SNMR measurement with 2 nV noise and 40 pulse moments.

| Parameter | MRS (Brooks & Corey) | MRS (van Genuchten) | MRS (Kosugi) | Model |
|---|---|---|---|---|
| $\Theta_S$ [%] | 35.0 ± 0.1 | 35.0 ± 0.1 | 35.0 ± 0.1 | 35 |
| $h_0$ [m] | 0.24 ± 0.07 | 0.30 ± 0.10 | 0.24 ± 0.07 | 0.25 |
| Distribution index | 2.0 ± 0.8 | 3.3 ± 1.3 | 1.1 ± 0.3 | 2.0 3.0 1.0 |

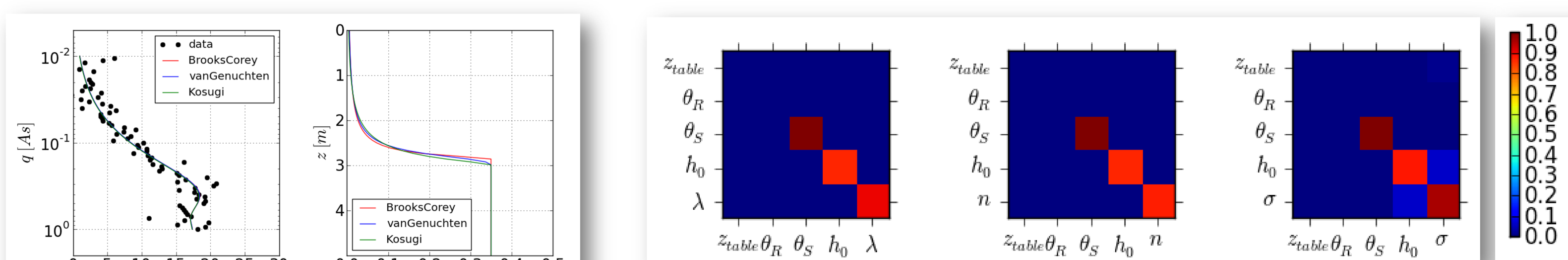

**Figure 6:** Simulated SNMR measurement with 2 nV noise and 80 pulse moments.

| Parameter | MRS (Brooks & Corey) | MRS (van Genuchten) | MRS (Kosugi) | Model |
|---|---|---|---|---|
| $\Theta_S$ [%] | 35.0 ± 0.1 | 35.0 ± 0.1 | 35.0 ± 0.1 | 35 |
| $h_0$ [m] | 0.17 ± 0.05 | 0.21 ± 0.05 | 0.23 ± 0.05 | 0.25 |
| Distribution index | 1.5 ± 0.4 | 2.6 ± 0.5 | 1.1 ± 0.2 | 2.0 3.0 1.0 |

➢Resolution/accuracy of $\theta_S$ is exellent for a wide range of noise levels, also for small numbers of $q$

➢Resolution/accuracy of WR parameters increases with number of $q$ and decreases with $z_{table}$

➢Reliable WR parameter estimation not possible for $z_{table}$ > 6m (Fig. 7)

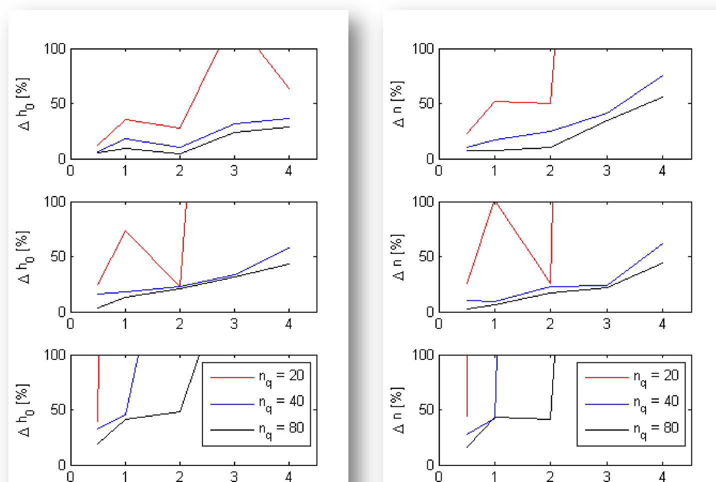


**Figure 7:** Uncertainty of WR-parameter estimates for the van-Genuchten model for different $z_{table}$

## Real data

➢Water table $z_{table}$ at 3.25m, reference values of WR parameters from tension infiltrometry (WR measurements on the saturating path)

➢SNMR measurements with 11.3-m circle loop, noise level: 0.3 to 0.7 nV, number of $q$: 13 and 52, measurement time: 1.5 and 3.5 h (Fig. 8 and 9)

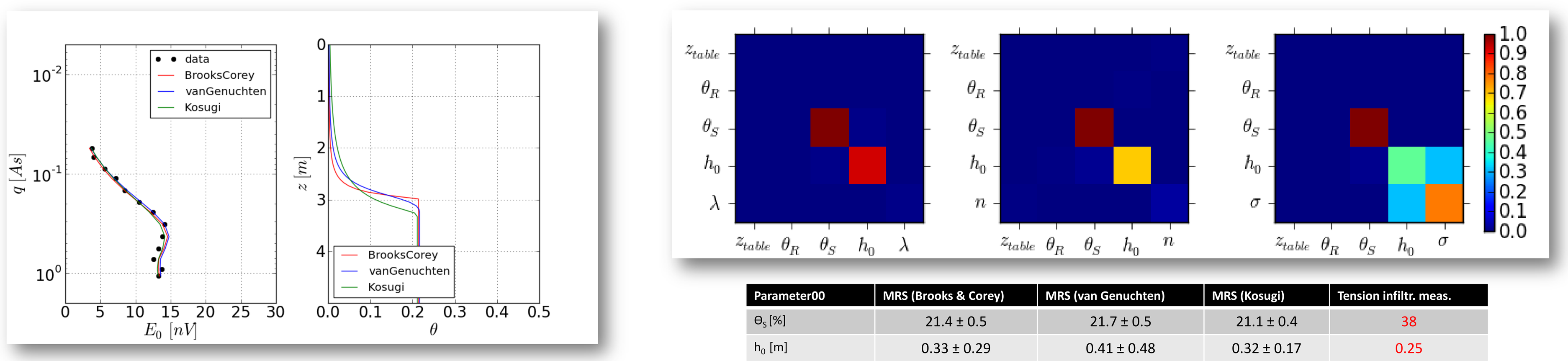

**Figure 8:** SNMR measurement with 0.7 nV noise and 13 pulse moments.

| Parameter00 | MRS (Brooks & Corey) | MRS (van Genuchten) | MRS (Kosugi) | Tension infiltr. meas. |
|---|---|---|---|---|
| $\Theta_S$ [%] | 21.4 ± 0.5 | 21.7 ± 0.5 | 21.1 ± 0.4 | 38 |
| $h_0$ [m] | 0.33 ± 0.29 | 0.41 ± 0.48 | 0.32 ± 0.17 | 0.25 |
| Distribution index | 2.8 ± 2.5 | 3.6 ± 2.9 | 1.1 ± 0.7 | 1.8 2.8 0.8 |

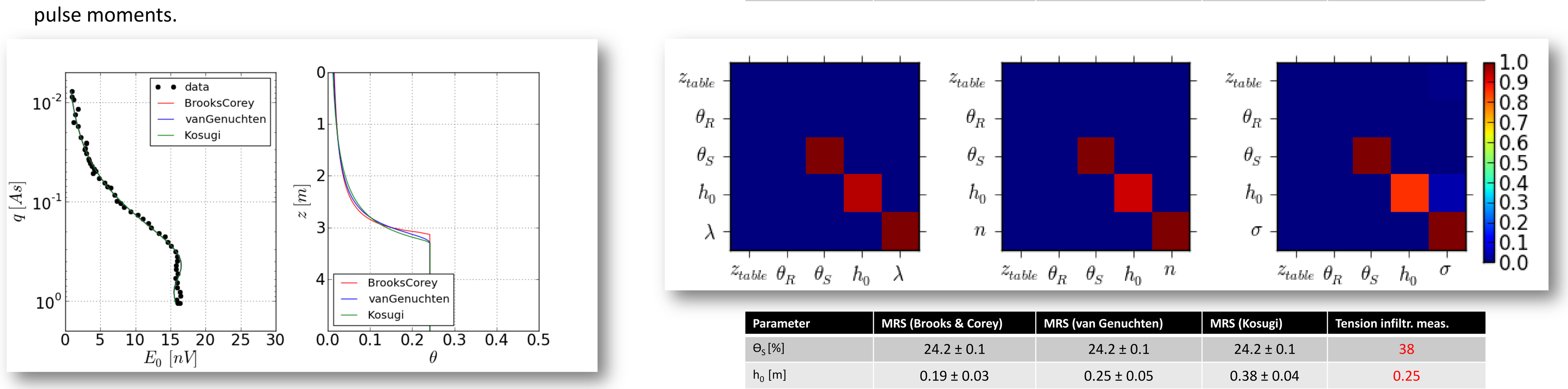

**Figure 9:** SNMR measurement with 0.3 nV noise and 52 pulse moments.

| Parameter | MRS (Brooks & Corey) | MRS (van Genuchten) | MRS (Kosugi) | Tension infiltr. meas. |
|---|---|---|---|---|
| $\Theta_S$ [%] | 24.2 ± 0.1 | 24.2 ± 0.1 | 24.2 ± 0.1 | 38 |
| $h_0$ [m] | 0.19 ± 0.03 | 0.25 ± 0.05 | 0.38 ± 0.04 | 0.25 |
| Distribution index | 1.0 ± 0.1 | 2.1 ± 0.1 | 1.3 ± 0.1 | 1.8 2.8 0.8 |

➢Resolution and accuracy equivalent to the results of the simulations, reliable estimation of WR parameters is only possible for SNMR measurement with the higher number of $q$

➢However, SNMR results (WR measurement at equilibrium) differ from reference values provided by dynamic WR measurements!

## Simulation: SNMR monitoring of an irrigation experiment

➢Simulation of an irrigation experiment with HYDRUS 1D (Šimůnek et al., 2009, Fig. 10):

•Duration: 4 h, Irrigation rate: 37 mm/h, sandy soil
•Bottom boundary condition: zero pressure head (i.e., no changes of $z_{table}$ with time)

➢Time-dependend SNMR measurements with adequate repetition rate are only possible for certain pulse moments (Fig. 11)!

➢Loss of vertical resolution compared to conventional SNMR measurements, however, time-dependend changes in certain depth ranges can be observed with adequate resolution in time.

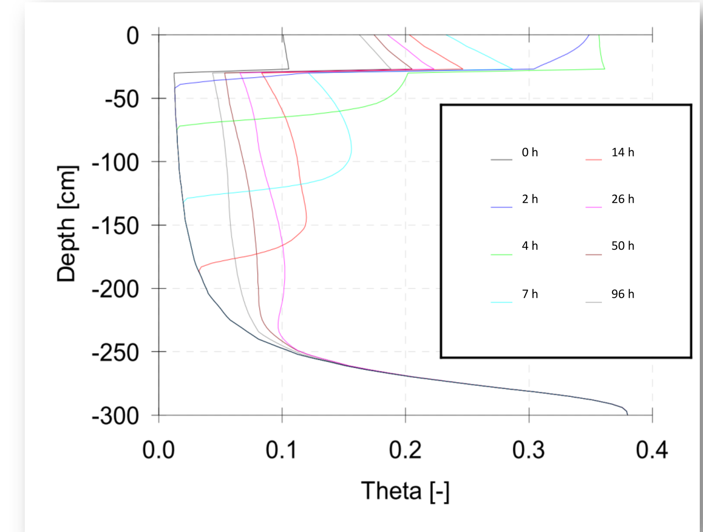


**Figure 10:** Distributions of $\theta$ during the simulated infiltration.

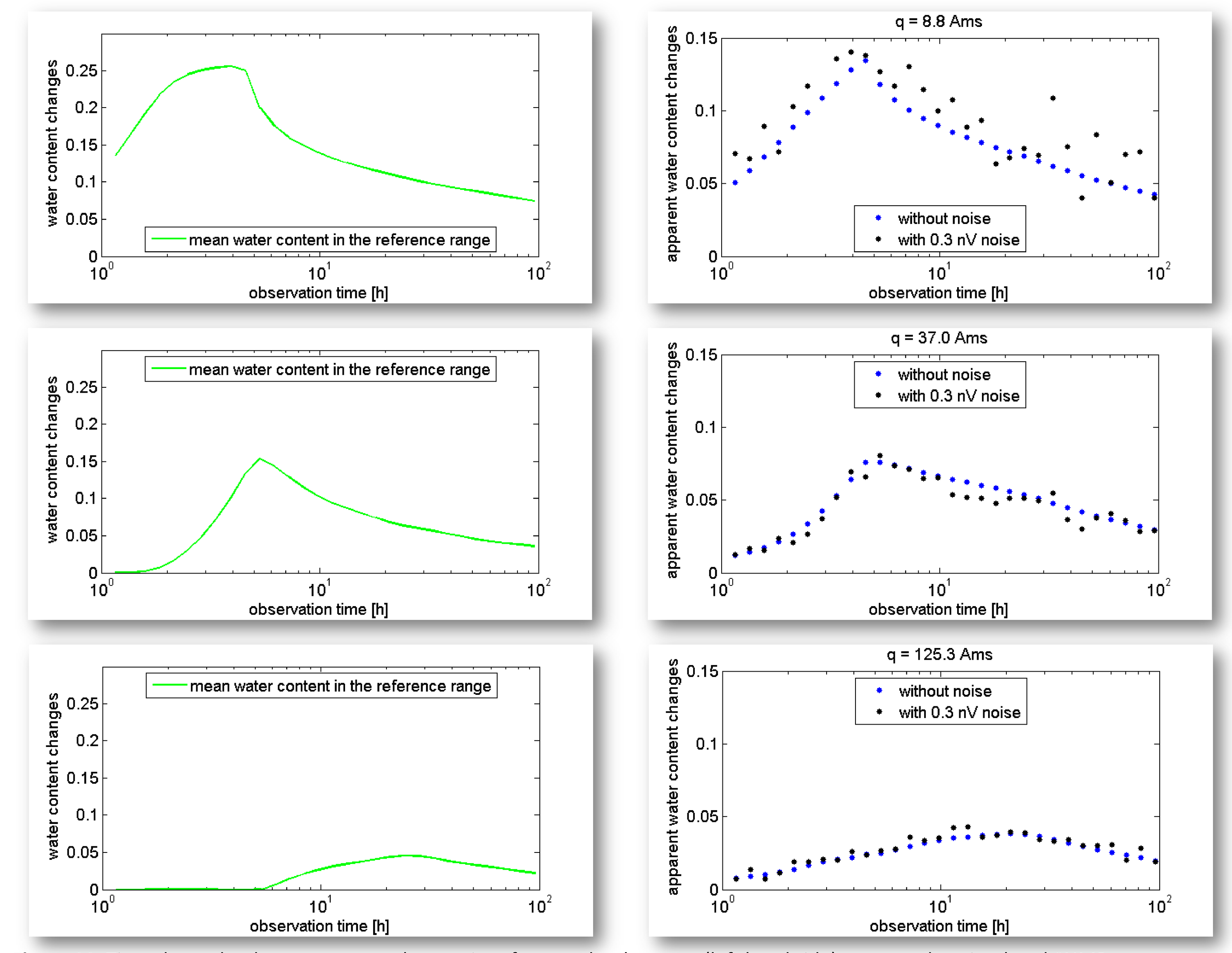


**Figure 11:** Time-dependend water content changes in reference depth ranges (left hand side) compared to simulated SNMR measurements for certain pulse moments (right hand side).

## Conclusions, Outlook

**➢If $z_{table}$ is given or can reliably be predicted, WR parameters can be estimated from non-invasive SNMR measurements with useful accuracy.**

**➢Accuracy increases with decreasing noise level, decreasing $z_{table}$, and increasing number of $q$.**

**➢ Accuracy can be improved by increasing the number of $q$ rather than increasing the number of repeated measurements for averaging (stacking).**

**➢The limit of a reliable WR parameter estimation is achieved at a noise level of 20 to 30% (percentage of NMR signal amplitude).**

**➢Future research is focused on monitoring of infiltration experiments with SNMR .**

**➢To achieve high repetition rates of SNMR measurement during fast infiltration processes, observation is possible only in certain depth ranges, i.e., no or very low vertical resolution of the SNMR measurements during the infiltration process.**

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