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## Key Points:

- First detailed comparison of laboratory and logging NMR estimated parameters in unconsolidated aquifers
- Proposing drilling and sampling methodologies to overcome the challenges facing laboratory and logging NMR measurements in unconsolidated aquifers
- The methods employed in this study support the use of laboratory NMR to develop the interpretation of NMR logging for aquifer characterization

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## Successful Sampling Strategy Advances Laboratory Studies of NMR Logging in Unconsolidated Aquifers

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**Abstract** The nuclear magnetic resonance (NMR) technique has become popular in groundwater studies because it responds directly to the presence and mobility of water in a porous medium. There is a need to conduct laboratory experiments to aid in the development of NMR hydraulic conductivity models, as is typically done in the petroleum industry. However, the challenge has been obtaining high-quality laboratory samples from unconsolidated aquifers. At a study site in Denmark, we employed sonic drilling, which minimizes the disturbance of the surrounding material, and extracted twelve 7.6 cm diameter samples for laboratory measurements. We present a detailed comparison of the acquired laboratory and logging NMR data. The agreement observed between the laboratory and logging data suggests that the methodologies proposed in this study provide good conditions for studying NMR measurements of unconsolidated near-surface aquifers. Finally, we show how laboratory sample size and condition impact the NMR measurements.

### 1. Introduction

Geophysical methods have been used widely for groundwater investigations (Butler, 2005; Schubert, 2015). But the physical parameters obtained from geophysics must be linked to the aquifer properties of interest. Recently, there has been significant interest in using the nuclear magnetic resonance (NMR) method for groundwater characterization because it responds directly to the amount and mobility of water in porous media (Behroozmand et al., 2015; Dlubac et al., 2013; Dlugosch et al., 2013; Falzone & Keating, 2016; Müller-Petke et al., 2015). In a fully saturated medium, the NMR-inferred water content is a good proxy for the total porosity (Coates et al., 1999; Dunn et al., 2002). The relaxation time constant of the NMR signal, that is, the time it takes for the nuclear spins to reequilibrate to their initial state after being perturbed by an energizing pulse, contains information about the pore size distribution (Bird et al., 2005; Brownstein & Tarr, 1979; Hinedi et al., 1997; Müller-Petke et al., 2015). Taken together, the NMR parameters have been linked to hydraulic conductivity ( $K$ ) through the use of various empirical relationships (Daigle & Dugan, 2009; Daigle et al., 2014; Dlubac et al., 2014, 2013; Dlugosch et al., 2013; Knight et al., 2016; Legchenko et al., 2004; Vilhelmsen et al., 2014).

NMR logging has been used for decades in the petroleum industry to estimate the hydraulic properties of reservoirs (Coates et al., 1999; Daigle & Dugan, 2009, 2011; Dunn et al., 2002; Kleinberg & Jackson, 2001). To support this work, extensive laboratory research has been conducted on core samples to develop an understanding of the NMR response of reservoir rocks and to establish the relationships that can be used to estimate permeability from the NMR parameters (Daigle & Dugan, 2009, 2011; Daigle et al., 2014; Kenyon et al., 1988; Seevers, 1966; Timur, 1969). Demonstrated success in the petroleum industry and increased interest in the use of NMR in the top few hundred meters of the subsurface (referred to here as the near surface) have led to the development of instruments that are suitable for groundwater studies (Walsh et al., 2013). While we have decades of publications describing the NMR response of sandstones and carbonates for petroleum applications, what we now need are studies combining logging and laboratory NMR of near-surface materials for groundwater applications.

Of specific interest in this study are unconsolidated near-surface aquifer materials. Working with these materials offers unique challenges. Here we enumerate three of the main challenges both for the actual NMR logging and for the sampling of materials needed for laboratory experiments.

1. *Borehole conditions.* The recent development of an NMR tool designed specifically for use in small-diameter water boreholes (Walsh et al., 2013) has motivated considerable interest in high-resolution NMR logging of shallow aquifers. The NMR logging instrument used in this study senses a thin cylindrical shell located ~10–20 cm radially from the tool's centerline. For this reason, boreholes that have a drilled diameter much larger than the casing diameter may not be appropriate for NMR logging. In addition, standard drilling in unconsolidated aquifers can lead to mud invasion and severe washout of formation materials during drilling (Kobr et al., 2005) and thus further disturbance beyond the borehole wall (Dlubac et al., 2013). This can raise questions about whether the NMR logging measurements are representative of the undisturbed formation materials.
2. *Laboratory sample conditions.* Laboratory NMR studies can provide high-quality data from well-controlled experiments that can be used to better understand the physics governing the logging measurements and the relationship between the NMR parameters and other material properties. Unlike the petroleum samples that are provided for laboratory experiments as undisturbed rock cores, unconsolidated samples, under near-surface pressure conditions, are often provided in a highly disturbed manner or even as repacked drill cuttings. As a consequence, it is difficult to know whether the samples used for laboratory measurements represent the materials sampled by the logging measurements.
3. *Laboratory sample size.* A related issue (of importance in studies of both consolidated and unconsolidated materials) is the size of the standard laboratory samples which typically have a volume of ~40 cm<sup>3</sup> or smaller. The question arises as to whether these standard samples are representative of logging NMR measurements, which have a sensitive volume of about 1,000–2,000 cm<sup>3</sup>.

We note here that there have been studies conducted in the marine environment that successfully compare logging NMR measurements with measurements on the core samples obtained in unconsolidated sediments (Daigle & Dugan, 2009, 2011; Daigle et al., 2014). However, marine sediments are found under conditions of much higher confining pressure and coring was successfully conducted using, for example, a hydraulic piston corer. When a similar coring tool was tested in the study by Dlubac et al. (2013), it was found to be incapable of providing high-quality samples of shallow unconsolidated and semiconsolidated aquifer materials; most of the core samples fell apart on removal.

Given the challenge of obtaining high-quality samples in unconsolidated near-surface aquifer materials, there have been no studies to date that have used laboratory samples to support the assessment or interpretation of NMR logging data in these materials. Yet such studies are needed to determine a robust relationship between the measured NMR parameters and  $K$ . In this study, we propose methodologies for obtaining reliable NMR logging and laboratory measurements in unconsolidated aquifers. We present a comparison of laboratory and logging NMR data under the best possible conditions from a study site in Denmark and show how a careful selection of drilling method, sample cutting, sample size, and preparation results in high-quality logging and laboratory NMR data.

## 2. Background

The fundamental concepts of NMR are similar when measured in consolidated or unconsolidated porous media (Dunn et al., 2002). At a thermal equilibrium state in a background static magnetic field, the alignment of the spin magnetic moments (spins) associated with the hydrogen protons of water molecules results in a small net nuclear magnetization. The magnetization precesses about the background magnetic field ( $\mathbf{B}_0$ ) at the resonance frequency. The system is first perturbed from equilibrium using an energizing radio frequency (RF) pulse. After the pulse is shut down, the spins relax back to thermal equilibrium, and their precession in the transverse plane generates a detectable, decaying signal, called the free induction decay (FID). The signal amplitude at the start of the relaxation is directly proportional to the total amount of sampled water. The relaxation of the NMR decay curve occurs as a consequence of interactions among nuclear spins and with the surrounding medium. The simplest NMR experiment, measurement of the FID, is sensitive to inhomogeneities in the magnetic field. As a result, the measured signal often undergoes a more rapid decay due to this dephasing. To eliminate this effect, the Carr-Purcell-Meiboom-Gill (CPMG) pulse sequence (Carr & Purcell, 1954; Meiboom & Gill, 1958), designed to rephase the spins, is typically used in standard laboratory and logging NMR measurements. A series of spin echoes, generated using refocusing pulses and separated by an echo spacing time, form a decay curve with a relaxation time  $T_2$  without the influence of dephasing.

The distribution of the  $T_2$  relaxation times contains information about pore size distribution and plays a key role in estimation of  $K$  from the NMR data.

The  $T_2$  relaxation of fluids in a porous medium is controlled by three relaxation processes, each of which is described with a relaxation rate. The rate of the bulk fluid relaxation process depends only on the physical properties of the fluid, such as viscosity, and chemical composition (Coates et al., 1999). Because this rate is very low compared to the other relaxation rates, its contribution to the overall relaxation rate is typically neglected. The surface relaxation rate depends on the surface relaxivity (varying with mineralogy) and the surface-area-to-volume ratio of the pore space (Brownstein & Tarr, 1979). The third relaxation rate describes relaxation that occurs due to the diffusion of spins in an inhomogeneous magnetic field. The diffusion relaxation rate is affected mainly by the strength of the field gradient, which itself depends on the strength and uniformity of the applied field and concentration of magnetic minerals, and echo spacing (Carr & Purcell, 1954; Hürlimann, 1998; Mitchell et al., 2010; Washburn et al., 2008). Working at low field strengths and/or shortening the echo spacing can minimize the effect of the diffusion relaxation.

Laboratory NMR typically uses a small-volume ( $\leq 40 \text{ cm}^3$ ) sample, which is placed inside an apparatus consisting of permanent magnets to provide the background field and an inductive coil to record the NMR signal (Dunn et al., 2002). The energizing pulse is tuned to efficiently turn the spins in the entire sample into the transverse plane.

In NMR logging, a probe composed of one magnet or an array of magnets and an RF coil is lowered into a borehole. The tool used in this study senses a thin cylindrical shell centered about the probe. The length of the sensitive cylinder depends on the probe length and defines the vertical resolution of the probe. Because the static fields have a gradient, different Larmor frequencies (up to four) are normally tuned to sense regions with different radial distances (on the order of several centimeters) from the center of the probe.

In the petroleum industry, laboratory experiments have been routinely used to develop models that have successfully linked the NMR parameters, water content, and relaxation time, with permeability (Coates & Dumanoir, 1974; Daigle & Dugan, 2009, 2011; Kenyon et al., 1988; Seevers, 1966; Timur, 1969) and used in NMR logging applications. This has not been the case in near-surface groundwater studies because of the above mentioned challenges. As a result, the models developed for petroleum applications have been used in the interpretation of near-surface NMR logging but derived estimates of permeability or hydraulic conductivity were found to underestimate the measured property (Dlubac et al., 2013; Knight et al., 2016).

### 3. Logging and Laboratory Experiments

The field site is located in the Ristrup area, NW of Aarhus, Denmark. The geology of the area is a complicated glaciotectonic complex and consists of multiple buried valley structures, which are incised into thick hemipelagic Paleogene clays (Høyer et al., 2015; Jørgensen et al., 2003). The valleys are filled mainly with meltwater clay, sand, and gravel and often contain significant volumes of groundwater.

The field site was selected based on the hydrogeological interest in the area, ease of access, and the electromagnetic noise conditions. A 32 m deep borehole with a diameter of 10.2 cm was drilled in April 2014 using a sonic rig (Barrow, 1994; Lawrie et al., 2012; Ruda & Farrar, 2006) to get good borehole conditions for logging (i.e., a borehole with a drilled diameter close to the casing diameter and with minimal disturbance beyond the borehole wall) and core samples for laboratory studies. The sonic method uses high-frequency, high-force vibration to penetrate into the formation. The drilling started by advancing a 2 m sampling barrel into the formation. Then, an outer case of the same length was lowered over the sampling barrel. The sampling barrel was removed from the borehole and the sample removed from the sampling barrel into liners. This procedure was repeated for the entire depth of the borehole. Then, the borehole was cased to the bottom with a PVC pipe (with an outside/inside diameter of 9 cm/8.1 cm and with the screen at the bottom) and the samples were preserved in a cooling room for future study. The size of the borehole and casing was chosen to be compatible with the NMR logging probe used in this study. The soil samples were continuous and undisturbed ( $\sim 7.6$  cm in diameter). The water level was 8.0 m below ground surface.

In May 2014, the logging data consisting of NMR logging, electromagnetic (EM) induction, gamma, and magnetic susceptibility were acquired. We measured NMR logging data using the Javelin equipment (Vista Clara

Inc.; Walsh et al., 2013). We used the JP175 downhole probe that is 2.1 m long with an outer diameter of 4.4 cm. A sensitive zone with a radius of  $\sim 12$  cm, from the center of the probe, and a nominal vertical resolution of 1 m are expected for this tool. However, we conducted overlapping measurements to obtain data in 0.5 m increments in the depth interval 8 to 19 m. Given the probe used in this study, with a radius of 2.2 and a depth of investigation of 12 cm, and the borehole radius of 5.1 cm, we are confident that the probe always sampled the in situ formation, even in the worst-case scenario when the probe was positioned against one side of the borehole. The NMR CPMG data with an echo spacing of 2 ms and a stack size of 100 were acquired at 245 kHz and 290 kHz (corresponding to radial distances of 12.7 cm and 11.7 cm, respectively), leading to a signal-to-noise-ratios (SNR) between 10 and 170 at different depths, with a mean SNR of 32. After logging NMR measurements, we acquired complementary logging data in the borehole consisting of gamma, EM induction, and magnetic susceptibility data.

Before cutting the cores for the laboratory NMR measurements, we measured DC resistivity and induced polarization directly on the cores. These measurements provided complementary data used to validate the identification of the clay/sand units. Afterward, we ran a cluster analysis to support selection of depth intervals for cutting laboratory samples, with the objective of sampling the full variety of subsurface conditions with a limited number of total samples. Sections were identified based on all field and laboratory data from the study site and two other nearby sites. Care was taken to balance the total number of samples for each geologic unit and to select the samples from each cluster and from any interesting feature like a thin layer of a different cluster type. As a result, 12 depths in the borehole were selected. The sample heights and diameters were  $\sim 10$  cm and  $\sim 7.6$  cm, respectively (we refer to them as “large” samples in the following). At the same time, geologic descriptions of the borehole were; these descriptions were used to develop the lithologic log.

Prior to laboratory NMR measurements, we saturated our samples with a 0.01 M  $\text{CaCl}_2$  solution, as is commonly used for  $K$  measurements of similar soils (Bo V. Iversen, personal communication, 2015). The samples were kept in their initial conditions in liners, with the lower end of the samples covered by cheesecloth. The saturation procedure involved placing the samples on a mesh inside a tank and wetting them gradually from the bottom. We increased the water level by  $\sim 1$  cm and waited 30–60 min for coarse sands, 1–2 h for fine sands, and 2–3 days for clay-rich materials before the next increase in the water level. At the end of the saturation process, we visually inspected the top of the samples to ensure full saturation. Because both ends of the sample were open during the saturation and the pores were filled slowly from the bottom with positive pressure, air saturation is expected to be low. Therefore, the laboratory NMR data should be representative of the total porosity.

Our laboratory NMR measurements were made using a 2 MHz Rock Core Analyzer (Magritek Ltd.). To ensure that our laboratory NMR samples were sufficiently large to represent in situ conditions, we used the Magritek P108 probe that supports samples of up to 10.2 cm in diameter. Therefore, our samples were placed directly inside the instrument in their initial condition and size. We collected  $T_2$  data with an echo spacing of 300  $\mu\text{s}$ : the measurements were stacked until a SNR of 200 was achieved. Next, to investigate the importance of sample size and condition on the NMR laboratory measurement, we prepared two sets of smaller subsamples using a sample holder with a diameter of 3.1 cm and a height of 5.6 cm. The first set of samples was undisturbed and prepared by advancing a sample holder into the large samples to investigate the influence of sample size on the results. The remaining sediments from the large samples were then repacked into a sample holder to form the second set of samples. These samples were disturbed because they were no longer in their in situ condition and were used to investigate the influence of sample condition on the results. We refer to these two sets as “small-undisturbed” and “small-disturbed” samples. We saturated the samples and measured a second round of laboratory NMR data on the 3 cm diameter subsamples using the Magritek P54 probe that supports up to 3.8 cm diameter cores with the same measurement procedure as described above.

The laboratory CPMG data were inverted to obtain  $T_2$  spectra. The inversion assumes a distribution of some known  $T_2$  values (here 200 logarithmically spaced values) and solves for the amplitudes with application of a regularization parameter to support minimal structure in the distribution (Whittall et al., 1991). The inversion was repeated for a range of regularization parameters, and an optimal regularization parameter was selected representing the smoothest solution that achieves a  $\chi^2$  of 1. Table 1 presents the regularization parameters and  $\chi^2$  values for the final inversions of the laboratory data. The  $T_2$  spectra were then corrected to remove

**Table 1**  
*Regularization Parameters ( $\lambda$ ) and the  $\chi^2$  values for Final Inversions of the Laboratory Large, Small-Undisturbed, and Small-Disturbed Samples Taken at 12 Depths in the Borehole*

Depth (m)	Large		Small undisturbed		Small disturbed	
	$\lambda$	$\chi^2$	$\lambda$	$\chi^2$	$\lambda$	$\chi^2$
2.55	330	0.99	530	0.98	190	0.97
5	220	1.03	3,800	0.99	195	1.00
7.5	240	1.00	1,350	1.00	320	1.01
9.6	1,100	1.00	3,400	1.02	75	0.99
12.05	1,800	1.02	9,000	0.99	710	1.00
14.65	400	1.30	19,200	0.98	8,500	1.01
16.33	500	1.30	9,000	1.01	6,900	0.99
19.39	5,500	1.02	220	0.99	3,500	1.00
23.09	6,000	0.99	22,700	1.01	1,000	0.99
24.47	8,000	0.99	25,000	1.00	1,750	0.98
27.11	200	0.98	5,000	1.02	1,900	1.01
30.18	4,500	1.00	15,000	0.99	7,500	1.00

the response of bulk fluid that could be seen, in a few cases, to have accumulated at the top of the sample during saturation. As is common practice, the relaxation response of each sample was represented by a single value calculated as the weighted logarithmic mean of the  $T_2$  distribution ( $T_{2ML}$ ). The logging NMR CPMG data collected at each measurement depth were inverted with the same approach used for the laboratory. We found a regularization parameter of 100 to be an appropriate parameter for the logging NMR data.

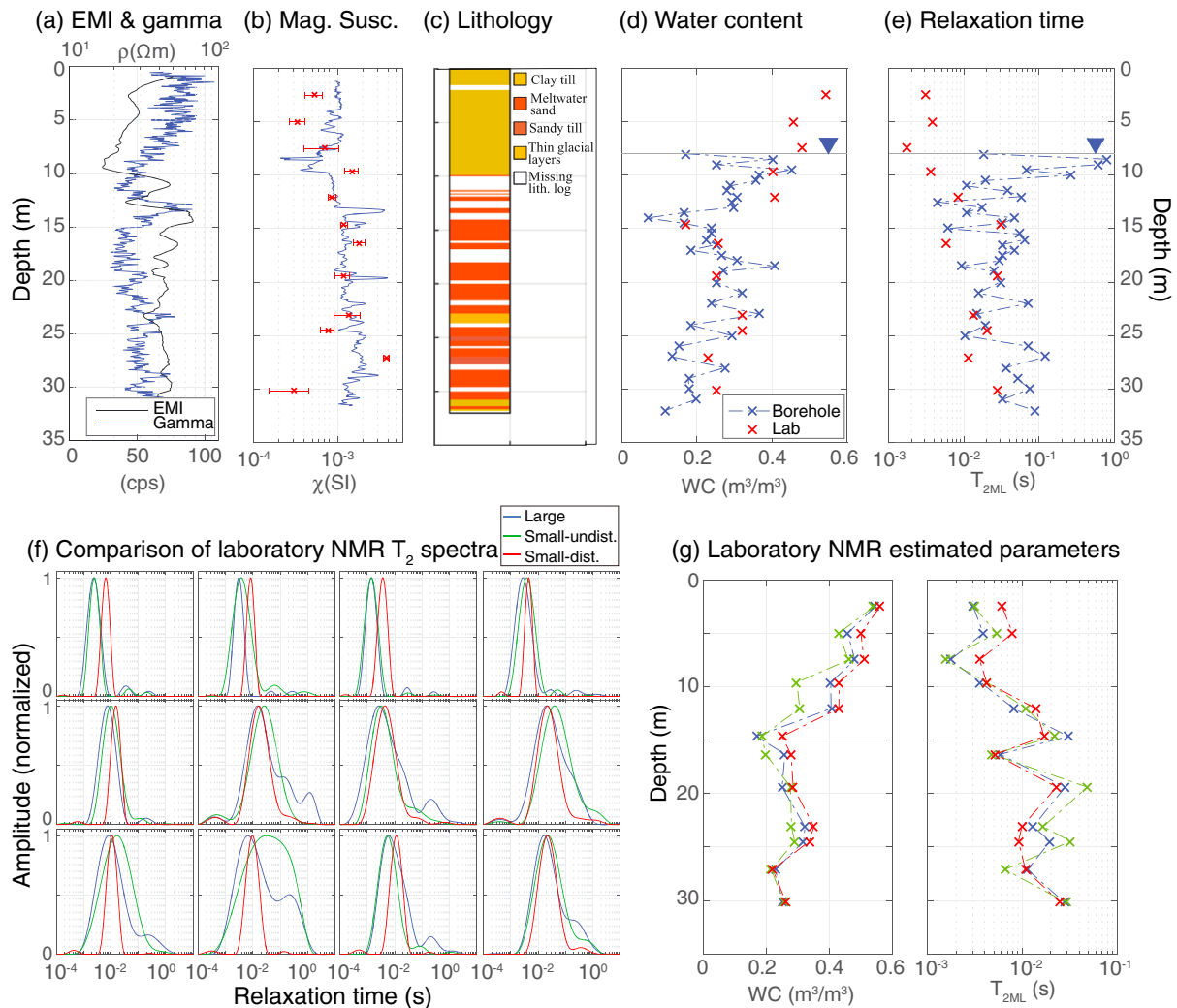
After the NMR measurements, we collected volumetric magnetic susceptibility data to assess the magnetic properties of the laboratory samples and to compare them with similar data acquired in the borehole. These data were measured on four 20 mL subsamples, and the measurements were repeated more than 3 times, with the average value and standard deviation reported.

#### 4. Results and Discussion

In this section we present and discuss the results of our laboratory and logging NMR measurements along with complementary data collected in the laboratory and borehole and the lithologic log. The natural gamma (blue—bottom x axis) and EM induction (black—top x axis) logs are shown in Figure 1a. These logs are acquired for the entire depth of the borehole and at a depth increment of 5 cm. Figure 1b displays the continuous magnetic susceptibility log (blue) and the volumetric susceptibility data measured on the 12 laboratory NMR samples (red). Red error bars show one standard deviation interval. As mentioned earlier, these data were measured to gain insight into the level and variation of the susceptibility in the subsurface. The lithologic log is shown in Figure 1c. There are mainly clay/till units in the upper 9.8 m; the unit below is identified as a sandy aquifer. Thin sandy till and glacial layers (of alternating sand and clay) are also observed within the aquifer. Figure 1d shows the water content estimates from the NMR laboratory and logging measurements as red and blue crosses, respectively. Estimates of laboratory water content were obtained by calibration of the NMR initial amplitude data with those obtained from a sample with known water volume. The relaxation time estimates are in Figure 1e, with the laboratory results shown as red crosses and the logging as blue crosses. In Figure 1f, we present laboratory  $T_2$  distributions obtained from the inversion of the NMR data from the large samples (blue), small-undisturbed samples (green), and small-disturbed samples (red). Finally, to get a quantitative comparison of the sampling techniques, Figure 1g compares water contents and  $T_{2ML}$  values for each sample. The same colors as in Figure 1f are used to display the data. The y axis shows depths in the borehole at which the samples were taken.

The gamma log (Figure 1a, blue) shows relatively high values in the upper ~10 m then decreases to reach an almost constant level below 10 m with the exception of a 2–3 m thick layer at ~ 12 m depth with higher values. The EM induction log (Figure 1a, black) shows a low resistivity layer in the uppermost part of the borehole (top ~10 m) that transitions to more resistive values toward the bottom of the borehole. A lower resistivity layer is observed at a depth of ~ 12 m, which is consistent with the rise in the gamma log at the same depth. The laboratory susceptibility data (Figure 1b, red) generally agree with the logging data (Figure 1b, blue). Overall, the measurements shown in Figures 1a and 1b are compatible with what we see in the lithologic log shown in Figure 1c.

Let us now compare the laboratory and logging NMR water content estimates shown in Figure 1d. Above the water table (blue triangle) the logging NMR data were dominated by noise and are thus not reliable. We assume that the laboratory NMR measurements, however, do accurately measure water content and see the high water content that would be expected in the clay-rich samples; note that these samples were fully water saturated, not measured in the unsaturated state they were in at the field site. Beneath the water table, the water content estimates from the laboratory and logging NMR measurements display very similar trends. The laboratory samples at 12.05 m, 27.1 m, and 30.2 m show water content values greater than estimated from the NMR logging (at closest corresponding depths of 12.0 m, 27.0 m, and 30.0 m, respectively), with absolute differences of 0.10 m<sup>3</sup>/m<sup>3</sup>, 0.09 m<sup>3</sup>/m<sup>3</sup>, and 0.07 m<sup>3</sup>/m<sup>3</sup>. The simplest explanation is that the sampling for the laboratory study acquired material in a zone within the logging NMR sampled volume



**Figure 1.** Results of laboratory and logging measurements. (a) Natural gamma (blue) and EM induction (black) logs. (b) Continuous magnetic susceptibility log (blue) and volumetric susceptibility data measured in the laboratory (red). Error bars show 1 standard deviation intervals. (c) Lithologic log. Logging (blue) and laboratory (red) NMR estimated (d) water contents and (e) relaxation times. The water table is shown with a blue triangle. (f)  $T_2$  distributions obtained from inversion of the laboratory large (blue), small-undisturbed samples (green), and small-disturbed samples (red) data. The spectra are normalized to their peak values. (g) Comparison of the laboratory NMR  $T_2$  distributions in terms of the water contents and relaxation time estimates. Same colors as in Figure 1f are used to display the data. The y axis shows depths in the borehole at which the samples were taken.

that consists primarily of finer-grained material. This explanation is supported by the relaxation time data (discussed below) where corresponding laboratory  $T_{2ML}$  values are shorter than logging  $T_{2ML}$  values.

With respect to the laboratory and logging NMR relaxation time estimates (Figure 1e), as mentioned in discussing Figure 1d, above the water table the logging NMR data are not reliable. In the laboratory NMR data we see low  $T_{2ML}$  values that correspond well to the clay unit seen in the lithologic log. Below the water table, we observe very good agreement between the two data sets. Given the challenges faced when working in unconsolidated environments and the scale difference between the laboratory and logging samples, we consider this to be a significant achievement. With the exception of the three data points (depths of 9.6 m, 16.3 m, and 27.1 m), the absolute differences between the two measurements are 47 ms at one depth and between 0.3 ms and 3.7 ms at all other depths.

The three samples with laboratory  $T_{2ML}$  values notably shorter than the logging values had laboratory-measured magnetic susceptibilities higher than the logging-measured values, suggesting that the sampling for the laboratory study acquired material in a zone with higher-than-average iron content (i.e., the averaged iron content within the logging NMR sampled volume). The presence of iron minerals can result in the

formation of internal magnetic field gradients (Brown, 1961), which can enhance the relaxation due to diffusion, leading to shorter measured  $T_{2ML}$ . We hypothesize that this is responsible for the observed differences. We note that if the iron content were the same in the materials sampled by the laboratory and logging instruments, we would expect the impact of diffusion relaxation on the two measurements to be the same, resulting in no difference in the measured  $T_{2ML}$ . The magnitude of internal gradients is affected by the background magnetic field strength and the echo spacing, but, as shown in Fay et al. (2015), for the combination of field strengths and echo spacing used in this study (2 MHz and 0.3 ms for the laboratory data;  $\sim$ 0.3 MHz and 2 ms for the logging data), the internal field contribution to the  $T_2$  measurements should be the same.

At the start of this study we questioned whether the laboratory samples, typically acquired with standard drilling and sampling procedures, are representative of the material sampled by logging NMR measurements, given their relatively small size of 40 cm<sup>3</sup> or less. Our sampling strategy, in contrast, obtains samples that are 10 times larger than this, so are more likely to be similar in internal structure to that of the in situ materials. Figure 1f allows us to compare, qualitatively,  $T_2$  distributions obtained from the inversion of the NMR data from the large samples (blue), small-undisturbed samples (green), and small-disturbed samples (red). We emphasize here that a similar SNR was achieved for all laboratory data in Figure 1f. The results are shown for samples at different depths from top (top left panel) to the bottom (bottom right panel) of the borehole. We observe that the  $T_2$  distributions for the large- and small-undisturbed samples are similar at shallow depths but differ both in shape and  $T_2$  values at depth. The reason for this is that the shallow units are relatively homogeneous and composed primarily of well-sorted materials. Therefore, similar composition and pore structure will be present in the large samples and the small-undisturbed samples. In contrast, the aquifer materials are composed of materials with different grain sizes including sands and gravels. As a result, the small-undisturbed samples are very likely to have compositions and pore structures that differ from those of the large samples.

Greater differences are observed between the large samples and the small-disturbed samples (red). Symmetric and narrow distributions are obtained for the disturbed samples across the entire depth; sampling "disturbed" materials results in samples that are more homogeneous than the in situ formations. For the shallowest depths, there is a shift toward longer relaxation times, because the clay-rich disturbed samples are less compacted than in situ formations; for deeper depths, the shape of the distribution is also altered, because disturbed samples are composed of materials with different grain size distributions.

Although there is a change in the regularization parameters in Table 1, we observe no correlation between high and low regularization and differences between the distributions of the samples in terms of broadness and peak positions. Consequently, the difference between the distributions can be associated with a change in the samples.

Comparison of the laboratory NMR  $T_2$  distributions in terms of the water contents and relaxation time estimates, as shown in Figure 1g, also demonstrates how the estimated parameters can vary depending on the sampling techniques. For the samples used in this study, the absolute water content and relaxation time differences of up to 0.13 m<sup>3</sup>/m<sup>3</sup> and 25.7 ms are observed between the measurements. The results in Figures 1f and 1g clearly demonstrate that both sample size and condition can influence the results. We expect that other problems with typical sampling of near-surface materials (e.g., inexact depth attribution and changes in the sediment properties) may result in even more biased estimates of the NMR parameters.

This study has clearly demonstrated that the combination of sonic drilling, along with careful collection and preparation of laboratory samples, can provide a data set of the quality needed when using laboratory measurements to support the interpretation of logging NMR data.

## 5. Conclusions

This study addresses the main challenges inherent in conducting laboratory and logging NMR in unconsolidated near-surface aquifers: the borehole conditions and the sample conditions and size. We present a detailed comparison of laboratory and logging NMR data from a study site in Denmark, under conditions intended to provide laboratory samples that are as representative as possible of the in situ materials. We

found sonic drilling to be a suitable drilling method. It is known to produce essentially no disturbed zone around the PVC casing and provide continuous, undisturbed samples of the unconsolidated materials. With this and with our careful sample preparation, the results of our study show good agreement between the logging and laboratory NMR estimated water contents and relaxation times.

We investigated the influence of sample size and condition by acquiring NMR data on two sets of undisturbed and disturbed smaller subsamples (comparable in size to standard laboratory NMR sample sizes). When the  $T_2$  distributions of the small-disturbed and small-undisturbed samples were compared to the  $T_2$  distributions of the large samples, we observed different distributions both in shape and time. We conclude that larger samples should be used for laboratory NMR experiments and that repacking of samples has a large impact on the NMR measurements.

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### References

- Barrow, J. C. (1994). The resonant sonic drilling method: An innovative technology for environmental restoration programs. *Ground Water Monitoring & Remediation*, 14(2), 153–160. <https://doi.org/10.1111/j.1745-6592.1994.tb00110.x>
- Behroozmand, A. A., Keating, K., & Auken, E. (2015). A review of the principles and applications of the NMR technique for near-surface characterization. *Surveys in Geophysics*, 36(1), 27–85. <https://doi.org/10.1007/s10712-014-9304-0>
- Bird, N. R. A., Preston, A. R., Randall, E. W., Whalley, W. R., & Whitmore, A. P. (2005). Measurement of the size distribution of water-filled pores at different matric potentials by stray field nuclear magnetic resonance. *European Journal of Soil Science*, 56(1), 135–143. <https://doi.org/10.1111/j.1351-0754.2004.00658.x>
- Brown, R. J. S. (1961). Distribution of fields from randomly placed dipoles: Free-precession signal decay as result of magnetic grains. *Physical Review*, 121(5), 1379–1382. <https://doi.org/10.1103/PhysRev.121.1379>
- Brownstein, K. R., & Tarr, C. E. (1979). Importance of classical diffusion in NMR studies of water in biological cells. *Physical Review A*, 19(6), 2446–2453. <https://doi.org/10.1103/PhysRevA.19.2446>
- Butler, D. (2005). Near-surface geophysics. *Society of Exploration Geophysicists* (758 pp.). <https://doi.org/10.1190/1.9781560801719>
- Carr, H. Y., & Purcell, E. M. (1954). Effects of diffusion on free precession in nuclear magnetic resonance experiments. *Physical Review*, 94(3), 630–638. <https://doi.org/10.1103/PhysRev.94.630>
- Coates, G. R., & Dumanoir, J. L. (1974). New approach to improved log-derived permeability. *Logic and Analysis*, 15, 17–31.
- Coates, G. R., Xiao, L., & Prammer, M. G. (1999). *NMR logging: Principles and applications*. Houston: Haliburton Energy Services.
- Daigle, H., & Dugan, B. (2009). Extending NMR data for permeability estimation in fine-grained sediments. *Marine and Petroleum Geology*, 26(8), 1419–1427. <https://doi.org/10.1016/j.marpetgeo.2009.02.008>
- Daigle, H., & Dugan, B. (2011). An improved technique for computing permeability from NMR measurements in mudstones. *Journal of Geophysical Research*, 116, B08101. <https://doi.org/10.1029/2011JB008353>
- Daigle, H., Thomas, B., Rowe, H., & Nieto, M. (2014). Nuclear magnetic resonance characterization of shallow marine sediments from the Nankai Trough, Integrated Ocean Drilling Program Expedition 333. *Journal of Geophysical Research: Solid Earth*, 119, 2631–2650. <https://doi.org/10.1002/2013JB010784>
- Dlubac, K., Knight, R., & Keating, K. (2014). A numerical study of the relationship between NMR relaxation and permeability in sands and gravels. *Near Surface Geophysics*, 12(2), 219–230. <https://doi.org/10.3997/1873-0604.2013042>
- Dlubac, K., Knight, R., Song, Y., Bachman, N., Grau, B., Cannia, J., & Williams, J. (2013). Use of NMR logging to obtain estimates of hydraulic conductivity in the High Plains aquifer, Nebraska, USA. *Water Resources Research*, 49, 1871–1886. <https://doi.org/10.1002/wrcr.20151>
- Dlugosch, R., Günther, T., Müller-Petke, M., & Yaramanci, U. (2013). Improved prediction of hydraulic conductivity for coarse-grained, unconsolidated material from nuclear magnetic resonance. *Geophysics*, 78(4), EN55–EN64. <https://doi.org/10.1190/geo2012-0187.1>
- Dunn, K.-J., Bergman, D. J., & Latorraca, G. A. (2002). *Nuclear magnetic resonance: Petrophysical and logging applications*. Pergamon.
- Falzone, S., & Keating, K. (2016). The NMR relaxation response of unconsolidated sediments during drainage and imbibition. *Vadose Zone Journal*, 15(6), 1–13. <https://doi.org/10.2136/vzj2015.11.0153>
- Fay, E., Knight, R., & Song, Y. (2015). Investigating internal magnetic field gradients in aquifer sediments. *Geophysics*, 80(3), D281–D294. <https://doi.org/10.1190/geo2014-0445.1>
- Hinedi, Z. R., Chang, A. C., Anderson, M. A., & Borchardt, D. B. (1997). Quantification of microporosity by nuclear magnetic resonance relaxation of water imbibed in porous media. *Water Resources Research*, 33(12), 2697–2704. <https://doi.org/10.1029/97WR02408>
- Høyer, A.-S., Jørgensen, F., Sandersen, P. B. E., Viezzoli, A., & Møller, I. (2015). 3D geological modelling of a complex buried-valley network delineated from borehole and AEM data. *Journal of Applied Geophysics*, 122, 94–102. <https://doi.org/10.1016/j.jappgeo.2015.09.004>
- Hürlimann, M. D. (1998). Effective gradients in porous media due to susceptibility differences. *Journal of Magnetic Resonance*, 131(2), 232–240. <https://doi.org/10.1006/jmre.1998.1364>
- Jørgensen, F., Sandersen, P. B. E., & Auken, E. (2003). Imaging buried quaternary valleys using the transient electromagnetic method. *Journal of Applied Geophysics*, 53(4), 199–213. <https://doi.org/10.1016/j.jappgeo.2003.08.016>
- Kenyon, W. E., Day, P. I., Straley, C., & Willemsen, J. F. (1988). Three-part study of NMR longitudinal relaxation properties of water-saturated sandstones. *SPE Formation Evaluation*, 3(03), 622–636. <https://doi.org/10.2118/15643-PA>
- Kleinberg, R. L., & Jackson, J. A. (2001). An introduction to the history of NMR well logging. *Concepts in Magnetic Resonance*, 13(6), 340–342. <https://doi.org/10.1002/cmr.1018>
- Knight, R., Walsh, D. O., Butler, J. J., Grunewald, E., Liu, G., Parsekian, A. D., ... Barrows, M. (2016). NMR logging to estimate hydraulic conductivity in unconsolidated aquifers. *Groundwater*, 54(1), 104–114. <https://doi.org/10.1111/gwat.12324>
- Kobr, M., Mareš, S., & Paillet, F. (2005). Geophysical well logging. In Y. Rubin & S. S. Hubbard (Eds.), *Hydrogeophysics* (pp. 291–331). Netherlands: Springer. [https://doi.org/10.1007/1-4020-3102-5\\_10](https://doi.org/10.1007/1-4020-3102-5_10)
- Lawrie, K. C., Brodie, R. S., Dillon, P., Tan, K. P., Gibson, D., Magee, J., ... Levett, K. (2012). BHMAR Project: Assessment of conjunctive water supply options involving Managed Aquifer Recharge options at Menindee Lakes (499 pp.). Geoscience Australia Record 2012/13.
- Legchenko, A., Baltassat, J.-M., Bobachev, A., Martin, C., Robain, H., & Vouillamoz, J.-M. (2004). Magnetic resonance sounding applied to aquifer characterization. *Ground Water*, 42(3), 363–373. <https://doi.org/10.1111/j.1745-6584.2004.tb02684.x>



- Meiboom, S., & Gill, D. (1958). Modified spin-echo method for measuring nuclear relaxation times. *Review of Scientific Instruments*, 29(8), 688–691. <https://doi.org/10.1063/1.1716296>
- Mitchell, J., Chandrasekera, T. C., Johns, M. L., Gladden, L. F., & Fordham, E. J. (2010). Nuclear magnetic resonance relaxation and diffusion in the presence of internal gradients: The effect of magnetic field strength. *Physical Review. E, Statistical, Nonlinear, and Soft Matter Physics*, 81(2), 026101. <https://doi.org/10.1103/PhysRevE.81.026101>
- Müller-Petke, M., Dlugosch, R., Lehmann-Horn, J., & Ronczka, M. (2015). Nuclear magnetic resonance average pore-size estimations outside the fast-diffusion regime. *Geophysics*, 80(3), D195–D206. <https://doi.org/10.1190/geo2014-0167.1>
- Ruda, T., & Farrar, J. (2006). Environmental drilling for soil sampling, rock coring, borehole logging, and monitoring well installation. In *Practical handbook of environmental site characterization and ground-water monitoring* (Second ed., Vol. 1–0, pp. 297–344). Boca Rato, FL: CRC Press. Retrieved from <https://doi.org/http://www.crcnetbase.com/doi/abs/10.1201/9781420032246.ch5>
- Schubert, G. (Ed) (2015). *Treatise on geophysics, second edition*, (Vol. 11). Oxford: Elsevier.
- SeEVERS, D. O. (1966). A nuclear magnetic method for determining the permeability of sandstones. Presented at the paper L presented at the SPWLA 7th annual logging symposium, Soc. of Petrophys. And well Logic and Analysis Retrieved from <https://www.onepetro.org/conference-paper/SPWLA-1966-L>
- Timur, A. (1969). Producibility porosity and permeability of sandstone investigated through nuclear magnetic resonance principles. *The Log Analyst*, 10(1), 3–11.
- Vilhelmsen, T. N., Behroozmand, A. A., Christensen, S., & Nielsen, T. H. (2014). Joint inversion of aquifer test, MRS, and TEM data. *Water Resources Research*, 50, 3956–3975. <https://doi.org/10.1002/2013WR014679>
- Walsh, D., Turner, P., Grunewald, E., Zhang, H., Butler, J. J., Reboulet, E., ... Fitzpatrick, A. (2013). A small-diameter NMR logging tool for groundwater investigations. *Ground Water*, 51(6), 914–926. <https://doi.org/10.1111/gwat.12024>
- Washburn, K. E., Eccles, C. D., & Callaghan, P. T. (2008). The dependence on magnetic field strength of correlated internal gradient relaxation time distributions in heterogeneous materials. *Journal of Magnetic Resonance*, 194(1), 33–40. <https://doi.org/10.1016/j.jmr.2008.05.025>
- Whittall, K. P., Bronskill, M. J., & Henkelman, R. M. (1991). Investigation of analysis techniques for complicated NMR relaxation data. *Journal of Magnetic Resonance* (1969), 95(2), 221–234. [https://doi.org/10.1016/0022-2364\(91\)90213-D](https://doi.org/10.1016/0022-2364(91)90213-D)