First Measurements of Surface Nuclear Magnetic Resonance Signals Without an Oscillating Excitation Pulse – Exploiting Non-Adiabatic Prepolarization Switch-Off

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Abstract Recently, small-scale surface nuclear magnetic resonance (SNMR) measurements with a footprint of about a few square meters have gained interest in the soil geophysics community as they directly provide water content and pore geometry information. Here, the application of strong prepolarization (PP) fields enables the detection of water in the vadose zone. Introducing PP into SNMR shifts the reference for the decay of the SNMR signal from the excitation pulse to the end of the PP, effectively increasing the instrumental dead time, which is already too long to measure short signals associated with unsaturated fine-grained soil. In an approach to overcome this limitation, we present the first measurements of SNMR signals from a water reservoir without an oscillating excitation pulse. Instead, we use the non-adiabatic, that is, imperfect, switch-off of the PP-field as an effective excitation mechanism. We complement our field experiments with numerical simulations of the corresponding SNMR spin dynamics.

Plain Language Summary Surface nuclear magnetic resonance (SNMR) is a geophysical method that can directly detect water in the subsurface. Typically, an electromagnetic pulse at a frequency determined by the local Earth’s magnetic field is applied to stimulate the water molecules. After this excitation, the water molecules relax to their equilibrium state and thereby generate a measurable signal at the surface. Water stored in small pores generates a short signal, whereas water stored in larger pores generates a longer signal. When small cable layouts are used to investigate the upper few meters of the soil, a strong prepolarizing (PP) magnetic field prior to the electromagnetic pulse is needed to amplify the response of the water molecules. We have successfully tested a new measurement approach to stimulate the water molecules without an oscillating electromagnetic pulse. Instead, we used the switch-off of the strong magnetic PP-field as an effective excitation. This should not only enable the development of simpler, and therefore cheaper, SNMR-PP devices but also the detection of water stored in very small pores. This is because in our approach the overall excitation time is significantly shorter compared to the classical stimulation, which employs an electromagnetic pulse.

1. Introduction

Surface nuclear magnetic resonance (SNMR) is a well-established method for groundwater exploration and non-invasive aquifer characterization (Costabel et al., 2017; Legchenko et al., 2004; Müller-Petke & Yaramanci, 2015; Vilhelmsen et al., 2016). Its main benefit is the direct sensitivity towards the hydrogen proton spin magnetization of the water molecule and therefore the ability to detect mobile pore water, that is, groundwater in sufficiently large pores. The amplitude of the spin magnetization linearly depends on the number of excited protons and thus on the amount of water in the sensitive area of the loop configuration on the surface (Behrozmand et al., 2014; Legchenko & Valla, 2002; Müller-Petke & Yaramanci, 2015). Whereas most of the SNMR case studies in the literature are related to the saturated zone, few studies focus on specific vadose zone characteristics and their corresponding water dynamics (Costabel & Günther, 2014; Legchenko et al., 2020; Walsh et al., 2014). This is mainly because the conventionally measured signal strength scales with the dimension of the surface loop layout. Hence, a signal from a small surface loop with a diameter of one to two meters can only be observed after long averaging, which in turn is too time-consuming for practical applications (Costabel, 2019). The introduction of the prepolarization (PP) technique into SNMR is expected to overcome this limitation.

The PP technique is usually applied in Earth’s field magnetic resonance at the laboratory scale (Callaghan et al., 1997; Melton & Pollak, 1971; Packard & Varian, 1954; Planinšič et al., 1994). Prepolarization adds a strong static polarizing magnetic field \( B_{pp} \) to the primary Earth’s magnetic field \( B_0 \) to increase the weak NMR
signal. Generally, an adiabatic switch-off of the PP-field is desired because it aligns the magnetization components perfectly parallel with the homogeneous background field. Subsequently, this enhanced magnetization can be conveniently stimulated from an equilibrium-like state by an oscillating excitation pulse.

In the context of the geophysical application of prepolarized SNMR (SNMR-PP), a few theoretical and experimental studies have been published recently. While de Pasquale and Mohnke (2014) assumed the ratio $B_{pp}/B_0$ to be the predominant amplification factor, Hiller et al. (2020) have shown that, depending on the surface loop layout and $B_0$ inclination, this concept of modeling the SNMR-PP amplitudes is insufficient for a realistic PP switch-off. This leads to large misinterpretations regarding the observed water content, if the switch-off characteristics, especially close to the PP-loop, are not properly accounted for. Besides promising experiments on water reservoirs by Costabel et al. (2019) and Lin et al. (2018) that show a signal amplification of up to five fold at a depth of about 1 m when using a measurement setup with a PP-loop diameter of 2 m, Hiller et al. (2021) have additionally shown the feasibility of SNMR-PP to measure reliable signals from the uppermost few decimeters of the soil. In addition, while not being a classical geophysical SNMR-PP application in terms of soil moisture characterization, the detection of oil under sea ice from a mobile, helicopter-borne NMR device also makes use of PP to amplify the measured NMR signals (Altobelli et al., 2019; Conradi et al., 2018).

However, a general limitation of SNMR-PP applications is the several milliseconds up to tens of milliseconds long dead time between the end of the PP and the record of the corresponding NMR signal. As sketched in Figure 1a, this dead time consists of the PP switch-off ramp (green solid), the alternating current electromagnetic pulse to excite the proton spins (black solid) and two wait time intervals (black dashed) after the PP switch-off ramp and excitation pulse, respectively. The two wait time intervals are needed to protect the electronic parts from high voltage pulses due to the fast switching of the PP or excitation pulse currents. Depending on the $T_1$ and $T_2^*$ relaxation times, this effective PP dead time prevents the detection of very fast decaying NMR signals related to clay- or other tightly bound pore water, which are therefore generally excluded from SNMR results (Costabel et al., 2017; Legchenko et al., 2004; Müller-Petke et al., 2011). This effect is expected to be even more pronounced in the vadose zone, where the pores are generally not fully saturated and therefore exhibit very short relaxation times. This was demonstrated by Hiller et al. (2021), where the authors used supporting laboratory NMR data to determine the amplitude loss due to the effective PP dead time to be about 60%. One possibility to overcome the effective PP dead time limitation may be the development of future SNMR-PP devices with more advanced electronic components that enable an operation at higher excitation pulse currents and hence, shorter excitation pulses and wait times. However, a more straightforward approach would be to significantly reduce the effective PP dead time by not applying an excitation pulse at all (cf. Figure 1b). In line with the classical approach of Packard and Varian (1954) and encouraged by the findings of Hiller et al. (2020), we hypothesized that it should be possible to utilize a non-adiabatic PP switch-off as an alternative excitation mechanism. That is, under realistic conditions a PP switch-off is never perfectly adiabatic over the whole subsurface volume, and therefore, always creates magnetization components that are not parallel to $B_0$ after the PP switch-off. This is especially true for short PP switch-off ramps. Consequently, these perpendicular magnetization components precess about $B_0$ and generate a measurable free induction decay (FID) at the local Larmor frequency $f_L \propto B_0$.

In this letter, we present the first experimental measurements of SNMR-PP signals without an oscillating excitation pulse. We support our experimental findings by employing full spin dynamics simulations of the magnetization evolution during and after the PP switch-off and, by doing so, we demonstrate that the method can be used to effectively quantify soil moisture content.

2. Experimental Setup

To easily control the experimental conditions, we conducted our experiment on a water reservoir: that is, a commercially available swimming pool made of plastic (Figure 1c). The pool has a diameter of 5.4 m and at its maximum, the height of the water body inside the pool was about 0.9 m with an accuracy of about ±0.01 m. To conduct SNMR-PP measurements at different water levels, the water was lowered in steps of about 0.05 m to a maximum distance between the platform and the water surface of 0.25 m. The pool was installed on the Test Site for Technical Safety of the Federal Institute for Materials Research and Testing in Horstwalde, about 70 km south of Berlin (Germany). A detailed description of the site and measurement conditions can be found in Hiller et al. (2021).
In this study, we use a device which is optimized for shallow investigations at depths not larger than 10 m (Radic, 2009; Radic & Lehmann-Horn, 2011). A PP-module is available as optional add-on, which generates a strong direct current in a multi-turn copper cable coil for an adjustable duration of a few seconds. For the utilized circular PP-loop, with a mean diameter of 1.6 m and 63 turns, this leads to an effective current of almost 1,150 A (18.2 A per turn) corresponding to a magnetic field $B_{PP}$ of about 1,000 μT in the center of the loop setup and about 200 μT at a depth of 1 m (Hiller et al., 2020). As it can be seen from Figure 1c, we installed the PP-loop in a spiral manner with an average diameter of 1.6 m; note, that not all layouts used in this study are visible in the photograph in panel (c); the colors used in panel (d) conform to the colors used in Figures 3c–3f to present the results.

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We use two different receiver (Rx) loop configurations. The first one is a simple circular Rx-loop setup with diameters for the individual loops ranging from 1 to 2.1 m and being concentrically installed with the PP-loop (cf. Figure 1d dashed circles). The second one is a set of Figure-Of-Eight (FOE) loops that are either inside the PP-loop (oriented north-south or west-east) or placed asymmetrically at the PP-loop cable with one eye of the FOE-loop inside and one eye outside, respectively (cf. Figure 1d solid circles). Due to the spatial extent of the FOE-loop, we refer to the latter type as separated FOE-loop. FOE-loops have successfully been applied before for SNMR measurements as they directly increase the signal-to-noise ratio due to their noise reduction capabilities (e.g., Girard et al., 2020; Trushkin et al., 1994). This may be advantageous for future mobile applications, where noise compensation with reference loops might not be possible. In contrast to the separated FOE-loop, we expect a decreased signal quality for the interior FOE-loops. Especially in the case of the west-east FOE-loop (blue), which should be least influenced by an asymmetry due to the local $B_0$ inclination, almost similar values (as probed by each FOE eye) are subtracted from each other and should therefore result in very small signal amplitudes.

Our measurement protocol is sketched in Figure 1b. After an on-time of 5 s (blue), the PP-field is switched-off within 1 ms (green). The effective PP dead time in our setup is 10.5 ms, because the device we are using is originally not designed to be used without an oscillating excitation pulse and its measurement protocol enforces certain timings that need to be obeyed (Hiller et al., 2021). We expect that the effective PP dead time can be shortened to the length of the PP switch-off ramp, that is, few ms, in an optimized device. The resulting FID was recorded for about 1.3 s (red).

Please note that the build-up of the enhanced magnetization $M_{pp}$ does not happen instantaneously but with a relaxation time constant $T_1$ (e.g., Levitt, 2002). Therefore, the PP on-time of 5 s just achieves about 97.5% effectiveness due to the increased $T_1 = 1.35$s relaxation time of the bulk water inside the pool. We account for this difference (about 2.5%) in the evaluation of the results by applying the same correction as described in Hiller et al. (2021). This correction is not necessary for soil measurements, where due to the shorter relaxation times, a shorter PP on-time is sufficient to reach 100% effectiveness (e.g., 0.5 s for $T_1 = 100$ ms).

### 3. Forward Modeling

To evaluate the measurement results, the experimental conditions are reproduced inside the SNMR-PP forward modeling as accurate as possible. The spatial distribution of perpendicular magnetization components $M_{pp}^\perp$ in the subsurface depends strongly on the local PP-field strength, the relative orientation between $B_{pp}$ and $B_0$, and the applied PP switch-off ramp characteristics (ramp shape and ramp time) (Hiller et al., 2020). The time evolution of $B_{pp}$ after the PP switch-off is modeled with the software BLOCHUS (Hiller, 2020) and uses the macroscopic Bloch equations (Bloch, 1946) to account for the full spin dynamics. Subsequently, the general form of the sensitivity kernel for separated transmitter and receiver loops, as given by for example, Hertrich (2008), is adapted to

$$K(r) = 2\omega_0 M_{pp}^\perp \times [B_{0}^\perp(r) \cdot \exp[i(\zeta_{pp}(r) + \zeta_{R}(r)))]$$

$$\times [b^\perp_{R}(r) \cdot b_{pp}^\perp(r) + i b_0 \cdot (b_{R}(r) \times b_{pp}^\perp(r))],$$

where $B_{0}^\perp$ is the counter-rotating (rotating against the spin precession direction) part of the Rx-field. The subscripts PP and R denote components belonging either to the PP- or Rx-loop, respectively. The phases $\zeta_{pp}$ and $\zeta_{R}$ in the exponential term in Equation 1 account for phase lags associated with subsurface conductivity structures. The unit vectors $b_{pp}^\perp$, $b_{pp}^\perp$, and $b_{R}$ in the third row of Equation 1 account for the relative orientations of PP-loop, Rx-loop and Earth’s magnetic field, respectively. Note that the spin dynamics simulation of $M_{pp}$ is carried out in a local Bloch frame where the azimuthal angle between the PP-axis and positive x-axis is always 0°. By doing so, we can directly adapt the notation of the classical SNMR kernel with excitation pulse and replace the excitation term with $M_{pp}^\perp$, which is the component of $M_{pp}$ perpendicular to $B_{0}^\perp$. Furthermore, note that $M_{pp}^\perp$ in Equation 1 is complex valued because we use the x- and y-components of $M_{pp}$ after the PP switch-off as real and imaginary parts. In this study, this has no practical consequences, as we are only interested in the absolute value of the kernel and the
corresponding SNMR-PP signals. The initial amplitude \( s_0 = \int K(r) w(r) \, dr \) of the FID is then given by the integral product of the sensitivity kernel and the water content distribution \( w(r) \). All \( B \)-field and kernel calculations were performed with MRSMatlab (Müller-Petke et al., 2016).

To present the spatial sensitivity of our approach, Figure 2 shows four vertical slices out of the three-dimensional sensitivity kernel for two different field setups. For both scenarios, the kernel calculation was carried out with a PP-loop with a mean diameter of 1.6 m and an effective current of 1,150 A being concentric with a Rx-loop (20 turns) with a diameter of 0.8 m. Because of the small scale of the loop configuration, assuming a resistive half-space for the subsurface is a valid simplification. The local Larmor frequency is set to \( f_L = 2110 \text{ Hz} \) and the Earth’s field inclination to 67° as measured on the experimental test site. For visibility reasons all kernel values smaller than \( 10^3 \text{nVm}^{-2} \) or larger than \( 10^7 \text{nVm}^{-2} \) are combined in the colors violet and dark red, respectively. Panels (a + b) show the sensitivity kernel for a positive PP current direction in a south-north and west-east slice, respectively. We define the PP current direction in the following way: if the z-components of the resulting PP-field and the Earth’s magnetic field in the center of the PP-loop have the same sign, then the PP current direction is positive (PP+). Correspondingly, if the signs are different, then the PP current direction is negative (PP−). The regions of high sensitivity (red colors) are concentrated very close to the PP-loop and Rx-loop cables. The sensitivity decreases to about 1% of the maximum value at about 0.5 m distance from the PP-loop (yellow colors). For a negative PP current direction (c + d) the sensitivity is generally larger and decreases to about 1% at about 0.8 m distance from the PP-loop. The effect of an increased sensitivity is due to the favorable spatial distribution of relative orientation between the Earth's magnetic field and the PP-field. For the case of negative PP current direction and considering the local Earth's field inclination, there are more perpendicular magnetization components generated inside the PP-loop setup (Hiller et al., 2020).

4. Results

In Figure 3, we present the results of our field experiments and the corresponding forward simulations. To obtain good data quality, the number of measurement repetitions (repetition time: 14.5 s) for circular Rx-loops and FOE-loops was set to 64 and 16, respectively. All field data was processed with standard SNMR post-processing workflows that include for example, despiking, reference noise cancellation, band pass filtering and stacking (Costabel, 2019). As an example for a measurement with a circular Rx-loop, panel (a) shows a measured PP
switch-off ramp (gray circles) and panel (b) the corresponding processed FID (gray) and its mono-exponential fit (black). The black line in panel (a) depicts the simulated PP switch-off ramp that is used for the numerical simulations. The inset in panel (b) depicts the corresponding frequency spectrum of the FID. Both panels impressively show that NMR signal responses with sufficiently large signal-to-noise ratios can be induced by a non-adiabatic switch-off of the PP-field.

In panels (c–f) we plot measured (dots) and forward modeled (dashed lines) initial amplitudes $s_0$ either for circular Rx-loops (c + d) or FOE-loops (e + f) as a function of water table distance for circular (center row) and FOE (bottom row) loop layouts, each for positive (left column) and negative (right column) PP-current directions. The dashed lines in panels (c) to (f) refer to results of the forward modeling.

Figure 3. Panels (a) and (b) show a measured (gray circles) PP switch-off ramp and a processed FID (gray curve) with its corresponding frequency spectrum in an inset; the corresponding data point is marked with a black circle in panel (c); Panels (c–f) show the normalized initial amplitudes $s_0$ as a function of water table distance for circular (center row) and FOE (bottom row) loop layouts, each for positive (left column) and negative (right column) PP-current directions. The dashed lines in panels (c) to (f) refer to results of the forward modeling.
Considering all loop configurations and PP current directions, we see an excellent agreement between the measured and forward modeled data. The forward modeling very well reproduces the overall trend, as well as the relative deviations between the different curves (loop layouts). Sporadic deviations are visible but are limited to a few percent difference and can probably be attributed to minor irregularities in the geometric layout of the loops (cf. Figure 1c). Because of the strong sensitivity close to the PP-loop (cf. Figure 2), the measured amplitudes decrease with an increasing distance between the loops and the water level. For both loop configurations the negative PP current direction has higher signal amplitudes than the positive PP current direction, due to the creation of more perpendicular magnetization components.

For circular Rx-loops and a positive PP current direction (panel c), the majority of perpendicular magnetization components is generated close to the PP-loop cable (cf. Figure 2a + b and Hiller et al., 2020). Therefore, for a high water table, the Rx-loop closest to the PP-loop cable (blue) has the largest amplitude (normalized to the effective loop area). When the water table is lowered, the regions close to the PP-loop cable do not contribute to the signal. Because the sensitivity of the outer Rx-loops (blue and green) focuses in these regions, their amplitude becomes smaller compared to the inner Rx-loop (red) which has a higher sensitivity to regions inside the PP-loop that still get excited. A corresponding effect is visible for the negative PP current direction (panel d) where the outermost Rx-loop (green) again has smaller amplitudes compared to the Rx-loop that is closer to the PP-loop cable (blue). Here, and in contrast to the positive PP current direction, most perpendicular magnetization components are generated closer to the center of the PP-loop (cf. Figure 2c + d and Hiller et al., 2020). Therefore, the inner Rx-loop (red) has always larger amplitudes compared to the outer ones, also for high water tables.

For the FOE-loops (e + f), the strongest signal for both PP current directions, and comparable to the circular Rx-loops, is measured with the separated FOE-loop (red). This is because for this FOE configuration, the orientation of the virtual magnetic Rx-field in the center of each FOE eye (inside and outside of the PP-loop) due to a potential current in the FOE, points in the same direction as the local PP-field and therefore leads to a constructive interference. On the contrary, for the two interior FOE-loops (blue and green), the orientations of the virtual magnetic Rx-fields in the center of each FOE eye point in different directions as the local PP-field. Therefore, this destructive interference will lead to a significantly decreased signal. As expected, for the interior FOE-loops shown in panel (e), the signal quality is also decreased due to the very weak sensitivity. Nevertheless, for example, the dip between 5 and 10 cm visible for the west-east FOE-loop (blue), is also reproduced by the forward simulation and is therefore in turn, a very strong indicator for the quality of our forward model.

5. Discussion

In Figure 3 we have shown that it is possible to detect FIDs due to a non-adiabatic PP-field switch-off. With this approach, we measure an average water content belonging to the corresponding excited subsurface volume of the particular measurement configuration. This obviously has certain advantages and disadvantages and the obtained value assumes a homogeneous water content distribution in the sensitive volume. To us, the most intriguing application is a mobile device that enables a relatively fast soil moisture measurement. With a footprint of about two square meters, it should be possible to sufficiently map the average soil moisture up to depths of about 0.5–1 m. We believe that the benefits of such an approach far outweigh the drawback of a limited depth resolution, even more so, when considering the large spatial heterogeneity of the water distribution in the uppermost soil layers.

However, there may be the potential to gather some kind of spatially resolved soil moisture data. As we have shown, by varying the PP current direction it is possible to probe deeper regions of the subsurface. This approach could be further generalized to not only reverse the PP current direction but to also modify the PP switch-off characteristics. Keeping the PP-loop layout constant and varying for example, PP switch-off ramp shape or length, and thereby varying the adiabatic performance of the switch-off, it may be possible to shift the focus regions below the PP-loop setup. Additionally, also the PP-Rx-loop configurations can be adapted, so that the simultaneous use of multiple Rx-loops leads to an increased spatial resolution. Then, a combined interpretation, or even inversion, should be possible. Now, with the modeling tools at hand, it is possible to review and evaluate such approaches. However, these questions are left for future research.

A new generation of simple and cost-efficient SNMR-PP devices is easily imaginable, if the need for sophisticated transmitter electronics is omitted. Basically, the presented approach only needs electronic components to control the power of the PP-loop and a synchronized receiver, which not necessarily needs to be hardwired to the
PP device. If the receiver unit is able to constantly record incoming data, any dead time, that is the delay between PP switch-off ramp and signal record, is essentially reduced to the length of the PP switch-off ramp. This should be a major improvement over currently available SNMR-PP devices.

6. Conclusions
We have successfully demonstrated the first measurements of surface NMR signals without an oscillating excitation pulse. We have shown that it is possible to exploit a non-adiabatic, that is, imperfect, PP-field switch-off to generate sufficient perpendicular magnetization components, which are recorded at the surface as a free induction decay. Our measurements are supported by forward modeling results that account for the full spin dynamics during the PP switch-off. Furthermore, we have shown that it is possible to excite different regions in the subsurface by for example, reversing the PP current direction and thereby exploiting more favorable B-field orientations. This can be further optimized by the implementation of different loop layouts and/or switch-off characteristics, maybe even to an extent where a rudimentary inversion approach is feasible. The measurement approach presented in this letter may enable the future development of cost-efficient SNMR-PP devices that enable non-invasive and fast soil moisture mapping applications.

Conflict of Interest
The authors declare no conflicts of interest relevant to this study.

Data Availability Statement
Data are available from Zenodo (Hiller, 2021).

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