Designing Adiabatic Pulses for Surface NMR

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SUMMARY

Surface nuclear magnetic resonance (NMR) is a powerful technique providing non-invasive imaging of groundwater. One challenge with the method is that it commonly suffers from low signal to noise ratios (SNR). Two methods to increase SNR are to either develop noise cancellation approaches to reduce the noise level, or to perform the experiment in a manner capable of increasing the signal amplitude. A recent study adopted the latter approach by employing a novel transmit strategy. An adiabatic pulse was employed and observed to produce significant signal improvements compared to the standard transmit method in surface NMR. The advantage of an adiabatic pulse is that it is capable of producing a uniform excitation in the presence of a heterogeneous magnetic field, which describes exactly the transmit conditions in surface NMR.

Given the great potential of adiabatic pulses for surface NMR, we explore several factors related to the design of adiabatic pulses intended for application in surface NMR conditions. We investigate how various adiabatic pulses perform in a heterogeneous magnetic field given the limitation that current instrumentation couples the modulation of the current amplitude during the pulse to the instantaneous transmit frequency. That is, only the duration of the adiabatic sweep, the bandwidth through which the pulse sweeps, and frequency modulation throughout the pulse can be directly controlled. A numerical sensitivity analysis of each of these parameters is performed to gain insight into how to design optimal adiabatic pulses for surface NMR. Additionally, a numerically optimized modulation (NOM) approach is implemented to optimize the frequency sweep. The spatial resolution and depth penetration provided by an example adiabatic pulse is also investigated. A trade off between signal amplitude and spatial resolution is observed to be present when employing adiabatic pulses.

Key words: surface NMR, adiabatic, SNR

INTRODUCTION

Surface nuclear magnetic resonance (NMR) is a geophysical technique capable of non-invasively imaging aquifers. One challenge commonly confronted when using this method is a low signal to noise ratio (SNR). To address this concern two approaches may be employed; the first is the development of noise cancellation techniques better equipped to reduce the noise level (Walsh, 2008; Dalgaard et al., 2012). The second is to perform the survey in a manner that directly produces a larger amplitude signal. A recent study by Grunewald et al., (2015) adopted the second approach, where an adiabatic excitation pulse (Tannus and Garwood, 1997) was implemented in place of the standard on-resonance pulse. They observed a significant enhancement of the signal amplitude when using the adiabatic pulse. The main difference between an adiabatic pulse and the standard pulse type used in surface NMR, called an on-resonance pulse, is that the adiabatic pulse modulates the transmit frequency throughout the duration of the pulse, while the transmit frequency is fixed during an on-resonance pulse. As a result, the net perturbation of the magnetization during an adiabatic pulse is different than that due to an on-resonance pulse. This difference results in the adiabatic pulse having several attractive features. For example, an adiabatic pulse can be designed to provide insensitivity to heterogeneity in the applied magnetic field (B_1 field) (Ugurbil et al., 1987), which can be exploited to improve the signal amplitude in surface NMR (Grunewald et al., 2015).

Given the great potential of adiabatic pulses to enhance SNR in surface NMR we investigate how to optimize adiabatic pulses for performance in surface NMR conditions. Existing instrumentation couples the modulation of the current amplitude during the pulse to the instantaneous transmit frequency. Therefore, adiabatic pulses in surface NMR may be defined by three parameters: 1) the bandwidth of swept frequencies (A), 2) the pulse duration (τ), and 3) the shape of the frequency modulation function. We conduct a sensitivity analysis of the ability of adiabatic pulses to generate a fully transverse magnetization (i.e. maximize the signal amplitude) in the presence of B_1 heterogeneity for varying A and τ to gain insight into how each parameter affects performance in surface NMR conditions. The numerically optimized modulations (NOM) approach (Ugurbil et al., 1987; Rosenfeld et al., 1997) is also implemented to determine the optimal frequency modulation function. The spatial resolution provided by a survey employing an adiabatic pulse is also contrasted against that provided by the standard on-resonance pulse. Results indicate that a trade off between signal amplitude and spatial resolution exists for adiabatic pulses in surface NMR.

EXCITATION IN SURFACE NMR

The surface NMR method provides insight into the spatial distribution of aquifer properties in the subsurface by measuring the properties of a magnetization present in the subsurface. This magnetization originates from the immersion of hydrogen atoms in the Earth's magnetic field. At equilibrium this magnetization is too small to measure directly and must be perturbed out of its equilibrium state in order to generate a measurable NMR signal. This perturbation is accomplished by using a transmit coil at the

surface to generate a secondary magnetic field (B_{eff}) that extends away from the coil into the subsurface. The perturbation of the magnetization due to the presence of the applied magnetic field is governed by the Bloch equation (Bloch, 1946),

$$\frac{\partial \boldsymbol{M}}{\partial t} = \gamma \boldsymbol{M} \times \boldsymbol{B_{eff}} \,. \quad (1)$$

The B_{eff} field induces a precession of the magnetization about an axis oriented in the B_{eff} direction at a rate determined by the magnitude of B_{eff}. We have not included the relaxation terms in equation 1; we consider the case of slow relaxation, where these terms are negligible. This assumption is not always valid, but is taken here for to simplify the discussion. In practise the inclusion of these terms would act to reduce the effectiveness of long duration pulses. Following the transmit pulse the magnetization is in a perturbed state, which contains a component transverse to the direction of the Earth's field. In surface NMR we are only sensitive to the amplitude of this transverse component.

In a reference frame that rotates at the instantaneous transmit frequency, ω_t, the B_{eff} field responsible for rotating the magnetization is described by,

$$\boldsymbol{B_{eff}} = \begin{bmatrix} B_1 \\ 0 \\ \frac{\omega_0 - \omega_t}{\gamma} \end{bmatrix}. \quad (2)$$

The z- and x-axes of this frame are oriented in the direction of the Earth's field and the direction of the applied magnetic field perpendicular to the Earth's field, respectively. The B_1 term represents the amplitude of the secondary field produced by the surface coil, while the magnitude of the z-component of B_{eff} is determined by the difference between the Larmor (ω_0) and transmit frequencies. The γ term is the gyromagnetic ratio of the hydrogen nuclei.

The standard transmit method uses an on-resonance pulse, which produces a current that oscillates at a fixed transmit frequency selected to be equal to the Larmor frequency. In this case, the z-component of the B_{eff} field is equal to zero and the magnetization precesses about an axis oriented in the x-direction. This results in a transverse magnetization oriented either along the +y axis or the –y axis (observed by noting in equation 1 that a magnetization initially oriented along the z-axis is restricted to the y-z plane when the rotation axis is parallel to the x-axis). The presence of transverse magnetization with both positive and negative signs, which is a result of B_1 heterogeneity generating transverse magnetization with both positive and negative y components, leads to destructive interference and signal loss. Given that surface NMR commonly suffers from low SNR, if this destructive interference were eliminated the signal amplitude and consequently the SNR would be improved. To eliminate this destructive interference an adiabatic pulse may be used.

In contrast to the on-resonance pulse, the orientation of the B_{eff} field during an adiabatic pulse varies throughout the duration of the pulse. To rotate the magnetization into the transverse plane, an adiabatic half passage (Bendall and Pegg, 1986)) is employed. This pulse begins with a transmit frequency that is offset from the Larmor frequency in order to produce a B_{eff} field oriented as close to the z-axis as possible (i.e. the z-component in equation 2 is much larger than the x-component). This confines the magnetization's precession to a tiny cone centered about the B_{eff} axis. The transmit frequency is then swept towards the Larmor frequency, and the pulse is terminated when these two frequencies become equal. This results in a B_{eff} axis that collinear with the x-axis at the end of the pulse. If the frequency sweep is performed adiabatically, meaning that the change in the orientation of the B_{eff} axis is much slower than the precessional rate of the magnetization, the magnetization will precess about a small cone oriented along the B_{eff} axis throughout the entire pulse. That is, the magnetization will follow the trajectory of the B_{eff} axis ultimately ending in a final perturbed state oriented in the +x direction. The advantage of the adiabatic pulse arises from the fact that at the end of the pulse, when ω_t=ω_0, the B_{eff} field will be oriented in the x-direction regardless of the amplitude of B_1. This means that as long as the frequency sweep is performed adiabatically the magnetization can be fully rotated into the transverse plane regardless of the B_1 amplitude. Thus, the adiabatic pulse has the potential to increase the signal amplitude for situations where the B_1 field is heterogeneous. Grunewald et al., (2015) demonstrated that this potential for significant signal enhancements when using an adiabatic pulse in surface NMR can be realized in the field, where an adiabatic pulse produced signals that were a factor of 2-3 larger than those produced by an on-resonance pulse.

ADIABATIC PULSES IN SURFACE NMR

Given the potential of adiabatic pulses to improve SNR in surface NMR we investigate the performance of various frequency sweeps in a heterogeneous B_1 field in order to gain insight into how to design adiabatic pulses optimally suited for surface NMR conditions. Current surface NMR hardware allows the user to control the transmit frequency throughout the duration of pulse, but does not allow independent control of the amplitude of the current throughout the pulse. The current can be manipulated from pulse to pulse, but not modulated freely during a single pulse. Instead the current amplitude is determined by the response of the tuned coil when driven off-resonance; that is, the coil quality factor Q will control the extent of the amplitude modulation throughout the pulse. In this situation, the adiabatic sweep is defined by three parameters: 1) the bandwidth (A) swept during the pulse, 2) the pulse duration (τ), and 3) the frequency modulation function that defines how the frequency sweep is performed. We present a sensitivity analysis investigating the performance of an adiabatic pulse in the presence of heterogeneous B_1 (spanning the range of B_1 likely to be encountered in a surface NMR survey) for various A, τ, and frequency modulation functions.

Consider first the impact of the swept bandwidth A, which controls the initial offset between the transmit and Larmor frequencies. In the top row of Figure 1 we illustrate the Mx and My components produced for adiabatic sweeps with various A; the Mx component represents the transverse magnetization collinear with the final B_{eff} orientation, while M_y represents the component of the transverse magnetization orthogonal to the final orientation of B_{eff}. A value of Mx or My equal to 1 indicates that the magnetization has been fully rotated into the transverse plane, equivalent to maximizing the signal amplitude for that given B_1 amplitude. In each case τ=50 ms, Q=5, and the frequency is swept linearly with time (similar to a chirp pulse) from ω_0-A to ω_0 ($\omega_0/2\pi$=2000 Hz). For large A (red line), the adiabatic pulse has a broad Mx profile (Figure 1A) and fully rotates the magnetization into the x-direction for a range of B_1 spaning nearly 2 orders of magnitude. As the A factor decreases the width of the Mx profile narrows and shifts to smaller B_1 amplitudes. The reason for the shift to smaller B_1 is that the rate of change of the B_{eff} axis

is slower for small A given fixed τ; the transmit frequency varies more slowly allowing the adiabatic condition to be satisfied at smaller B_1 amplitudes. Note also the behaviour of the My component, where it initially rises to form a bump at B_1 amplitudes corresponding to the initial rise of Mx profile (the position of the rise on the left hand side of the Mx profile in 1A), and it eventually begins to oscillate rapidly between My equal to +1 and -1 for strong B_1. The bump in the My at lower B_1 amplitudes represents the B_1 range where the magnetization struggles to follow the B_{eff} axis; that is, the precession of the magnetization about the B_{eff} axis is not much larger than rate of change of the orientation of the B_{eff} axis. In contrast, the erratic behaviour observed in the My profile for large B_1 is due to a poor initial condition, where the orientation of B_{eff} at the start of the adiabatic pulse is not along the z-direction giving rise to a precession of the magnetization about a larger cone. This ultimately causes the large My component at the end of the adiabatic pulse since the component of the magnetization collinear with the B_{eff} axis is reduced. This indicates that the A parameter may be varied to target regions of the subsurface with different B_1 amplitudes. For example, small A can be used to target deeper regions where B_1 will be smallest, while large A will be effective at generating large signals from the shallowest depths where the largest B_1 amplitudes are present.

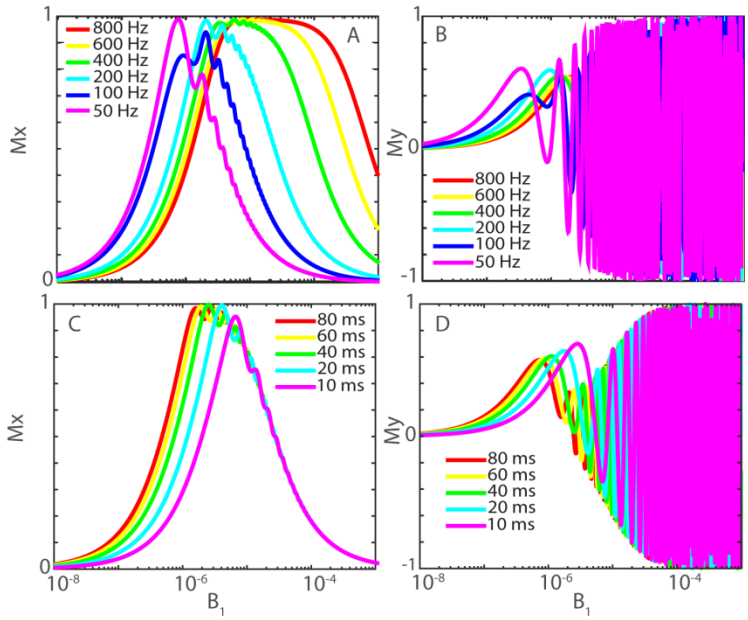

Figure 1. The top row illustrates the performance of adiabatic pulses with τ=50 ms and Q=5, where A/2π is varied from 50 to 800 Hz. The frequency is swept linearly with time. A) and B) indicate the Mx and My components for the varying A case, respectively. The bottom row illustrates the performance of adiabatic pulses with A/2π=200 Hz and Q=5, where τ varies from 10 to 80 ms. The frequency is swept linearly with time. C) and D) indicate the Mx and My components for the varying τ case, respectively.

Consider next the influence of the pulse duration, illustrated in the bottom row of Figure 1. In this case, A/2π=200 Hz, and Q=5 are constant. The frequency is again swept linearly with time beginning at ω_0 - 200Hz*2π and ending at ω_0. Figure 1C indicates that increasing τ extends the Mx profile to smaller B_1 amplitudes, equivalent to increasing depth penetration. The pulse duration also does not appear to have a significant impact on the position of the Mx profile's edge at larger B_1 amplitudes. The My profiles in this case (1D) demonstrate similar behaviour to Figure 1B, where a bump is observed at the same B_1 amplitudes as the rise of the Mx profile (rise of the left side of the Mx profile in 1C) that transitions into a region of quickly oscillating My values at large B_1 amplitudes. This indicates that increasing τ improves performance at low B_1 amplitudes but does not have a significant impact at larger B_1 amplitudes.

The pulses investigated in Figure 1 used a linear frequency sweep, the same type employed by Grunewald et al. (2015). To investigate whether a linear sweep is optimal we employ a technique called numerically optimized modulation (NOM) (Ugurbil et al. 1987, Rosenfeld et al., 1997) that allows the timing of the frequency sweep to be optimized given a particular shape of the frequency and amplitude modulation functions. In our case the timing, frequency modulation, and amplitude modulation functions are given by,

$$t = \xi(t), \quad \Delta\omega(t) = A\xi(t), \quad \omega_1(t) = \frac{B_1\left(\frac{T}{2}\right)^2}{(A\xi(t))^2+(T/2)^2}, \qquad (3)$$

where ξ(t) is a variable used to determine the sweep timing. The Δω(t) function describes the offset between the transmit and Larmor frequency, and $\omega_1(t)$ is the corresponding amplitude modulation function (determined by treating the coil response as a Lorentzian function whose full width at half maximum is equal to $T = \frac{\omega_0}{Q(\sqrt{2}-1)}$). The function ξ(t) is found using the method discussed in detail in Rosenfeld et al., (1997). Briefly, ξ(t) is a parametric function used to determine the pulse timing. In this case it is equal to 1 and 0 at the start and the end of the pulse, respectively. Given these boundary conditions ξ(t) is determined by optimizing the frequency sweep such that a minimum adiabaticity (ratio of the precession frequency of the magnetization about the B_{eff} axis and the rate of change of the B_{eff} axis orientation) is maintained over the B_1 range of interest. After determining ξ(t) the timing of the optimal frequency sweep providing a minimum adiabaticity is found. To demonstrate the performance of a NOM sweep compared to a linear frequency sweep consider Figure 2, which illustrates the Mx and My profiles for a NOM and frequency sweep where A/2π=200 Hz

and Q=5, in both cases. The duration of the linear sweep is 50 ms. For the NOM sweep, the minimum adiabaticity factor is equal to 5, and the target B_1 is 3.33e-6 T. The B_1 heterogeneity factors, ν_{min} and ν_{max} (the notation used in Rosenfeld et al., 1997), needed to determine $\xi(t)$ are both equal to 1 in this example. These parameters effectively control the width of the Mx profile.

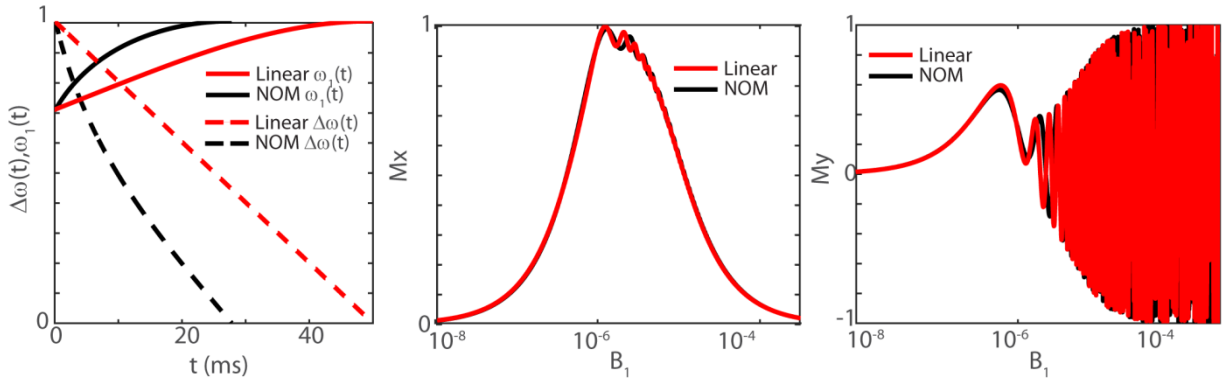

Figure 2. Comparison of the performance of a linear frequency sweep (red line) where τ=50 ms, A/2π=200 Hz, and Q=5 and a NOM sweep (black line). The NOM sweep is determined using equations 3 along with the method discussed in Rosenfeld et al., (1997) to determine the sweep given a minimum adiabaticity of 5 and a target B_1=3.3e-7 T. The left panel indicates the frequency and amplitude modulation functions in each case, while the center and right panels show the Mx and My components produced by each pulse, respectively.

Figure 2 demonstrates that the NOM approach can be used to generate an adiabatic pulse that produces extremely similar Mx and My profiles as in the linear sweep, but where the pulse duration and power requirements are reduced. In this example, the linear sweep duration is 50 ms, while the NOM pulse is only 28 ms in duration. The NOM pulse would also require less power than the linear pulse; if we approximate the required power as the integration of the square of the ω_1 curves in the left panel of Figure 2 (equivalent to integrating the square of the envelope of the current waveform) the NOM pulse requires only 59% of the power used in by the linear sweep. The advantage of the NOM pulse is that it allows the frequency to be swept quickly during times when the adiabaticity is high (early times in Figure 2), while recognizing that the sweep must be slowed during critical times in order to maintain a minimum adiabaticity (the reduction of the slope at later times in Figure 2). This demonstrates that the linear sweep can be substituted for a different frequency modulation providing similar Mx and My profiles with less power consumption. The power reduction provided by the NOM approach was observed to vary (both lower and greater power reductions than that observed in Figure 2) for different Mx profiles.

It is important to keep in mind that the goal in surface NMR is ultimately to produce an image of aquifer properties in the subsurface. To ensure high-quality images are produced we require transmit techniques capable of producing images with high spatial resolution and satisfactory depth penetration. Figure 3 illustrates the resolution matrices associated describing the kernels describing a synthetic survey employing a 25 m diameter circular loop, and 16 pulse moments where the current amplitudes are logarithmically sampled on the range from 5 A to 100 A for a resistive subsurface. MRSmatlab (Müller-Petke et al., 2012) was used to produce kernels necessary to generate the resolution matrices and sounding curves. The resolution matrix and sounding curve for a survey employing an on-resonance pulse of duration 20 ms is illustrated in the left column of Figure 3. The resolution matrix represents the ability to resolve each model parameter given a particular sampling method (Müller-Petke and Yaramanci, 2008) (eg. 20ms on-resonance pulses with currents ranging from 5 to 100 A). Perfect resolution would be described by an identity matrix. Deviation from diagonal behaviour indicates loss of resolution. The sounding curve in this case represents the signal that would be measured following each pulse given a subsurface described by a half space of 100% water content. The resolution matrix and sounding curve corresponding to an equivalent survey where all parameters are the same except that an adiabatic pulse with A/2π=200 Hz, τ=50 ms, and Q=5 with a linear frequency sweep is employed in place of an on-resonance pulse is illustrated in the right column of Figure 3. The same current amplitudes are employed in the adiabatic survey; varying the current amplitude alters the B_1 distribution in the subsurface, effectively varying where a particular adiabatic pulse would produce a transverse magnetization. Figure 3 serves to contrast the expected spatial resolution and depth penetration of the adiabatic pulse against that provided by an on-resonance pulse. The on-resonance resolution matrix is observed to have values closer to 1 on the diagonal and to maintain diagonal behaviour to a greater depth. The adiabatic pulse is observed to provide larger signal amplitudes for the higher pulse numbers (the larger current amplitudes), with the range of enhanced SNR depending on the current amplitude. The optimal distribution of current amplitudes is likely to be different for the on-resonance pulse and the adiabatic pulse. The adiabatic pulse is anticipated to be optimally implemented using large current amplitudes. This demonstrates that the adiabatic pulse is expected to capable of improving signal amplitudes, as was observed by Grunewald et al., (2015), but this signal enhancement potentially comes at the expense of a loss of spatial resolution. Furthermore, the on-resonance pulse provides greater depth penetration given that its resolution matrix retains diagonal behaviour to greater depths than the adiabatic case.

CONCLUSIONS

Adiabatic pulses present an opportunity to improve the signal to noise ratio in surface NMR. To maximize the benefits of employing an adiabatic pulse we present a sensitivity analysis investigating how the size of the swept bandwidth, the pulse duration, and the shape of the frequency modulation function impact the performance of an adiabatic pulse for a range of magnetic field heterogeneity

typical of surface NMR conditions. For linear frequency sweeps the width of the bandwidth swept is observed to play a strong role in determining the range of B_1 where the adiabatic pulse is effective at producing a transverse magnetization. Sweeping a large bandwidth (equivalent to starting far off-resonance) allows the magnetization to be rotated fully into the transverse plane for a broad range of B_1 amplitudes, focused mostly at stronger B_1. In contrast, sweeping a smaller bandwidth produces a magnetization that lies in the transverse plane for a reduced range of B_1 amplitudes, but is able to produce a transverse magnetization for smaller B_1 amplitudes given a fixed pulse duration. The duration of a linear sweep is observed to affect primarily the performance of the adiabatic pulse at low B_1 amplitudes, where longer pulses are able to produce a transverse magnetization for smaller B_1. A numerically optimized modulation approach was also observed numerically to provide equivalent performance to the linear frequency sweep, but while using a shorter pulse duration and requiring less power. Given the limitation that the current amplitude modulation cannot be freely controlled throughout the pulse, the NOM method presents an opportunity to optimize the frequency modulation function.

Adiabatic pulses represent a promising technique to improve signal to noise ratio in surface NMR However, a trade off between signal improvement and spatial resolution loss is observed. Future work will investigate how to optimally design a suite of adiabatic pulses to ensure high SNR while maintaining sharp spatial resolution and satisfactory depth penetration.

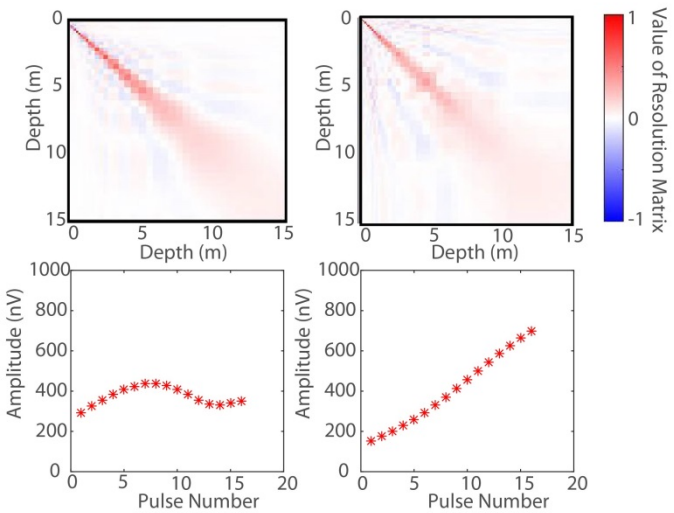

Figure 3. The resolution matrices (top row) and sounding curves (bottom row) for surveys employing a 20 ms on-resonance pulse (left column) and an adiabatic pulse where A/2π=200 Hz, τ=50 ms, Q=5, and the frequency is swept linearly (right column). The survey used a 25 m loop with 16 current amplitudes logarithmically sampled on the interval from 5 A to 100 A.

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REFERENCES

Bendall, M.R., and Pegg, D.T, 1986, Uniform sample excitation with surface coils for in vivo spectroscopy by adiabatic rapid half passage: Journal of Magnetic Resonance, 67, 376-381.

Bloch, F., 1946, Nuclear induction: Physical Review, 79 (7-8), 460-474.

Dalgaard, E., Auken, E., and Larsen, J.J., 2012, Adaptive noise cancelling of multichannel magnetic resonane sounding signals: Geophysical Journal International, 191 (1), 88-100.

Grunewald, E., Grombacher, D., and Walsh, D.O., 2015, Adiabatic pulses enhance speed and sensitivity of geophysical surface NMR measurments for groundwater investigations: 24th ASEG-PESA meeting, Perth, Australia, Extended Abstracts.

Müller-Petke, M., and Yaramanci, U., 2008, Resolution studies for magnetic resonance sounding (MRS) using the singular value decomposition: Journal of Applied Geophysics, 66 (3-4), 165-175.

Müller-Petke, M., Walbrecker, J.O., Costabel, S., Günther, T., and Hertrich, M., 2012, MRSmatlab – a toolbox for modeling, processing, and inverting surface-NMR data: Magnetic Resonance in the Subsurface 5th International Meeting, Hanover, Germany.

Rosenfeld, D., Panfil, S.L., and Zur, Y., 1997, Design of selective adiabatic inversion pulses using the adiabatic condition: Journal of Magnetic Resonacne, 129, 115-124.

Tannus, A., and Garwood, M., 1997, Adiabatic pulses: NMR in Biomedicine, 10, 423-434.

Ugurbil, K., Garwood, M., and Bendall, R., 1987, Amplitude- and frequency-modulated pulses to achieve 90^0 plane rotations with inhomogeneous B_1 fields: Journal of Magnetic Resonance, 72, 177-185.

Walsh, D.O., 2008, Multi-channel surface NMR instrumentation and software for 1D/2D groundwater investigations: Journal of Applied Geophysics, 66 (3-4), 140-150.