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Estimating T_2 from surface NMR FID data using a forward model based on the full-Bloch equation

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SUMMARY

An integral component of the surface nuclear magnetic resonance forward model involves predicting the magnitude of the transverse magnetization following excitation. To predict the transverse magnetization, the Bloch equation must be solved. Traditional surface NMR forward models solve a simplified version of the Bloch equation where the relaxation terms are neglected. A shortcoming of this approach is that it can struggle to accurately describe the impact of relaxation during pulse effects. To address this concern, an alternative forward model based on solution of the full-Bloch equation is proposed. The advantage of the proposed scheme is that it implicitly accounts for relaxation during pulse effects, increases the flexibility to implement alternative parametrizations of the inverse model, and can readily describe an arbitrary excitation protocol given that it no longer requires closed form expressions of the transverse magnetizations. To demonstrate the potential of the updated forward modelling scheme, a novel approach for the inversion of complex-valued free-induction decay (FID) data is presented. The inverse model is reparametrized in order to produce depth profiles of the water content, T_2^* and T_2 . This approach has great potential to enhance the ability of FID measurements to provide insights into pore size and permeability as it can provide direct sensitivity to T_2 . In contrast, traditional approaches that employ a forward model based on the simplified Bloch equation and estimate only T_2^* are plagued by uncertainty surrounding the link between T_2^* and pore size/permeability. Synthetic and field results are presented to demonstrate the feasibility of the proposed forward model and FID inversion framework.

Key words: Hydrogeophysics; Inverse problem; Numerical techniques; Electromagnetic methods.

INTRODUCTION

To ensure reliable images of groundwater systems are produced by the surface nuclear magnetic resonance (NMR) method, it is imperative that the excitation process is modelled accurately. A key component of accurate excitation modelling is the ability to predict the transverse magnetization at each location in the subsurface following the excitation pulse, a process that requires solving the Bloch equation. Traditionally, surface NMR forward models solve a simplified version of the Bloch equation where the relaxation terms are neglected (Legchenko and Shushakov 1998; Legchenko and Valla 2002; Hertrich 2008). The advantage of this simplification is that the transverse magnetization is described by a simple closed form expression and the inversion can be linearized given certain experimental designs. Even for alternative experiments that employ pulse types without an analytic expression of the transverse magnetization (such as for adiabatic half-passage pulses; Grunewald *et al.* 2016), the forward model can still be linearized by calculating the transverse magnetization numerically to form a look-up table. The

transverse magnetization at all locations in the subsurface can then be calculated using the local applied magnetic field and the look-up table.

Although neglecting the relaxation terms can be justified in the long relaxation time/short pulse duration limit it can lead to significant inaccuracies when describing the signal in the presence of short relaxation times (Weichman *et al.* 2000). To extend the range of conditions where this simplification remains accurate the extrapolation to mid-pulse approach can be used, which can improve water content estimates in the presence of relaxation during pulse (RDP) effects (Walbrecker *et al.* 2009). However, even the extrapolation to mid-pulse approach breaks down at fast relaxation times and can lead to challenges describing alternative pulse types, such as adiabatic half-passage pulses (Grombacher *et al.* 2017a).

To further expand the range of conditions where the surface NMR forward model can reliably predict the transverse magnetization, we present a surface NMR forward model based on the solution of the full-Bloch equation. This solution includes the relaxation terms that

are neglected in the traditional forward model. In the following, we aim to:

- (1) demonstrate the feasibility of a forward model based on the full-Bloch equation, and
- (2) highlight the flexibility and discuss advantages of such a forward modelling framework.

We consider the mostly widely implemented surface NMR measurement, the free-induction decay (FID). We aim to highlight the advantages of the proposed forward model through presentation of a novel approach for handling FID data, where the updated forward model is paired with an alternative model parametrization to enhance the value of FID measurements. Several synthetic results and a field example are presented to demonstrate that the updated forward model is capable of constraining both T_2^* and T_2 from complex-valued FID data. This work builds upon the results of Grombacher and Aiken (2018), where it was shown that the T_2^* – T_2 relationship could be constrained from FID data by performing inversions using a range of forward models each employing a distinct but plausible T_2^* – T_2 relationship. This initial work employed a simplification where a single T_2^* – T_2 relationship was present in the entire subsurface; in this work we now allow for depth dependent T_2^* and T_2 , where FID data is inverted using a Gauss–Newton inversion scheme to produce depth profiles of the water content, T_2^* and T_2 . This approach has great potential to enhance the ability of FID data to provide insight into pore sizes and permeability. Adaptation of the proposed scheme and potential benefits for multipulse experiments are discussed as well.

BACKGROUND THEORY

The surface NMR forward model is described by

$$V(I, t) = \int_{\text{vol}} \omega_0 M_0 e^{2i\zeta(r, \omega_0)} m_{\perp}(\mathbf{r}, I) B_{\perp}^-(\mathbf{r}) w(\mathbf{r}) e^{-\frac{t}{T_2^*(\mathbf{r})}} d^3r, \quad (1)$$

where $V(I, t)$ is the voltage at time t measured following a pulse with a peak current I . The ω_0 and M_0 terms are the Larmor frequency and the equilibrium magnetization magnitude, respectively. The term containing ζ describes a phase shift that arises due to the electrical conductivity structure of the subsurface. The $m_{\perp}(\mathbf{r}, I)$ term is the transverse magnetization at each location in the subsurface, and is dependent on the excitation pulse waveform. $B_{\perp}^-(\mathbf{r})$ is the receive field sensitivity. $w(\mathbf{r})$ is the water content, and ranges in value from 0 to 1. The exponential containing T_2^* describes the decaying envelope. In practice, eq. (1) is simplified by linearizing the forward operator to give (Müller-Petke and Yaramanci 2010)

$$\mathbf{d} = \mathbf{K}\mathbf{m}, \quad (2)$$

where $\mathbf{K}$ is the kernel matrix described by (Weichmann *et al.* 2000)

$$K(I, z) = \int_{x,y} \omega_0 M_0 e^{2i\zeta(r, \omega_0)} m_{\perp}(\mathbf{r}, I) B_{\perp}^-(\mathbf{r}) dx dy, \quad (3)$$

and $\mathbf{m}$ is a model vector describing the water content in each depth layer. Of interest in this work is the $m_{\perp}$ term that describes the transverse component of the magnetization following excitation, which is obtained through a solution of the Bloch equation (Bloch 1946)

$$\frac{\partial \mathbf{M}(t)}{\partial t} = \gamma \mathbf{M} \times \mathbf{B}_{\text{eff}} - \frac{M_x}{T_2} - \frac{M_y}{T_2} - \frac{M_z - M_0}{T_1}, \quad (4)$$

where γ is the gyromagnetic ratio of the hydrogen nuclei, $\mathbf{M}(t)$ describes the magnetization vector at time t , and T_2 and T_1 are the transverse and longitudinal relaxation times, respectively. M_x , M_y and M_z represent the x -, y - and z -components of $\mathbf{M}$. $\mathbf{B}_{\text{eff}}$ is the effective magnetic field defined in the reference frame rotating at the instantaneous transmit frequency ω_t , where

$$\mathbf{B}_{\text{eff}} = \begin{bmatrix} B_1 \\ 0 \\ \Delta\omega/\gamma \end{bmatrix}. \quad (5)$$

B_1 is the corotating component of the applied magnetic field (Weichmann *et al.* 2000) and $\Delta\omega = (\omega_0 - \omega_t)$. The cross-product term in eq. (4) describes the perturbation of the magnetization due to the applied field $\mathbf{B}_{\text{eff}}$, while the relaxation terms act to return the magnetization back to its equilibrium orientation. Note that forming $m_{\perp}(\mathbf{r}, I)$ requires solving eq. (4) at each location $\mathbf{r}$ in the subsurface.

Consider first the case where $m_{\perp}$ is determined by solving the Bloch equation without relaxation terms (as is standard in surface NMR). For experiments employing on-resonance or off-resonance pulses $m_{\perp}$ can be described by a simple analytic expression depending on the local B_1 amplitude, pulse duration and offset between the Larmor and transmit frequencies (Mansfield *et al.* 1979; Trushkin *et al.* 1993). For more complex pulse types, such as adiabatic half-passage pulses, $m_{\perp}$ no longer has a simple expression but instead must be calculated numerically. In practice, the lack of an analytic expression is handled by calculating $m_{\perp}$ as a function of B_1 numerically, and then generating the required $m_{\perp}(\mathbf{r})$ from $B_1(\mathbf{r})$ and a look-up table based on $m_{\perp}(B_1)$ (Grunewald *et al.* 2016). Note that in each of these cases, $m_{\perp}$ depends only on B_1 and pulse specific parameters—that is, $m_{\perp}$ does not depend on any inversion parameters (i.e. no T_2^* or water content dependence). This has the distinct advantage that the kernel does not need to be recalculated during the inversion (as long as the electrical conductivity structure is unchanged) and effectively linearizes the forward problem. Note that the same look-up table may be used for data collected at multiple sites as long as the pulse specific parameters remain unchanged (such as the current waveform and offset during the pulse). In principle, $m_{\perp}$ also depends on $\Delta\omega$, however in this study we consider the situation where $\Delta\omega$ is spatially homogenous for simplicity. To include $m_{\perp}$'s $\Delta\omega$ dependence, the look-up table is given a second dimension.

Typical inversion schemes for FID data that employ smooth models estimate the water content and T_2^* in each depth layer, while the layer thicknesses are kept constant during inversion. An inversion with N layers will therefore estimate $2N$ parameters (N is often in the range of 20–30), and regularization is required to stabilize the inversion. For joint inversions of NMR and electrical/electromagnetic data, the conductivity in each depth layer is also estimated in addition to water content and T_2^* (Behroozmand *et al.* 2012b; Günther & Müller-Petke 2012) (i.e. the inversion will estimate $3N$ parameters). In this case, the kernel has to be recalculated at each iteration. Braun *et al.* (2009) have also performed inversions to estimate conductivity, water content, and T_2^* using only FID data. A second common approach is to employ a few layer inversion scheme (Guillen and Legchenko 2002) where few layers are used (typically less than ~ 5) and a regularization term is no longer needed. In this case, the layer thicknesses are estimated in addition to the water contents and T_2^* (and conductivities); these inversions estimate $3N-1$ parameters (the minus 1 is because the bottom layer extends to infinity and the thickness is not defined). If the conductivity is also estimated in a few layer inversion the number of model parameters increases to $4N-1$.

To estimate the distribution of subsurface parameters a model minimizing the objective function $\Phi(\mathbf{m})$,

$$\Phi(\mathbf{m}) = \phi_d(\mathbf{m}) + \phi_s(\mathbf{m}) \quad (6)$$

is sought. $\phi_d(\mathbf{m})$ is the L_2 norm of the misfit between the observed and predicted data given model $\mathbf{m}$, while $\phi_s(\mathbf{m})$ is the stabilizer function. Minimizing the objective functions requires balancing the data misfit term with a stabilizer function that penalizes models with particular characteristics (e.g. sharp variations between neighbouring layers). Multiple stabilizer functions have been employed in surface NMR including from L_2 norms, L_1 norms (Mohnke and Yaramanci 2002) and minimum gradient support (MGS, Grombacher et al. 2017). A Gauss–Newton scheme is employed to find a model that minimizes the objective function, where the corresponding model is taken as the best estimate of the subsurface parameters. The employed inversion framework builds upon the magnetic resonance sounding forward implementation (Behroozmand et al. 2012a) within the AarhusInv software package (Auken et al. 2015). A thorough discussion about the inversion workflow used to minimize eq. (6) is given in Auker and Christiansen (2004).

Solution of the simplified Bloch equation and the corresponding inversion in terms of water content and T_2^* has two primary shortcomings. The first stems from the need to account for RDP, which if neglected can significantly bias water content estimates (Walbrecker et al. 2009). Walbrecker et al. (2009) demonstrate that an extrapolation to mid-pulse approach can improve the reliability of modelling based on the simplified Bloch equation in the limit where the relaxation time is long compared to the pulse duration for an on-resonance pulse. However, in certain relaxation conditions and/or for alternative pulse types the extrapolation to mid-pulse approach may break down and potentially bias water content estimates (Grombacher et al. 2017). A second limitation of approaches that involve extrapolation based on T_2^* estimates (such as the extrapolation to mid-pulse approach) is that they cannot readily describe variations in the underlying T_2 and T_{2IH} terms (which combine in parallel to form T_2^* ; Grunewald and Knight 2011). T_{2IH} describes signal loss due to static dephasing in an inhomogeneous background magnetic field. Multiple T_2 – T_{2IH} combinations could give rise to the observed T_2^* , yet the underlying T_2 and T_{2IH} can have significant impacts on how RDP effects manifest (Grombacher et al. 2017). The standard forward model based on the simplified Bloch equation cannot readily incorporate this effect given that T_2 and T_{2IH} do not affect calculation of the $m_\perp$ term.

Traditional FID inversion schemes that only estimate the relaxation time T_2^* do not provide enough information to solve the full-Bloch equation. This is not an issue with the traditional forward model as T_2 and T_1 never entered the solution. However, if one chooses to solve the full-Bloch equation T_2 and T_1 must be defined at all locations in the subsurface, which can be quite difficult given that these parameters are not known *a priori*. In an initial attempt to invert FID data using the full-Bloch equation, Grombacher and Auker (2018) addressed the uncertainty in T_2 and T_1 by performing inversions where $m_\perp$ was calculated by assigning all depths the same T_2 and T_1 value, but where multiple inversions were performed for a range of plausible T_2 and T_1 . This approach is limited in that it does not account for spatial variation in T_2 or T_1 , and does not allow the inversion to iterate towards a best estimate of T_2 .

Model Parameterization

$\sigma_1, \text{Thk}_1, \text{WC}_1, T_{2^*}, T_{2f,1}, T_{1f,1}$
$\sigma_2, \text{Thk}_2, \text{WC}_2, T_{2^*}, T_{2f,2}, T_{1f,2}$
$\vdots$
$\sigma_n, \text{Thk}_n, \text{WC}_n, T_{2^*}, T_{2f,n}, T_{1f,n}$

Figure 1. Subsurface model parametrization for the surface NMR forward model that solves the full-Bloch equation. The second subscript on T_{2^*} , T_{2f} and T_{1f} refers to the layer index.

MODELLING BASED ON THE FULL-BLOCH EQUATION

To address the shortcomings of approaches that solve a simplified version of the Bloch equation, we propose to use a forward model that solves the full-Bloch equation (with relaxation terms included) in combination with an alternative parametrization for the inversion that accounts for spatial variations in T_2^* , T_2 and T_1 . Fig. 1 illustrates the parametrization used to calculate the kernel (eq. 3) given the scenario where $m_\perp$ is determined using the full-Bloch equation. The i th layer is defined by its conductivity σ_i , thickness thk_i , water content WC_i , $T_{2^*}, T_{2f,i}, T_{1f,i}$. The factors T_{2f} and T_{1f} are not equal to T_2 and T_1 , rather they are scale factors, where

$$T_2 = T_{2f} T_{2^*}, \text{ and} \quad (7A)$$

$$T_1 = T_{1f} T_2. \quad (7B)$$

This parametrization is selected as it allows bounds on the T_2 and T_1 to be easily incorporated, where T_2 is forced to be greater than or equal to T_{2^*} by restricting T_{2f} to be greater than or equal to 1. Similarly, T_1 is forced to be greater than or equal to T_2 by restricting T_{1f} to be greater than or equal to 1. Positiveness is also ensured for all parameters by working in a log model space. In this work, we do not consider the stretching exponent C (Behroozmand et al. 2012a), (i.e. each layer is described with a mono-exponential decay in T_{2^*}), and we fix T_{1f} to be equal to 1 (equivalent to setting $T_2 = T_1$), in order to reduce the number of model parameters. In practice, T_{1f} typically varies from 1 to 3 (Kleinberg et al. 1993). For simplicity, we treat the conductivity structure as constant in the following examples (i.e. conductivity is not estimated during the inversion), which corresponds to inversions that estimate $3N$ parameters in the case of smooth inversions and $4N-1$ parameters for the few layer inversion.

The influence of T_{2IH} on the modelled $m_\perp$ at each location in the subsurface is dependent on the difference between the local T_2^* and T_2 , where

$$\frac{1}{T_2^*} = \frac{1}{T_2} + \frac{1}{T_{2IH}}. \quad (8)$$

Eq. (8) allows T_{2IH} to be quantified using T_2^* and T_{2f} . The T_{2IH} value is then used to constrain the width of a Lorentzian Larmor frequency distribution, as the exponential T_{2IH} decay is simply the

Fourier transform of the underlying Lorentzian Larmor frequency distribution. This distribution is discretized into a number of distinct Larmor frequencies $\omega_{0,i}$ each with an abundance A_i . To determine $m_{\perp}$ in the presence of a Larmor frequency distribution eq. (9) is used.

$$m_{\perp} = \sum_i A_i m_{\perp,i} \quad (9)$$

Each $m_{\perp,i}$, the transverse magnetization corresponding to the i th Larmor frequency, is determined by solving eq. (4) with the corresponding $\mathbf{B}_{\text{eff}}$ vector defined in eq. (5). Note that each $\omega_{0,i}$ has a distinct $\mathbf{B}_{\text{eff}}$ vector, which allows off-resonance effects during the pulse to be appropriately weighted based on the relevant offset, B_1 magnitude, and pulse waveform. The weighted sum of each individual Larmor frequency component in eq. (9) therefore reflects $m_{\perp}$ given the local T_2^* , T_{2H} , T_2 , T_1 and B_1 . In this work, the Larmor frequency distribution is discretized into 401 linearly spaced values ranging from -100 to 100 Hz, and the look-up tables are based on a B_1 discretization involving 2000 values logarithmically spaced from 10^{-11} to 10^{-5} T. Estimates of $m_{\perp}$ for B_1 values not directly appearing in the look-up table are estimated by interpolating between neighbouring B_1 values in the look-up table. Eq. (9) is relevant in the static dephasing limit, which occurs when the scale of B_0 heterogeneity exceeds the diffusion length of an individual water molecule during the pulse length (in this case). This is equivalent to assuming that each water molecule experiences a single B_0 value during the pulse.

Another important advantage to solving the full-Bloch equation is that it readily allows an arbitrary pulse to be modelled given that it does not require a closed form description of $m_{\perp}$. This allows one to define an arbitrary current amplitude waveform and frequency sweep. The pulse waveform is parametrized using two functions $F1(t)$ and $F2(t)$ and the initial offset A (Garwood and DelaBarre 2001). These two functions allow the B_1 amplitude and instantaneous offset $\Delta\omega$ ($\Delta\omega = \omega_0 - \omega_t$) during the pulse to be determined from

$$B_1(t) = B_{1,\text{ref}} \cdot F1(t) \cdot I \quad (10A)$$

$$\Delta\omega(t) = A \cdot F2(t) \quad (10B)$$

$F1(t)$ describes the amplitude of the normalized current envelope during the pulse, while I and $B_{1,\text{ref}}$ correspond to the peak current amplitude during the pulse and the B_1 value produced by a 1 A peak current, respectively. $F2(t)$ describes the normalized frequency sweep (i.e. variation of the offset between the Larmor and transmit frequencies during the pulse). The instantaneous offset in eq. (10B) corresponds to the offset between the dominant Larmor frequency (i.e. the central frequency of the Larmor frequency distribution) and the transmit frequency. The A term describes the offset between the dominant Larmor and transmit frequencies at the beginning of the pulse. For example, an adiabatic half-passage pulse that begins 100 Hz off-resonance corresponds to $A/2\pi$ equal to 100 Hz, where $F2(t=0) = 1$ and $F2(t=\tau) = 0$. The $F1(t)$ and $F2(t)$ functions range from $[-1, 1]$ are simply used to modulate the B_1 amplitude and offset throughout the pulse (i.e. they enter the Bloch equation through the $\mathbf{B}_{\text{eff}}$ term in eq. 4). Note that pulse waveforms are always included in the full-Bloch approach, which differs from traditional forward models where an effective constant current amplitude is typically adequate (where a parameter referred to as the pulse moment is used, which is equal to average peak current multiplied by the pulse duration). Fig. 2 illustrates the $F1(t)$ and $F2(t)$ functions for

Figure 2. Examples of the pulse parametrization for the AarhusInv forward implementation. The $F1(t)$ and $F2(t)$ functions describe the modulation of the current envelope and the modulation of the transmit frequency during the pulse, respectively. Grey and black curves correspond to two example pulses (the on-resonance case being a single-frequency pulse, and the NOM example representing an adiabatic half-passage pulse).

two example pulses (the pulses used in the field example). The grey curve describes an on-resonance pulse, where $F1(t)$ rises to an initial peak and then droops over the course of the pulse. The $F2(t)$ function in this case is equal to 0 at all times indicating that there is no offset between the Larmor and transmit frequencies. For the example adiabatic half-passage pulse (black), which is described by a sweep defined using a numerically optimized modulation (NOM) approach (Uburgil *et al.* 1988; Grombacher 2018) the $F1(t)$ function shows a similar shape first rising to a peak and then drooping over the course of the pulse. The $F2(t)$ function in this case starts at 1 and sweeps smoothly towards 0 at the end of the pulse, which corresponds to a frequency sweep beginning at an initial offset A and terminating at an offset of 0 (as is required for an adiabatic half-passage pulse (Tannus and Garwood 1997)). Note that in Fig. 2, the $F1(t)$ function is zero for the final 8 ms in each case. This corresponds to the dead time, where by setting $F1(t)$ equal to zero over this interval we are able to calculate $m_{\perp}$ at the end of the dead time. The advantage of including the dead time in the modelling is that it eliminates the need for any extrapolation.

The primary shortcoming of the proposed approach is that the inversion is non-linear. The kernel must be recalculated in all depth layers during each iteration given the current best estimate of T_2^* and T_2 , which requires reweighting the relaxation terms in the Bloch equation and recalculating the width of the Larmor frequency distribution during each kernel calculation. This results in increased inversion times compared to the standard approach that uses the simplified Bloch equation and fixed conductivity structure. However, we do not consider this to be a significant issue given that the employed inversion scheme is already able to recalculate the kernel after each iteration as this must also be done for joint NMR-EM inversion schemes. Secondly, the solution of the full-Bloch equation and required use of a look-up table to populate $m_{\perp}(\mathbf{r})$ also result in longer inversion times compared to scenarios where $m_{\perp}$ has a closed form description.

In the following, we aim to highlight the advantages of this forward modelling/inversion scheme through demonstration of a novel approach for the inversion of complex-valued FID data.

ESTIMATING T_2 FROM COMPLEX-VALUED FID DATA

Parameter resolution tests

To investigate whether the proposed scheme and parametrization offers the ability to constrain T_2 from complex-valued FID data consider Fig. 3. Fig. 3 presents the results of a sensitivity analysis conducted using the approach outlined in Behroozmand *et al.* (2013) where the *a posteriori* covariance matrix is used to provide insight into model parameter uncertainty. The *a posteriori* covariance matrix is calculated for a three-layer model, where layer two is designated as the layer of interest (as it is given the highest water content of the three layers). The model space consists of 11 parameters: the water content, T_2^* , T_2 and layer thickness for each of the upper two layers, as well as a water content, T_2^* and T_2 for the bottom layer. The *a posteriori* covariance matrix is calculated without roughness or prior constraints. The forward model corresponds to a 75 m² coincident transmit/receive loop and 20 current amplitudes logarithmically spaced from 2 to 200 A. The data set consists of complex-valued FIDs produced by two excitation pulses, a 4 Hz off-resonance 40 ms pulse, and an adiabatic half-passage pulse described by an NOM [the recommended pulse in Grombacher (2018) involving a sweep over 100 Hz in 52 ms]. The use of two pulse types (an adiabatic and an off-resonance pulse) is better able to constrain T_2 compared to a survey employing a single-pulse type (Grombacher and Aiken 2018). Decays are gated into 25 linearly spaced time gates where the first and final gates are centred 1 ms after the end of the pulse and at a time equal to three times the value of T_2^* (which is a value that could be roughly determined from examination of the time series), respectively. From the *a posteriori* covariance matrix, a standard deviation factor (STDF) for each parameter is extracted from the square root of the relevant diagonal element. The analysis is conducted on the logarithm of the model parameters; therefore, a model parameter with value m has a 68 per cent likelihood of falling within the range described by eq. (11).

$$\frac{m}{\text{STDF}} < m < m \cdot \text{STDF} \quad (11)$$

Fig. 3 illustrates the STDF factor for T_2 in layer 2 (the layer of interest) for a range of different conditions. The STDF of the T_2 estimate is determined by the product of the STDF of T_2^* and the STDF of T_{2f} . The bottom left panel of Fig. 3 lists the value of all model parameters. The T_2 and T_2^* parameters vary for each pixel in the top four panels. The left- and right-hand columns correspond to layer two thicknesses of 10 and 20 m, respectively. Noise levels of 20 and 50 nV are also investigated (top and middle rows, respectively). The STDF values in each pixel are binned into categories representing how well resolved the parameter is—the colour scale for parameter resolution outlined in Behroozmand *et al.* (2013) is employed. Green, yellow, orange, red, light blue and dark blue colours correspond to parameters that are very-well determined, well-determined, determined, poorly determined, very-poorly determined and undetermined, respectively. White panels correspond to unphysical conditions (i.e. T_2^* is always less than or equal to T_2).

Several trends can be observed in Fig. 3. For each T_2^* value, the T_2 parameter is best resolved when it is similar in magnitude to T_2^* (observed by noting that the colours trend towards red/blue as one moves from left to right in each row). T_2 is also best resolved in the low T_2 limit (top left corner of each panel). In the long T_2 limit (rightmost columns of each panel), T_2 is poorly resolved. The reason for the reduced resolution in this limit is that the exact T_2 magnitude has little influence in these cases (e.g. if $T_2^* = 50$ ms, the

data are not significantly affected if T_2 is varied from 300 to 600 ms because the signal is dominated by T_{2f}). However, the large STDF in these cases does not necessarily indicate that the results are not of value. Consider the top right panel for the $\text{Thk}_2 = 20$ m and 50 nV of noise scenario, where $T_2^* = 50$ ms and $T_2 = 600$ ms. In this case, the STDF on layer two's T_2 is 2.7. Even though this corresponds to a very-poorly determined parameter, it is still possible to say with confidence that this layer's T_2 is likely to be greater than 600 ms/2.7, which is much greater than $T_2^* = 50$ ms. As such, one is still able to extract valuable insight that T_2^* is dominated by T_{2f} in this case and that it should not be used to make pore-size/permeability estimates. Note that the resolution of T_2 is also reduced at higher noise levels as expected.

Overall, Fig. 3 indicates that in many situations T_2 can be well resolved using standard FID acquisition schemes with complex-valued data and a forward modelling framework that solves the full-Bloch equation.

Inversion of synthetic data

To further investigate the ability of the updated forward model to reproduce depth varying T_2 consider Fig. 4, which illustrates the ability of the inversion to reproduce one-, two- and three-layer scenarios. In each row, four different models are investigated, each with an identical water content and T_2^* profile but with a different T_2 profile (colours). The same survey geometry/parameters and timing used to form Fig. 3 are again used, with the exception that the subsurface is now discretized into 25 layers whose thickness increases with depth. A smooth inversion employing an MGS regularization scheme is used to estimate the water content, T_2^* and T_2 in each depth layer. The employed regularization uses σ_{rel} and β values of 1.1 and 500. These parameters influence how strongly neighbouring layer parameters may vary and the likelihood of sharp transitions in the model; σ_{rel} and β are discussed further in Grombacher *et al.* (2017). In each case, 25 noise realizations (50 nV of noise) are added to the same underlying noise-free synthetic data set. Each noisy data set is inverted and the suite of inversion results is illustrated as a histogram, where the transparency corresponds to the number of counts in each bin (opaque bins correspond to bins with many counts while transparent (white) bins have no counts). The histogram width is used to provide insight into uncertainty in the estimated profiles. The true models are shown by the solid lines with circles. Note that all inversions are given the same initial model (a half-space with 20 per cent water content, $T_2^* = 150$ ms, and $T_2 = 225$ ms) and are observed to fit the data within the standard deviation following inversion.

In the top row, the subsurface is described by a half-space but where the T_2 is equal to 60 ms (black), 100 ms (blue), 150 ms (red) and 250 ms (green). In all cases, the water content and T_2^* profiles are the same and are accurately estimated, while the underlying T_2 profile is also well estimated. For the long T_2 case (green), the estimated T_2 histograms begin to widen at depth. This reduced accuracy at depth in the long T_2 limit is consistent with insights from Fig. 3 where it is expected that T_2 is more poorly resolved in the long T_2 limit. The middle row illustrates a two-layer example, representative of an upper unconfined aquifer underlain by a lower water content layer but where no T_2^* contrast is present. In all cases, the water content and T_2^* profiles are accurately resolved. Furthermore, the varying T_2 value in the upper layer is also well resolved. At greater depths, the reduction in T_2 is also reproduced, but with T_2 being overestimated (with the magnitude of the overestimate increasing

Figure 3. Sensitivity analysis of the T_2 parameter in the layer of interest (layer 2) for multiple T_2^* – T_2 scenarios when using the proposed forward model that solves the full-Bloch equation. The left- and right-hand columns correspond to the layer two thickness. The top and middle rows correspond to noise levels of 20 and 50 nV. All parameters for the three-layer model are listed in the bottom left panel. Pixel colours indicate the STDF for a particular T_2^* – T_2 combination. The colour scale is the same in all panels. Green, yellow, orange, red, light blue and dark blue colours correspond to parameters that are very-well determined, well-determined, determined, poorly determined, very-poorly determined and undetermined, respectively. White panels correspond to unphysical conditions (i.e. T_2^* is always less than or equal to T_2).

as T_2 in the upper layer increases). Note that ability to differentiate between these four scenarios could lead to significantly more accurate conceptual models of the subsurface. For example, the ability to differentiate between the black and green cases could be the difference between interpreting the upper layer as fine sands or as gravels, which is extremely important for permeability predictions. Note that the T_2^* profile alone provides no insight into these differences in this example. The final example in Fig. 4 (bottom row) corresponds to a three-layer scenario where a high water content layer is present in a low water content background, but where no T_2^* contrast is present. The water content and T_2^* profiles are again reproduced accurately in all cases, with the underlying T_2 also being well estimated in the upper two layers. T_2 is poorly resolved at depth for the three long T_2 cases. Taken together, Fig. 4 demonstrates a consistent ability to resolve the water content, T_2^* , and T_2 profile given only complex-valued FID data.

In the three examples investigated in Fig. 4, the water content and T_2 profiles shared a similar structure. To highlight that structure in

the T_2 profile can be resolved even if it does not accompany changes in the water content or T_2^* profile consider Fig. 5, where two two-layer scenarios are investigated. In each case, the water content and T_2^* profiles are described by a half-space. In the top column, the T_2 value in the upper 15 m is varied (colours) and the T_2 below that depth is the same in all cases. For the bottom row, the T_2 value in the upper 15 m is held constant, while the T_2 value below 15 m depth is varied (colours). In all investigated cases, the water content and T_2^* profiles are accurately reproduced, while the differences in the T_2 profiles are also reliably captured. Overall, Fig. 5 indicates that the proposed inversion has the potential to resolve structure in the T_2 profiles that does not coincide with similar structures in the water content or T_2^* profiles.

Taken together, Figs 3–5 highlight that the proposed forward modelling scheme based on solution of the full-Bloch equation is able to consistently estimate the T_2 profile from complex-valued FID data.

Figure 4. Synthetic inversion results for three different subsurface models (rows). The left-, centre and right-hand columns illustrate the estimated water content, T_2^* , and T_2 profiles. In each row, four different subsurface models are present—each with the same water content and T_2^* profiles but different T_2 profiles (colours). Each histogram is formed from 25 noisy synthetic inversions (50 nV of noise). The coloured histograms in the water content and T_2^* profiles are mostly overlapping.

Field example

To demonstrate the feasibility of the proposed scheme under field conditions a data set collected at Leque Island, Washington, USA is presented. Data were collected using a two-turn 42 m circular loop and two different excitation pulses. A 40 ms on-resonance and an adiabatic half-passage pulse described by an NOM (the NOM pulse recommended in Grombacher (2018)). In each case, 36 current amplitudes were collected ranging from approximately ~ 1.75 to ~ 296 A. The conductivity structure at the site is known from a previous EM investigation and is included in the forward modelling. The Larmor frequency was observed to be 2290 Hz. Prior to inversion, a phase correction is applied to both the on-resonance and adiabatic half-passage data sets; this is necessary to eliminate

any instrumental or processing phases imparted on the data. The phase correction is determined using the approach outlined in the appendix of Grombacher *et al.* (2016). The complex-valued data were inverted by treating the real and imaginary components separately, where the data vector $\mathbf{d}$ (eq. 2) was formed by concatenating the real and the imaginary data. This has the advantage that the data and kernels are real-valued, which naturally constrains the estimated water contents to also be real. The data are gated into 26 linearly spaced time gates, where the first and last time gate are centred 0.2 and 108 ms after the end of an 8 ms dead time, respectively.

Fig. 6 illustrates the inversion results, where the on-resonance and adiabatic half-passage data are jointly inverted to produce a single model. The starting model begins with a half-space of 20 per cent water content, $T_2^* = 50$ ms, and $T_{2f} = 1.5$. The water content and

Figure 5. Synthetic inversion results for two different subsurface models (rows). The left-, centre and right-hand columns illustrate the estimated water content, T_2^* , and T_2 profiles. In each row, four different subsurface models are present—each with the same water content and T_2^* profiles but different T_2 profiles (colours). Each histogram is formed from 25 noisy synthetic inversions (50 nV of noise). The coloured histograms in the water content and T_2^* profiles are mostly overlapping.

T_2^* profiles are observed to be consistent with previous knowledge of the site, where a thick water bearing layer appears to be present from ~ 5 to ~ 20 m depth. T_2^* is small at most depths ranging within ~ 30 – 50 ms, while the T_2 profile has much larger values ranging from ~ 200 to ~ 300 ms over much of the investigated depth range. To verify the reliability of the estimated T_2 profile, Fig. 7 plots the estimated T_2 profile (solid red line) on top of an NMR T_2 log collected at the same site using the Javelin logging tool (Walsh *et al.* 2010). Hot colours in the NMR T_2 log indicate T_2 values present at that depth interval. The resulting T_2 profile tracks the hot region of the NMR log for much of the investigated depths. The T_2 log deviates from the surface NMR T_2 estimate at depths ~ 7 m; the T_2 values measured by the log at these depths are quite small and would be difficult to detect using conventional surface NMR instrumentation. Overall, the agreement between the NMR T_2 log and the T_2 estimated from the proposed inversion scheme indicates that T_2 can be constrained using complex-valued FID data in the field. Note that the estimated T_2^* profile (dashed red line) significantly underestimates the logging T_2 values. As such, if T_2^* were considered to be approximately equal to T_2 it may lead to significant errors in pore size/permeability predictions in this case.

The estimated vertical profiles in Fig. 6 show several differences with the profiles estimated in Grombacher and Auker (2018), which was the previous best estimate of the subsurface using the same data sets. Specifically, the water content profile estimated in Grombacher and Auker (2018) show higher water content peaks at depths ~ 7

and ~ 20 m depth. The more homogeneous structure estimated in Fig. 6 likely stems from a differences in the employed regularization scheme (MGS in this case), model discretization and stopping criteria.

DISCUSSION

The presented forward model, which solves the full-Bloch equation has several attractive features. The first stems from its implicit compensation of RDP effects. Inclusion of the relaxation terms allows RDP to be weighted appropriately based on the current waveform, the local B_1 amplitude and the best estimate of the spatially varying T_2^* , T_2 and T_1 . This has the potential to improve the ability to fit complex-valued surface NMR data and may lead to broader exploitation of the benefits of complex inversion (such as improved resolution; Braun & Yaramanci 2005).

Secondly, this forward model can be readily adapted to handle alternative parametrizations. This potentially allows parameters to be estimated that could not have previously been constrained. For example, in the traditional approach for inverting FID data T_2 never enters the modelling, only T_2^* . Therefore, these types of approaches were unable to inform about T_2 . However, by altering the forward model and including T_2 in the parametrization, it allows the influence of T_2 to enter the inversion and allows it to be further constrained. Several alternative parametrizations for the inversion of FID data have been discussed previously, Legchenko *et al.* (2016)

Figure 6. Inversion results for a field data set collected at Leque Island, Washington. The left-, centre and right-hand panels of the top row illustrate the estimated water content, T_2^* and T_2 profiles, respectively; each estimated by inverting an adiabatic half-passage data set and an on-resonance data set jointly using the proposed forward model based on the full-Bloch equation. The bottom panel illustrates the misfit (observed data minus forward modelled data) for the profiles in the top panels.

presented an approach to invert for the offset between the Larmor and transmit frequencies as a function of depth, while Irons and Li (2014) include a parameter describing non-exponential behaviour at early times in their inversion. The proposed scheme can be readily adapted to include these types of parametrizations as both the offset and background field distribution shape/width enter the solution of the full-Bloch equation. One could even include T_1 in the inversion—however, the ability to resolve T_1 in the current FID scheme is an outstanding question. Although T_1 is expected to have some influence on the transverse magnetization in a single-pulse experiment (Grombacher *et al.* 2017), T_1 was fixed and set equal to T_2 in order to reduce the dimension of the model space and simplify the inversion. Deviation from $T_1 \sim T_2$ may degrade accuracy of the estimated transverse magnetization for the presented implementation where these two parameters are forced to be equal.

Another advantage of the presented forward model is that it eliminates the need for a closed form description of the transverse magnetization. Instead the Bloch equation is solved numerically, and the transverse magnetization can be predicted at any time for any arbitrary pulse waveform. This approach can readily incorporate a user

defined frequency sweep or an observed current modulation (e.g. drooping of the current). We also propose to model the transverse magnetization by solving the Bloch equation until the end of the dead time, which can be done by modelling the dead time with no B_1 present (i.e. only relaxation and dephasing occur during the dead time). This has the advantage that the estimated water contents are based only on observed data and not extrapolations to early times that can produce biased water content estimates in the presence of fast relaxation times.

The flexibility afforded by the proposed forward model allows a novel approach for the inversion of complex-valued FID data to be exploited. The ability to model local variations in T_2 and T_{2H} when combined with a reparametrized model domain allows an inversion to be performed where both T_2^* and T_2 can be constrained from only FID data. This may lead to enhanced value for FID measurements. Standard forward models and inversion of FID data that produce only T_2^* estimates are plagued by uncertainty about the process controlling T_2^* (Grunewald and Knight 2011), this uncertainty can be alleviated through the proposed approach. For example, in Figs 4 and 5, the ability to differentiate between the black (short T_2) and

Figure 7. Comparison of the surface NMR FID estimated T_2 profile (same as that illustrated in Fig. 6) and a T_2 log produced using the Javelin NMR logging tool. The T_2 log is illustrated as the background colourmap, where hot colours indicate which T_2 values are present in the greatest abundance in each depth layer. The black line illustrates the mean log of the T_2 distribution in the T_2 log. The dashed and solid red lines illustrate the T_2^* and T_2 profiles for the surface NMR inversion, respectively.

green (large T_2) cases is extremely important for building a more complete conceptual model of the subsurface. One scenario could be a low permeability unit (black), while the other could be an attractive target for groundwater extraction (green). If one is forced to make an interpretation based only on the water content and T_2^* , large uncertainty remains.

The proposed FID inversion scheme is best suited to use with complex-valued data. Similar tests based on amplitude-only inversions (where the phase is not used) were observed to more poorly resolve T_2 . Inversions that employed both a single frequency pulse (on- or off-resonance) and an adiabatic half-passage pulse were also observed to better constrain T_2 than cases that used only a single-pulse type. The two pulse types display opposite trends as T_2 and T_{2H} are varied, thus providing greater insight into the underlying $T_2^* - T_2$ relationship (Grombacher and Auker 2018).

Although this work discusses only FID measurements, the presented forward model has great potential for multipulse surface NMR experiments such as spin-echo (Legchenko *et al.* 2010; Grunewald *et al.* 2014), pseudo-saturation (Legchenko *et al.* 2004; Walbrecker *et al.* 2011) and multi-echo measurements (Grunewald and Walsh 2013). The parametrization of the transmit pulse can be expanded to describe the multipulse scenario by defining the $F1(t)$ and $F2(t)$ functions as a series of pulses separated by time intervals where $F1(t)$ and $F2(t)$ are zero. Future work will investigate the utility of this approach for multipulse scenarios.

Note that the proposed forward model does have several trade-offs. The first is that the inversion is no longer linear, as the kernel now depends upon several of the model parameters (T_2^* and T_2). This leads to increased inversion times compared to the traditional forward model. However, Jacobian calculations can be accelerated by storing information from previous iterations. A forward response for a 25 layer model that uses the on-resonance and NOM pulses discussed in the synthetic and field cases can be calculated in roughly 5–10 s using 12 threads, this leads to inversion times that average

~15–20 min for the results shown in Figs 4 and 5. Future work will focus on reducing inversion times. In contrast, the traditional inversion can be completed in several seconds. The inversions presented in Figs 4 and 5 typically required ~7–10 iterations. Secondly, the current approach to invert FID data does not include T_1 as an inversion parameter, which requires an assumption to be made about its relationship with T_2 .

CONCLUSIONS

Traditional inversion schemes for surface NMR FID data, which are based on solution of a simplified Bloch equation, can struggle to accurately describe the signal in the presence of strong RDP effects, particularly in the fast relaxation limit or when using alternative pulse types such as adiabatic half-passage pulses. To improve the ability of the forward model to account for RDP effects for a wider range of conditions and for arbitrary pulse types a forward model based on the full-Bloch equation is presented. The proposed approach requires inclusion of the relaxation terms in the Bloch equation during the forward model, which requires that the relaxation times T_2^* , T_2 and T_1 be specified (either by allowing them to become inversion parameters or defining them based on *a priori* knowledge of the site). The advantages of the updated forward model are an implicit ability to weight RDP effects based upon the best estimate of the spatially varying relaxation times and the specific excitation pulse employed. A further advantage is that the proposed scheme does not rely upon a closed form description of the transverse magnetization, making it straightforward to implement an arbitrary experimental design. Alternative parametrizations can also be readily employed using this type of scheme, as demonstrated by the ability to invert complex-valued FID data to constrain the T_2 profile. Overall, solving the full-Bloch equation has great potential to enhance the reliability of the surface NMR forward model and to improve inversion and survey design flexibility moving forward.

Standard FID inversion schemes are also often plagued by large uncertainties surrounding the interpretation of T_2^* —is T_2^* strongly linked to pore geometry or has it been contaminated by background magnetic field inhomogeneity? Such uncertainty has potential to lead to biased subsurface models. To enhance confidence in FID-based interpretations of pore size and permeability the updated forward model based on solution of the full-Bloch equation is employed with an alternative parametrization where the water content, T_2^* and T_2 profiles are simultaneously estimated using complex-valued data collected by standard FID acquisition protocols. This scheme has the benefit that it can extract valuable information that could not be gleaned from traditional inversion schemes, thus enhancing the utility of the FID. T_2 estimates using the presented scheme are shown to be best resolved in the low T_2 limit, with resolution decreasing for larger T_2 values.

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