Surface NMR Processing and Inversion – II: Data Fitting

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SUMMARY

I present a method for compressing the entire surface NMR data set for a set of basis parameters that is most in accord with the measured data. Each basis parameter generates an amplitude and phase for each pulse moment of the recorded SNMR experiment, and keeps track of all uncertainty in the data.

Key words: Surface NMR, groundwater, data fitting

INTRODUCTION

The ultimate goal of an SNMR experiment is to obtain a plausible image of the groundwater contained in the subsurface. From the time series of the set of pulse moments, the first step is to obtain the single exponential decay fit to the data (eg, Legchenko and Shushakov, 1998). The second natural step is to examine the data set for more exponentials: and this is typically done on a pulse moment by pulse moment basis using a regularisation in the fitting (Mohnke and Yaramanci, 2005), by the *QT*-inversion (Mueller-Petke and Yaramanci, 2010), or by a stretched-exponential distribution (Behroozmand et al., 2012). In this paper, I present an alternative method of data compression that explores the complete NMR experiment time series recording for a set of basis parameters that is most logically consistent with the measured data.

SNMR SIGNALS IN DATA

Data from an SNMR experiment can be proposed in a functional form as:

$$F_q(t) = \sum_i^m (A_i \cdot sin(\omega_i t) + B_i \cdot \cos(\omega_i t)) \cdot e^{-t/T_{2i}^*},$$

where ω_i are Larmor frequencies, T_{2i}^* are the characteristic decay times associated with each frequency, and A_i and B_i are amplitudes of the signal. Each $F_q(t)$ is the relevant time series for a given pulse moment q. By examining all the time series for all values of q in the experiment, relevant parameters ω_i and T_{2i}^* are sought. Amplitude and phase values (or, equivalently, in-phase and quadrature amplitudes A_i and B_i are found during the fitting process. Since a layer of groundwater in a 1D model can be found in the time series data of every pulse moment, the entire data set is used during fitting. We seek, then, for a mono-exponential decay signal, parameters ω_1 T_{21}^* that are, on a probabilistic basis, most consistent with the data measured.

RESULTS

Figure 1 shows the measured (black), modelled (red) and misfit (green) of the time series for the first 20000 points of each time series for each pulse moment of a complete SNMR experiment whereby a single Larmor frequency and a single characteristic time were solved for. Each panel of the figure shows the data for each pulse moment, but the parameters were fit using the complete set at once.

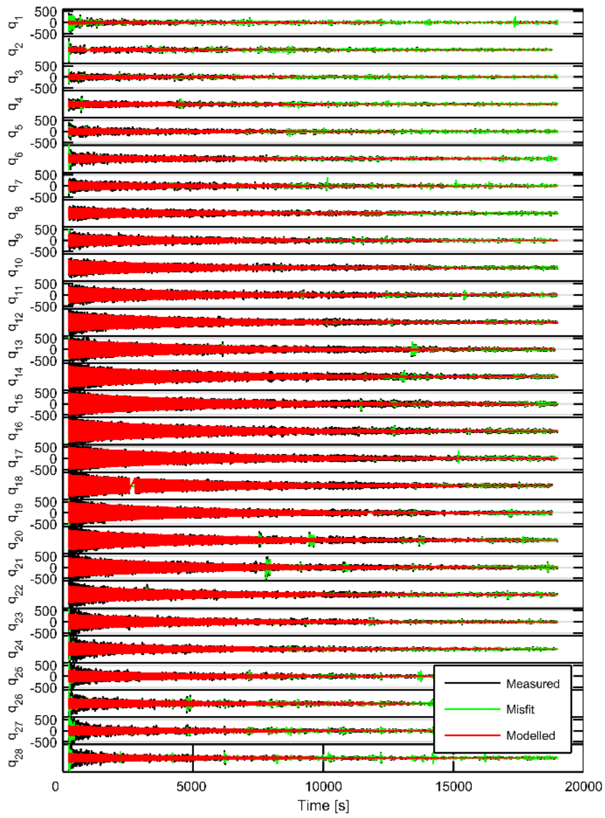

Figure 1: Measured (black), modelled (red) and misfit (green) of the first 20000 points of each time series from an SNMR experiment. Each panel represents the time series for an individual pulse moment, but the entire data set was fit for a single Larmor Frequency and characteristic time.

Figure 2 shows the migration path of the fitting parameters ω_1 T_{21}^* from 16 different Monte Carlo experiments of 1000 trial proposals. The chains were started from random proposal sites in the parameter space. The first 100 proposals from each chain are rejected as burn-in. It is very clear that the parameters quickly converge to a stable solution, and, looking at Figure 3, we see that the distributions of the parameters (approx. 14000 proposals) is extremely sharp.

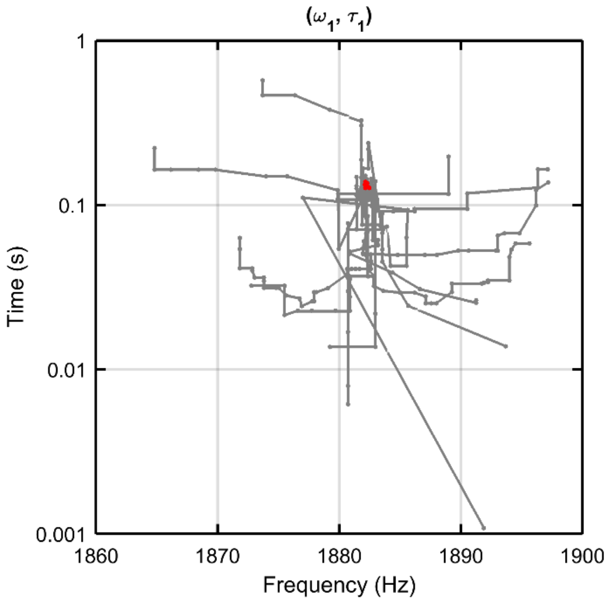

Figure 2: Results from 16 different Monte Carlo chains, starting from random locations in the parameter space, locating the best fitting frequency and characteristic time parameters. Each chain has the first 100 points greyed out due to burn-in. The remaining points are shown in red.

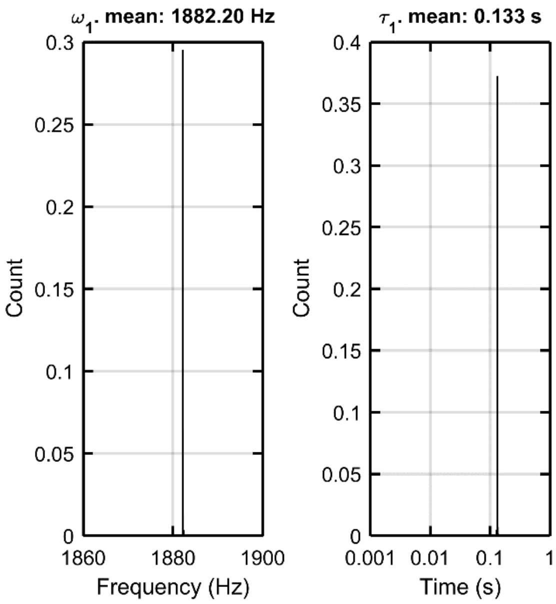

Figure 3: Distributions of ω_1 T_{21}^* parameters from the Monte Carlo chain. Each parameter is extremely well-determined.

Figure 4 shows the in-phase and quadrature components of the fitted data for this particular SNMR experiment. Total amplitude for each pulse moment is shown with open circles, in-phase is shown with dots, and the quadrature is shown with crosses. Each pulse moment amplitude has associated with it an uncertainty; and these are shown with error bars in the in-phase and quadrature components.

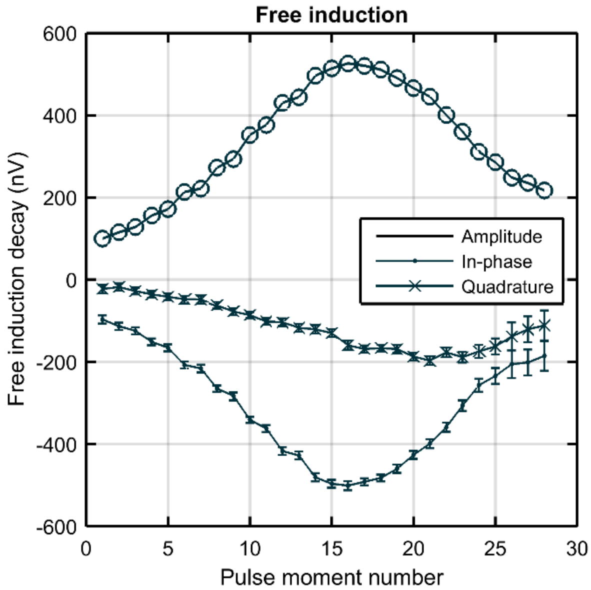

Figure 4: In-phase and quadrature amplitudes for SNMR experiment.

CONCLUSIONS

I have shown that the parameters of ω_1 and T_{21}^* from a SNMR experiment can be determined with great accuracy from the time series of the entire data stack recorded during the experiment. The result is a set of parameters that, given the model proposal, are most consistent with the measured data. The compressed data space is then given as a set of in-phase and quadrature amplitudes whose uncertainty is a reflection of the fitting process.

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