MRSMATLAB – processing, modelling and inversion of MRS data

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SUMMARY

MRSMATLAB is designed to provide tools for processing, modelling and inversion of MRS (Magnetic Resonance Sounding) data. The toolbox is MATLAB based. Ongoing from its origin, several researchers have implemented their work over the last years as the project intends to be open for the implementation of current developments. Latest progress includes the processing and inversion of spin echo data, off-resonance excitation and complex inversion.

This abstract reviews the general capabilities, provides insight into the handling of MRSMATLAB and in particular the used numerical implementation, and introduces current developments.

Key words: Processing, Modelling, Inversion

INTRODUCTION

MRSMATLAB originates from the need to process and invert surface NMR (Nuclear Magnetic Resonance) data independently from the tools provided by the manufactures. In particular, the development started with COSSMO (e.g. Hertrich et al., 2005, Braun et al., 2005) to calculate kernel functions according to Weichman et al. (2000), to simulate forward data and to invert field data. Further progress and a renaming to MRSMATLAB was triggered by the QT inversion, i.e. inversion of all pulse moments Q for the complete time T at once (Müller-Petke and Yaramanci, 2010) scheme and the ability to perform remote reference noise cancellation (Radic, 2006; Walsh, 2008). Ongoing from this state several features have been implemented by different researchers over the last years as the project is intended to be an open platform distributing new tools to the community.

In this abstract we give a brief overview of existing modules of the toolbox and review currently integrated features. We show how to handle field data and how to build synthetic data. Finally, we spotlight new features such as spin echo measurements and off-resonance complex inversion.

OVERVIEW OF MRSMATLAB

MRSMATLAB is separated into six modules each with a user interface (GUI) and the following general purpose:

1. ***MRSSignalPro***: Loads the measured raw data and processing can be conducted. Processed data is saved in MATLAB format as *.mrsd.
2. ***MRSFit***: Post-process field and synthetic data for inversion.
3. ***MRSKernel***: Calculates the 1D sensitivity function. Kernel is saved in MATLAB format as *.mrsk.
4. ***MRSQTInversion***: T2* and T2 Inversion of field or synthetic data in various kinds.
5. ***MRST1Inversion*** : T1 Inversion of field or synthetic data.
6. ***MRSModelling***: Calculates synthetic data for a given 1D model.

MRSSIGNALPRO

MRSSignalPro is the basic processing module of MRSMATLAB. An easy run through MRSSignalPro would be simply loading and saving the data. This would then include by default envelope detection, low-pass filtering (500~Hz), stacking and error calculation. The more challenging the data gets the more processing is necessary. The following processing tools are implemented.

Despiking

Spikes are either identified as (i) an amplitude above the standard deviation of all time gates of the same record or (ii) the standard deviation of all records of one stack for a specific time gate. After detecting the spike, a certain time range is replaced with the average of all stacks from this pulse moment. While this replacement is done with the complex signal, the detection is done with the amplitudes of the record because this amplitude does not contain any oscillations. A comparison of different replacement schemes can be found in Costabel and Müller-Petke (2014), other spike detection schemes are presented in Dalgaard et al. (2012) or Jiang et al. (2011).

Harmonic modelling noise cancellation

Principles are based on the paper of Larsen et al. (2014). The approach does not need a remote reference coil, instead the higher harmonics of a base frequency are modelled, with each higher harmonic owning an independent amplitude and phase. Baseband frequency, amplitude, and phase of each higher harmonics are estimated. We conduct a brute force search for the base-frequency. A range of base frequencies is set up and for each an inverse problem for phase and amplitudes is solved.

Remote reference noise cancellation

Principles and equations can be found in Müller-Petke and Costabel (2014). In MRSMATLAB, we solve this problem in the frequency domain but time domain solutions are also possible (Dalgaard et al. 2012). Two options are available:

- Global: take a (complete) set of records and get only one transfer function. Sometimes a global transfer function may not be suitable for the complete dataset as noise is changing during the measurements.
- Local: get a single transfer function for each record. The single record is split in several parts in advance to processing the record. You may also be careful if harmonic noise is close to the Larmor (resonance) frequency of your NMR signal. The global option is more robust in this context, so be careful not to cancel NMR signal.

Synchronous detection and low-pass filter

There are a couple of schemes around to calculate the complex envelope of the signal. We use the Hilbert transformation of the signal as this allows for avoiding additional filter. However, as signal-to-noise (SNR) is typically low and data is broadband a forward and reverse filter is applied that preserves the phase of the signal.

Error calculation

Reliable data errors are essential for inversion. We calculate the standard deviation for every time sample from the set of records used for stacking. To get reliable error this is to be done using the data after synchronous detection and at a sampling rate reduced according to the filter properties.

MRSFIT

MRSFit is the post-processing module. Concerning FID (free induction decay) data post-processing means fitting the data by a mono-exponential decay to obtain initial amplitude, T2* decay time, phase and frequency offset. Introducing QT inversion, initial amplitude and decay time became obsolete but phase and frequency offset are still necessary to rotate the dataset, which is explained below. With respect to complex inversion, the phase estimate becomes obsolete as well but in any case frequency estimation will remain necessary. Concerning T2-Echo data post-processing estimates the echo amplitude by fitting a Gaussian function. These echo-amplitudes are later used for QT inversion.

MRSKERNEL

MRSKernel calculates the MRS sensitivity function. Most field parameters (such as pulse moments, Larmor frequency and loop size) can be imported from field data or individually set for synthetic studies. B-fields of circular loops on a 1D layered space are calculated according to Ward and Homann (1988). In detail, a FORTRAN code from Peter Weidelt (personal communication) is translated to MATLAB. Ongoing from the B-fields, FID kernels are calculated according to Weichman et al. (2000). The impact of off-resonance excitation is implemented as given by Walbrecker et al. (2011a). As the T1 kernel depends on the distribution of T1 relaxation times in the subsurface (Walbrecker et al., 2011b) only the B-fields are saved while the actual kernel function is calculated during the inversion progress. T2-kernels are calculated based on the equations given by Legchenko et al. (2010) or Grunewald et al. (2014).

MRSQTINVERSION

General capabilities have been described in Müller-Petke and Yaramanci (2010) for smooth and multi-exponential FID inversion. MRSQTInversion, however, allows for smooth and mono-exponential inversion which reduces the number of free parameter dramatically, improves speed and reduces ambiguity. Mono-exponential decay refers to a single layer in depth not to the data. To our knowledge this assumption is valid in most cases. Furthermore, block and mono-exponential inversion is available based on a genetic algorithm code. This code allows for multiple parallel runs to calculate non-linear uncertainties. Besides these three options for the model, the data space used for inversion can be either, amplitude data, rotated amplitude data (rotated to minimize the imaginary part) or complex data. All of which have several pros and cons. Amplitude data does not decay to zero but to the noise level, thus the inversion contains a bias. Rotation of the data may fail if data is strongly multi-exponential and each component comes with another phase value. Complex inversion can circumvent these difficulties but adapted measurement sequences are necessary (Grombacher et al., 2015). Every option comes with regularisation parameter and model boundaries need to be chosen. We recommend to run the inversion with different parameter setting to evaluate the robustness of the result. Sufficient data fit is derived if (i) the data misfit plot show a random pattern with no structure (any remaining structure would indicate unexplained data) and the data fit is close to the calculated data error. As we use error weighting this means a chi^2 of 1. In summary, chose the highest regularisation that both give you a chi^2 of one and no remaining structure in the data misfit plot.

All types of model spaces are available not only for FID inversion but T2 as only the sensitivity function using the spin-echo data is different. However, currently only amplitude data derived from MRSFit can be used. Concerning T1 inversion, the FID results is necessary as a first step.

MRST1INVERSION

Referring to Walbrecker et al. (2011b), the T1 kernel depends on the T1 distribution in the subsurface, thus, is to be updated iteratively during the inversion. Consequently, the inversion is non-linear. We solve the T1 Inversion in a twostep process (Müller-Petke et al., 2013). First, the primary FID signal is inverted and the information obtained from this step is used for the T1 inversion, i.e. only the kernel is updated but the water content and T2* distribution remains constant in this second step. We further refer to the phase-cycled pseudo recovery scheme (PCPSR) to suppress unwanted signal components (Walbrecker et al, 2011b). MRSMATLAB allows for including an arbitrary number of secondary FIDs that contain the T1 information. T1 inversion is currently implemented as smooth and block but mono-exponential decay within a single layer.

MRSMODELLING

MRSModelling allows for simulating FID, T2 echo and T1 data. Modelling is carried out for a given block model. Gaussian noise can be added to the data. Concerning T1 and T2 the number and timing of tau, i.e. the time interval between two pulses, can be freely chosen. The synthetic data is saved in the same format as the stacked field data, thus data handling is the same as for field data. This also enables, for instance, carrying out a complete simulation to study appropriate field parameter in advance.

WORKFLOWS

Field data

The recommended workflow from field data to results is:

1. MRSSignalPro can directly load GMR and NUMIS data, for MRSMIDI data a converter is to be used. Some field parameter can be load from the measured data, some necessary parameter can be added during load. After individual processing the data is stacked and saved as *.mrsd file.
2. LOAD the *.mrsd file into MRSFit for post-processing and save the fitting results to the same file.
3. LOAD *.mrsd into MRSKernel to get most of the necessary field parameter. Typically z-discretization is derived from the loop size and may be adapted. A resistivity profile can be entered. After calculation the kernel is saved as *.mrsk file.
4. LOAD data and kernel file into MRSQTinversion. Select the type of data and model space. Check for instance if rotated data can be used.
5. If applicable start MRST1Inversion and load all relevant data sets.

Synthetic data

To carry out a synthetic study the workflow is:

1. Calculate the kernel function with appropriate parameters for your study
2. LOAD the kernel function into MRSModelling, define the model and measuring conditions, e.g. noise level and tau spacing’s and save the data as *.mrsd
3. Continue as with MRSFit and MRSQTInversion.

NEW FEATURES

Latest developments are:

1. The implementation of harmonic noise cancellation (HNC) that can be carried out in addition to the more common reference based noise cancelation (RNC). If the detected noise shows higher harmonics of a base frequency such as power line noise this approach typically allows for cancelling these components without using a reference coil. In some cases the combination of HNC first followed by RNC can lead to significant improvement compared to only using RNC.
2. Complex inversion is implemented to account for an additional constant phase factor for the complete dataset that can arise from processing and/or instrument calibration. To carry out complex inversion has several already reported advantages such as increased penetration depth (Braun et al., 2005). Grombacher et al. (2015) show that complex inversion is very sensitive to unknown frequency offsets and propose a sequence that auto-compensates for any unwanted artefacts using a frequency-cycling approach.
3. Besides T1, T2 data allows for improved hydrological interpretation as both T1 and T2 relaxation times are less affected by magnetic gradients. Therefore T1 and T2 provide a more reliable pore-size measure. T2 handling has been implemented for processing data, calculating the kernel function and data inversion and modelling.

CONCLUSIONS

MRSMATLAB is a comprehensive toolbox providing all essential tools for working with field data and carrying out synthetic studies. In MRSMATLAB current developments are continuously implemented and everyone is warmly welcome to participate and contribute latest improvements.
Download information for MRSMATLAB will be sent upon email request.

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