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MRS inversion for water volume

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SUMMARY

In this paper we present an approach for analyzing uncertainty in the MRS inversion. Additionally to any other inversion strategy we propose to use the total or partial volume of water under MRS loop as the criterion for estimation of possible variations in the selected solution so that the maximum and the minimum volumes of water correspond to two extreme but still equivalent inverse models. We apply jointly the Monte Carlo and regularization methods for investigating solution space using uncertainty in the water content provided by the SVD analysis. A big advantage of the Monte Carlo modeling is its suitability for both linear and non-linear inversion and the possibility to use the Monte Carlo method without specific assumptions about investigated inverse problem. Experience gained from the numerical modeling and processing of field data shows that this approach is very convenient and has particular advantage when the volume of water under MRS loop is one of the subjects of MRS study.

Key words: MRS, SNMR, inversion, uncertainty.

INTRODUCTION

It is known that inversion of Magnetic Resonance Sounding (MRS) data is ill-posed. It means that experimental signals can be fitted equally well by different inverse models. These models are called the equivalent models. Selection of the best model from the pool of equivalent models can be done using additional information about solution (boreholes, other methods) or assumptions about solution shape.

One of the most popular methods is the Tikhonov regularization (Legchenko and Shushakov, 1998). It allows obtaining unique solution based on the assumption of the smoothness of the inverse model. Assumptions on the solution shape can be also used for performing blocky inversion (Mohnke and Yaramanci, 2002). In both cases the smoothness constraint or the number of block for inversion may be not fully justified, especially when investigating 2-D and 3-D targets (Legchenko et al., 2011) and obtained equivalent solutions do not provide straightforward information about uncertainty in the inverse model.

Uncertainty in the inverse model can be estimated using different methods. The singular value decomposition (SVD) allows estimating resolution of the linear inverse problem for a general case without investigating particular data sets (Weichman *et al*., 2002). The Monte Carlo inverse modeling allows investigating solution space for both linear and non-linear inverse problems and could be applied to the analysis of any particular data set (Guillen and Legchenko, 2002; Chevalier *et al*., 2014). The linear programming technique was also reported to be used for investigating solution space considering different limitations applied to the solution selection (Guillen and Legchenko, 2002).

The majority of reported approaches to MRS data inversion do not take into account the fact that different volumes of water may produce similar signals and consequently different equivalent models may provide different volumes of water. We used this property of MRS inverse problem for developing a simple and practically convenient approach for investigation of the uncertainty in the inverse model. We propose to use the total or partial volume of water under MRS loop as the criterion for selection of the inverse models. Instead of using only one unique solution we propose additionally to take into account solutions that provide the minimum and the maximum volumes of water. Thus, we obtain three inverse models: an optimal model (considered to be the best for any justified reason) and two models that are equivalent to the best model but corresponding to the maximum and the minimum volumes of water. We applied this criterion to investigation of the Tête Rousse glacier where estimation of the maximum and the minimum possible volumes of water accumulated in the glacier was a matter of particular importance (Vincent *et al*., 2012; Legchenko *et al*., 2014).

METHOD

MRS measurements can be carried out by measuring either free induction decay (Legchenko and Valla, 2002) or spin echo (Legchenko *et al*., 2010) signals. In both cases MRS integral equation can be approximated by a system of algebraic equations and in a matrix notation the approximating equation can be written as

$$\mathbf{A}\mathbf{w}=\mathbf{e}_0, \tag{1}$$

where $\mathbf{A}=\left[a_{i,j}\right]$ is a rectangular matrix of $I\times J$, $\mathbf{e}_0=(e_{0,1},e_{0,2},...,e_{0,i},...,e_{0,I})^T$, $e_{0,i}=e_0(q_i)$ is the set of experimental data, $\mathbf{w}=(w_1,w_2,..,w_j,..,w_J)^T$, $w_j = w(\Delta z_j)$ is the water content and the symbol T denoting transposition.

For resolving Equation (1) we assume a non-negative solution ($w_i \geq 0$) and optimization is carried out so that

$$\sum_{i=1}^{I}\sum_{j=1}^{j}(a_{i,j}w_j - e_{0,i})^2 = \min \cdot \quad (2)$$

For inversion, one of the three approaches can be used.

1) If MRS signal has only real part (no dephasing) then inversion can be carried out using amplitudes (Legchenko and Shushakov, 1998). In this case $a_{i,j}$ and $e_{0,i}$ are real numbers. The amplitude inversion is simple and has advantage to be robust.

2) If dephasing takes place then $a_{i,j}$ and $e_{0,i}$ are complex numbers and inversion should be carried out using complex signals (Weichman *et al*., 2002; Braun *et al*., 2005). Inversion of complex signals has better resolution but requires data of a good quality and accurate mathematical model.

3) If the mathematical model or/and data quality are not accurate enough but dephasing takes place then inversion can be performed using complex numbers but optimizing only amplitudes. In this case experimental and theoretical signals ($e_{0,i}$ and $e_{mod,i}$ respectively) are complex numbers but optimization is carried out for the amplitudes. This procedure can be written as

$$\begin{cases} \mathrm{Re}(e_{\mathrm{mod},i}) = \sum_{j=1}^{J}\left(\mathrm{Re}(a_{i,j})\times w_j\right) \\ \mathrm{Im}(e_{\mathrm{mod},i}) = \sum_{j=1}^{J}\left(\mathrm{Im}(a_{i,j})\times w_j\right) \\ e_{\mathrm{mod},i} = \sqrt{\mathrm{Re}(e_{\mathrm{mod},i})^2 + \mathrm{Im}(e_{\mathrm{mod},i})^2} \\ e_{0i} = \sqrt{\mathrm{Re}(e_{0,i})^2 + \mathrm{Im}(e_{0,i})^2} \\ RMSE = \sqrt{I^{-1}\sum_{i=1}^{I}(e_{\mathrm{mod},i} - e_{0,i})^2} = \min \end{cases}, \quad (3)$$

This approach is a compromise between two previous cases and has the disadvantage to be a non-linear inversion.

For investigating resolution of Equation (1) we assume that the inverse problem is linear and noise is normally distributed. In this case we can use the SVD analysis (Aster *et al*., 2005). For that, we can present the matrix **A** as

$$\mathbf{A} = \mathbf{USV}^T, \quad (4)$$

where **U** is an of $I\times I$, orthogonal matrix representing the data space, **V** is an $J\times J$, orthogonal matrix representing the model space and **S** is $I\times J$ diagonal matrix with nonnegative diagonal elements called singular values. The resolution can be estimated using the model resolution matrix $\mathbf{R}_m$, which is a symmetric matrix $J\times J$ describing how well the recovered model is able to represent the original model

$$\mathbf{R}_m = \mathbf{VV}^T \cdot \quad (5)$$

Let **I** to be the identity matrix. If $\mathbf{R}_m = \mathbf{I}$ then the model will be perfectly recovered by the inversion. Otherwise the resolution is not perfect. SVD can be carried out so that the smallest singular values are significant and hence $\mathbf{R}_m = \mathbf{I}$. It is one of the possible ways to obtain a more stable regularized solution.

Another possibility is based on the well-known Tikhonov regularization method applying the smoothness-constrain. In order to find an approximate solution of the Equation (1), this method supposes minimization of the Tikhonov functional

$$M(\eta) = \left\|\mathbf{Aw} - \mathbf{e_0}\right\|_{L_2} + \eta^2 \left\|\mathbf{w}\right\|_{L_2} = \min, \quad (6)$$

where $\eta>0$ is the smoothing factor.

The model resolution matrix for the Tikhonov regularization can be written as

$$\mathbf{R}_{m,\eta} = \mathbf{VFV}^T, \quad (7)$$

where **F** is $J \times J$ diagonal matrix with diagonal elements given by the filter factors

$$f_j = \frac{s_j^2}{s_j^2+\eta^2}, \quad (8)$$

with s_j being the singular values.

For estimating inversion uncertainty caused by experimental noise we assume independent and identically distributed normal data errors $\sigma_N{}^2$. In this case the covariance for the model becomes

$$Cov(\mathbf{w}_\eta) = \sigma_N^2 \mathbf{VFS}^{-2}\mathbf{V}^T \cdot \quad (9)$$

The corresponding 95% confidence intervals for $\mathbf{w}_\eta$ can be computed as

$$\mathbf{w} = \mathbf{w}_\eta \pm \mathbf{w}_{0.95\eta}, \quad (10)$$

where

$$\mathbf{w}_{0.95\eta} = 1.96\times\sqrt{diag\left(Cov(\mathbf{w}_\eta)\right)}, \quad (11)$$

and the 1.96 factor arises from the definition of the 95% confidence intervals. Note that the use of regularization renders solution more stable but less accurate. Selection of the smoothing factor is a tradeoff between stability and accuracy.

It follows from Equation (9) that the data uncertainty σ is an important criterion for inversion. In MRS the data uncertainty is composed of three major components: experimental error caused by external and internal noise (σ_N), discretization of the integral equation (σ_A) and consistency of the mathematical model and the subsurface (σ_G).

$$\sigma = \sigma_N + \sigma_A + \sigma_G \cdot \quad (12)$$

In NUMIS system noise is estimated in the noise measuring window before injecting the first pulse. Measured average amplitude of the noise (E_N) is a relatively stable parameter characterizing noise and the phase of the noise records can be considered as random value relative to the pulse. If the noise magnitude stays relatively stable during measuring then we can assume that noise amplitude varies in the interval between $-E_N$ and $+E_N$. As the phase is random we can assume that noise has normal distribution around zero and that the measured noise amplitude corresponds to the 95% confidence interval of the normal distribution. Under these assumptions we obtain an estimation of the noise standard deviation as

$$\sigma_N = E_N/1.96 \approx E_N/2 \cdot \quad (13)$$

Note that the estimation given by Equation (13) is an approximation because noise is measured before the pulse and thus, the true noise added to the MRS signal is known only approximately. The second component of the data uncertainty

σ_A depends on the matrix **A** and on the regularization. Indeed, it is known that inversion acts as a filter. The bandwidth of this filter depends on the filter factor (Equation 8) and on the number of model layers. Larger number of layers makes the bandwidth larger and consequently σ_A smaller. Geological noise σ_G is usually unknown because the subsurface is unknown and thus we have an additional uncertainty caused by the imperfection of our mathematical model.

Discretization of the integral equation consists of defining in the matrix **A** the depth z_j and thickness Δz_j of model layers so that

$$0 \le z_j \le z_{\max},\ \Delta z_j = z_{j+1} - z_j,\ z_{\max} = \sum_{j=1}^{J} \Delta z_j \cdot \tag{14}$$

It is also recommended to respect (Legchenko and Shushakov, 1998)

$$\Delta z_1 \le \Delta z_2 \le .. \le \Delta z_j \le .. \le \Delta z_J . \tag{15}$$

Number of model layers for inversion can be selected with respects to Equations (14 and 15) so that $\mathbf{R}_m \approx \mathbf{I}$ (Equation 5).

When inversion is linear and noise has normal distribution Equation (10) allows estimating uncertainty for each value $w_{mod,j}$ given by the Tikhonov regularization. However, these conditions are not always respected and equivalent solutions can be additionally investigated using the Monte Carlo approach. For that, we generate models randomly varying each value w_j within the uncertainty given by SVD

$$w_j = (w_{\mathrm{mod}\, j} - w_{0.95\, j}) + 2 \times w_{0.95\, j} \times random\ (0 \div 1), \tag{16}$$

and considering only positive water contents $w_j \ge 0$. For generating pseudo-random numbers ranging between 0 and 1 the multiply-with-carry method was used (Marsaglia and Zaman, 1991).

For selecting equivalent solutions we propose to use such a physically justified parameter as the volume of water under MRS loop computed as

$$V(\mathbf{w}) = \sum_{j=1}^{J} w_j \Delta z_j , \tag{17}$$

were w_j and Δz_j are the water content and thickness of corresponding layer j. Note that this parameter can be easy extended to the 2-D and 3-D inversions.

Then, we consider the best model with $V=V_{mod}$ and two extreme models equivalent to the best model with corresponding volumes V_{max} and V_{min}. These extreme models can be selected by the Monte Carlo method for the data uncertainty σ so that

$$\begin{cases} V_{\min}(\mathbf{w}) = \min\limits_{N}(V_n) \\ V_{\max}(\mathbf{w}) = \max\limits_{N}(V_n) \\ RMSE(V_{\min}) = RMSE(V_{\mathrm{mod}}) = RMSE(V_{\max}) = \sigma \end{cases} ,(17)$$

where N is the number of models.

The extreme solutions corresponding to $V_{min}=V(\mathbf{w}_{min})$ and $V_{max}=V(\mathbf{w}_{max})$ can be also found by minimizing the following functions

$$M_{\min}(\alpha) = \left\| \mathbf{A}\mathbf{w}_{\min} - \mathbf{e_0} \right\|_{L_2} + \alpha V(\mathbf{w}_{\min}) = \min , \tag{18}$$

$$M_{\max}(\alpha) = \left\| \mathbf{A}\mathbf{w}_{\max} - \mathbf{e_0} \right\|_{L_2} + \alpha / V(\mathbf{w}_{\max}) = \min , \tag{19}$$

where $V(\mathbf{w})$ is computed using Equation (17) and for both V_{min} and V_{max}, the penalty function for volume is assumed to be linear and α is selected so that

$$RMSE(V_{\min}) = RMSE(V_{\max}) = \sigma \cdot \tag{20}$$

Optimization is carried out using the best model ($w_{mod,j}$) and varying the water content in each layer ($w_j \ge 0$) within the 95% confidence interval around the best model

$$(w_{\mathrm{mod}\, j} - w_{0.95\, j}) \le w_j \le (w_{\mathrm{mod}\, j} + w_{0.95\, j}) \cdot \tag{21}$$

Thus, the inversion flowchart consists of a few steps: SVD-based discretization of the linear equation with respect to Equations (5, 14, 15); inversion of MRS data with or without regularization and estimate of the uncertainty (Equation 11); investigation of the solution space with the Monte-Carlo method and selection of the equivalent models corresponding to the V_{max} and V_{min} criteria using the Monte Carlo (Equations 16, 17) or regularization methods (Equations 18-20).

RESULTS

We demonstrate our approach with a synthetic model consisting of a well-defined water-saturated layer (w=20%) located at a depth between 50 and 60 m. For modeling we assumed a 100×100 m^2 square loop and the Larmor frequency of 2000 Hz. Synthetic signal was contaminated by a 30-nV random noise. We discretize the integral equation using the resolution matrix as the criterion (Equations 14, 15). We consider three cases: non-damped inversion (η=0), smooth inversion ($\eta=\eta_T$ is selected after Tikhonov regularization) and damped inversion (a small regularization with $\eta=\eta_T/10$). Figure (1a) shows that without regularization inversion is too sensitive to noise and becomes stable with the smoothing factor η increasing. The width of the probability density function (PDF) obtained with the Monte Carlo modeling (Figures 1b and 1c) is in a good agreement with the SVD-provided estimates.

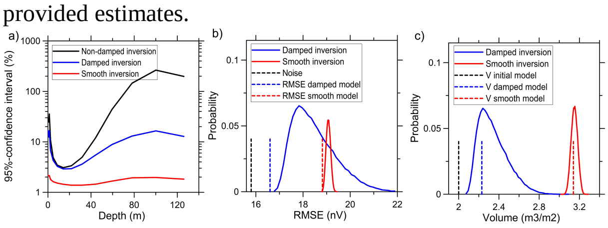

Figure 1. a) 95% confidence interval computed considering the non-damped inversion (black line), the damped inversion (blue line) and the smooth inversion (red line). b) PDF for RMSE computed considering the damped and smooth inversions (blue and red lines respectively), estimated noise level (black dashed line), RMSE of the damped inverse model (blue dashed line) and RMSE of the smooth inverse model (red dashed line). c) PDF of the volume of water of the corresponding models.

Figure (2) shows the minimum and maximum water volume corresponding to the damped and smooth solutions. In practice, noise is known only approximately and the inversion uncertainty can be estimated for noise assumed equal to the RMSE of the best model. Figure (3) shows the damped and the smooth solutions and corresponding synthetic signals. Summary of the inversion results is presented in Table (1).

One can see that estimated water volume is largely dependent on the assumed shape of the solution. Consequently, if reliable information about the solution is not available (sharp or smooth) then the extreme solutions should be selected considering different inversion algorithms. In our example V_{min} solution should be selected from the damped inversion and V_{max} – from the smooth inversion. In this case, extreme solutions corresponding to V_{min}=2.19 m^3/m^2 and V_{max}=3.23 m^3/m^2 are shown in Figures (3a) and 3b respectively.

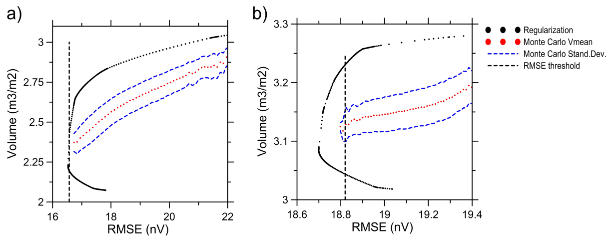

Figure 2. Volume of water versus RMSE for different models computed using the Monte Carlo and the regularization algorithms: a) damped inversion; b) smooth inversion.

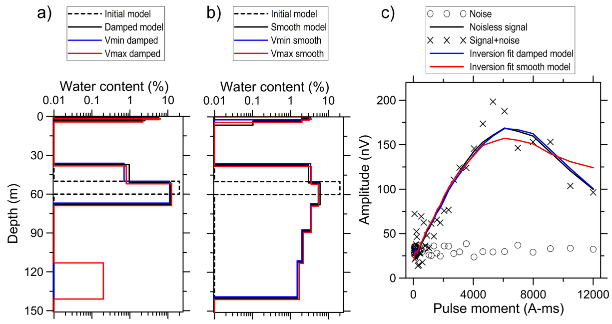

Figure 3. Equivalent models: a) the damped inversion; b) the smooth inversion. c) corresponding MRS signals (c).

Parameter	Damped	Smooth
Synthetic noise estimate (nV)	15.8	15.8
RMSE (nV)	16.57	18.82
Volume initial model (m^3/m^2)	2.0	2.0
Volume min (m^3/m^2)	2.19	3.04
Volume inverse model (m^3/m^2)	2.23	3.14
Volume max (m^3/m^2)	2.41	3.23

Table 1. Summary of the inversion results corresponding to the damped and smooth solutions.

CONCLUSIONS

In this paper we presented an approach for estimation of the inversion uncertainty based on computing the maximum and the minimum water volumes provided by different solutions as the criterion of selection of the extreme equivalent models. For the analysis we used the Monte Carlo and the regularization methods applied taking into account preliminary estimates of the solution uncertainty provided by the SVD analysis. We demonstrated numerical implementation of our approach for the 1-D case using a well-defined synthetic model contaminated by random noise.

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