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Inversion of Magnetic Resonance Sounding data

U. Yaramanci(1) and M. Hertrich(2)

(1) Berlin University of Technology
yaramanci@tu-berlin.de

(2) Eidgenössische Technische Hochschule Zürich
hertrich@aug.ig.erdw.ethz.ch

ABSTRACT

In this paper the basics, state of the art, current and future developments considering inversion of Magnetic Resonance Sounding (MRS) data are presented. A very brief account is given about the MRS method as such to an extent for better understanding of inversion and what it relates to. The inversion is introduced in general terms as usual for the geophysical data, with emphasis on major issues on schemes and their impact on the results in an extension necessary to follow the inversion for MRS. The most extensive and fundamental equation currently available for MRS modelling, the very basis of inversion, is presented, discussed and assessed for its completeness and properties. Based on this expression and its simplified forms for different purposes the current use of inversion in default and in research i.e. new developments are shown. For practical purposes an account on existing schemes and computer software is given and compared on their properties and abilities.

Key words: inversion, decay times, resistivity, Magnetic Resonance Sounding, MRS, modelling, water content

Inversión de datos de Sondeos de Resonancia Magnética

RESUMEN

En este trabajo se presentan sucintamente el estado del arte de la inversión de datos de Sondeos de Resonancia Magnética (SRM), así como el desarrollo actual y futuro de la misma. Se hace una breve reseña del método SRM, a fin de situar a qué se refiere la inversión de sus datos. Se explican los conceptos generales sobre inversión de datos geofísicos, resaltando las principales cuestiones sobre los diversos sistemas y su repercusión en los resultados, con la finalidad de que se pueda seguir la inversión de datos de SRM. Se presenta la ecuación fundamental más completa actualmente disponible para el modelado de SRM, que es la base de la inversión, valorando y analizando su grado de validez y propiedades. Basándose en esta expresión y en sus formas simplificadas para diferentes situaciones, se muestra el uso actual de la inversión en estudios ordinarios y de investigación. A efectos prácticos, se presenta un esquema de los sistemas y software existentes, comparando sus propiedades y aplicaciones.

Palabras clave: contenido en agua, inversión, modelado, resistividad, Sondeos de Resonancia Magnética, SRM, tiempo de decaimiento

Introduction

MRS is a new technology, made available for a larger community in the mid 1990s as a result of long research and development. It already has passed the experimental stage to become a promising surface measurements tool to investigate directly the existence, amount and productivity of ground water. The main principle of Nuclear Magnetic Resonance (NMR), well known since mid forties in physics, physical chemistry as well as in medicine, has now successfully been adapted to assess the aquifer properties, which are mostly needed in hydrogeological investigations.

The first high-precision observations of NMR signals from hydrogen nuclei were made in the 1940s. Meanwhile it is also a standard investigation technology on rock cores and in boreholes (Kenyon 1992). The first ideas for making use of NMR in groundwater exploration from the ground surface were developed as early as the 1960s, but only in the 1980s effective equipment was designed and put to operation (Semenov *et al.,* 1988; Legchenko *et al.,* 1990). In the last 10 years, after a commercial tool got available many groups worldwide took up on use and research for MRS. Some comprehensive resumes were given in two special issues following the International Workshops on MRS (Valla and Yaramanci, 2002; Yaramanci and Legchenko, 2005). Extensive surveys and testing have been conducted in different geological conditions particularly in sandy aquifers but also in clayey formations as well as in fractured limestone and at special test sites (Schirov *et al.,* 1991; Lieblich *et al.,* 1994; Goldman *et al.,* 1994; Legchenko *et al.,* 1995; Beauce *et al.,* 1996; Yaramanci *et al.,* 1999; Meju *et al.,* 2002; Plata and Rubio, 2002; Supper *et al.* 2002; Vouillamoz *et al.,* 2002; Yaramanci *et al.,* 2002; Dippel and Golden, 2003; Baltassat *et al.,* 2005; Lange *et al.,* 2005; Voillamoz *et al.,* 2005). Meanwhile the technique has found an increasing impact to hydrogeologists as a powerful tool for aquifer characterization (Legchenko *et al.,* 2004; Lachassagne *et al.,* 2005; Roy and Lubczynski, 2003; Lubczynski and Roy, 2004).

Basics of geophysical data inversion

Geophysical measurements consist of a set of data by which various parameters are measured (observed), which relate to one or more physical property of the subsurface (underground) and to the spatial distribution of these properties (Figure 1). Examples are given in Table 1.

In fact for MRS the Table 1 gives a simplification i.e. a first degree of approximation as will be shown later. In reality in MRS all observed data depend more or less on all the relevant NMR properties of the underground (see Plata and Rubio, 2007, this Issue).

In all geophysical work i.e. measurements, modeling and inversion, one of the most basic considerations is the dimensionality assumed of and assigned to the subsurface. Considering that geological units and for that geophysical parameters are somewhat constant over large areas, assumptions or simplifications, justified by geological or petrophysical reasoning or by other existing data, can be made.

This can be formalized by assigning a dimensionality to the underground. If the underground is assumed to consist of horizontal layers, this means a one dimensional (1D) structure i.e. the properties change only in vertical direction and not in other directions. This is the most simplification, but holds very often in practice. 2D structures mean formally that the structure holds constant into the direction (y) perpendicular to the section (x-z) under consideration. In practice the measured data than is along the x-direction. 3D obviously means that the subsurface

Method	**Observed data**	**Property of subsurface**
Gravimetry	Earth gravity field	Densities
Geomagnetics	Earth magnetic field	Magnetic susceptibilities
Seismics	Travel times of seismic waves Amplitudes of seismic waves	Seismic velocities, elastic constants Seismic attenuations Seismic reflectivites
Geoelectrics	Voltages and currents	Resistivities Induced Polarisations
Self potential	Voltages	Current systems
Electromagnetics	Artificial electromagnetic fields	Resistivities
Georadar	Travel times of electromagnetic waves Amplitudes of electromagnetic waves	Radar velocities, dielectric constants Resistivities Radar reflectivities
Magnetic Resonance Sounding	NMR amplitudes NMR relaxations NMR phases	Water contents Relaxation times Resistivities

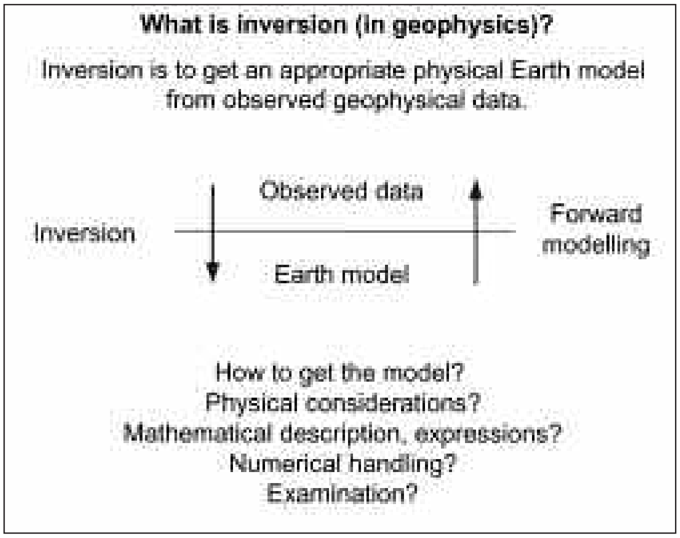
Table 1. Geophysical methods and mapped physical properties of the subsurface
Tabla 1. Métodos geofísicos y propiedades del subsuelo estudiados

property under investigation may vary in all directions equally.

There are basically two different approaches to account for the model geometry in inversion. The model can be assumed to consist out of constant model blocks differently. Most inversion schemes define basic layers (by 1D), cells (by 2D) or volumes (by 3D) and ask for the values of the physical parameters in these geometric units. However, the geometry itself can also be imposed as unknowns, which is very often the case in 1D inversion, where also the depths and thicknesses of layers are to be found.

The assumed dimensionality of the subsurface model is closely related to the survey design and the inversion approach applied. For example in the geoelectric method for a pure depth penetrating configuration (e.g. Vertical Electrical Sounding) a 1D model assumption is mandatory, whereas the same method in 2D configurations (e.g. 2D Wenner) requires a different measurement scheme, a 2D model discretisation, a modified mathematical formulation and finally a 2D inversion scheme to determine the physical properties of the model. Basically the assignment of a dimensionality to the model is a matter of how simple the structure actually is assumed to be, how much fieldwork can be done and how far the theoretical and numerical schemes are available for the modeling and inversion.

Basic tasks in geophysical survey design are to decide for the physical property of subsurface to be mapped, for the right geophysical method, for measurement lay-outs considering the assumed dimensionality, for the required depth of penetration and for the resolution to be achieved. Most essential for the derivation of subsurface properties from the measured data is the existence of a reasonable, robust, reliable and appropriate physical concept, called model. It is described by a more or less complex mathematical formulation and adapted for discrete data sampling and model discretisation in a numerical way.


What is inversion (in geophysics)?

Inversion is to get an appropriate physical Earth model from observed geophysical data.

How to get the model?
Physical considerations?
Mathematical description, expressions?
Numerical handling?
Examination?

Fig. 1. Schematic of geophysical data inversion
Fig. 1. Esquema conceptual de la inversión geofísica

A wide range of literature for inversion in geophysics gives the basics as well as examples for various applications (e.g. Tarantola, 1987; Menke, 1989; Gubbins, 2004; Oldenburg and Li, 2006). In the following, the style used by Menke is followed, which is well established in geophysical literature. Furthermore the analytical theory will be dropped and discretised matrix notation scheme is used as, in particular for MRS, data are discrete and all numerical models are in discretised form.

In a geophysical inversion problem, the most important part is to identify the model relating the physical property of the subsurface i.e. model parameter to the data, which would result from measurements on the model. The model parameters are the unknowns and sought for the solution. With the resulting data, which can be organized in a vector **d**, and the physical property of subsurface organized in a vector **m**, the relation can be expressed most generally with an implicit relation like

$$f(\mathbf{d}, \mathbf{m}) = 0$$

In many applications in geophysics and also for MRS the relation is explicit and linear:

$$\mathbf{d} = \mathbf{G}\mathbf{m} \qquad [1]$$

d = Data, $[d_i]$, i = 1, 2, … , N
m = Model parameter, $[m_j]$, j = 1, 2, … , M
G = Relation of the data to model parameter (Physical model !), $[G_{ij}]$

For MRS the **d** and **m** may contain:

d = Initial amplitudes, decay times (-spectra), phases (depending on excitation intensity, local Earth magnetic field, location(s), geometry(ies) and size(s) of loops, etc.)
m = Water contents, decay times, resistivities, layer thicknesses (sizes)

The main objective in inversion is to determine the best model parameter **m** i.e. to find a solution $\mathbf{m}^{est}$, so that the data resulting from the best model $\mathbf{m}^{est}$ i.e. the model response

$$\mathbf{d}^{pre} = \mathbf{G}\mathbf{m}^{est} \tag{2}$$

is as close as possible to the observed data $\mathbf{d}^{obs}$. Thus the misfit (error)

$$\mathbf{e} = \mathbf{d}^{obs} - \mathbf{d}^{pre}, ([e_i], i = 1, 2, \ldots, N) \tag{3}$$

has to be as small as possible. The measure for that is the mean square of the misfit:

$$E = ||\mathbf{d}^{obs} - \mathbf{d}^{pre}|| = \mathbf{e}^T\mathbf{e} = \sum_i (d_i^{obs} - d_i^{pre})^2 = Min! \tag{4}$$

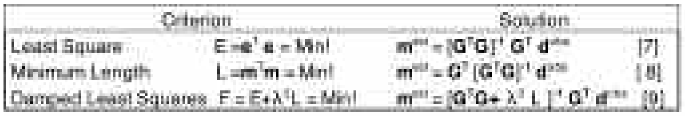
The calculation of $\mathbf{m}^{est}$ follows the usual matrix algebra:

$$\partial E / \partial \mathbf{m}^{est} = 0 \;\text{ i.e. }\; \partial E / \partial \mathbf{m}_j^{est} = 0, \quad j = 1, 2, \ldots, M \tag{5}$$

The solution, called least square solution, is:

$$\mathbf{m}^{est} = [\mathbf{G}^T\mathbf{G}]^{-1}\mathbf{G}^T\mathbf{d}^{obs} \tag{6}$$

provided a solution exists. The problem is underdetermined in case that the number of unknowns M in **m** is greater than the number of data N in **d** as it will be found for many geophysical inverse problems. In this case no unique solution to the inverse equations system exists and additional information on the model has to be implemented to make the inverse problem solvable. An objective approach if no other information is available is to expect the model to be "simple". A first order approximation is to demand the minimum length of the model $L = \mathbf{m}^T\mathbf{m}$, which means a minimum variability of model parameters. Combining the data functional E and the model functional L scaled by λ^2, a damped least square F can be formulated (Table 2).



Criterion		Solution	
Least Square	$E = e^T e = Min!$	$m^{est} = [G^TG]^{-1} G^T d^{obs}$	[7]
Minimum Length	$L = m^Tm = Min!$	$m^{est} = G^T [G^TG]^{-1} d^{obs}$	[8]
Damped Least Squares	$F = E + \lambda^2 L = Min!$	$m^{est} = [G^TG + \lambda^2 I]^{-1} G^T d^{obs}$	[9]

Table 2. Different criteria and solutions adopted in geophysical inversion

Tabla 2. Diferentes criterios y soluciones adoptados en la inversión de datos geofísicos

The weighting factor λ is also called damping factor. For λ=0, it is F=E and for λ=very large than F ≈ L.

For many geophysical problems the minimum length criterion L might not be a suitable measure since it only constraints implicitly the deviation of every model parameter from the model mean. To constrain the model to be "smooth", i.e. to minimize differences of adjacent model cells, L can be modified by using **C m** instead of **m**, with **C** being the approximate first order derivative matrix. This solution is equivalent to so-called first order Tikhonov regularization, which is used often in geophysical inversion. Higher order Tikhonov (derivative) approaches are possible, depending on the given inverse problem and expected model properties.

The Damped Least square criterion is not only applied in underdetermined systems, where no Least Square solution exists, but is also useful in overdetermined systems to stabilize the solution. In particular supplementary information (other geophysical results, geological conditions) may indicate a certain degree of smoothness of the inversion model parameters.

In addition to constraints on the model by damping and smoothing, further information about the data can be implemented into the inversion. In case that information of the data quality is available, each single data point can be weighted individually for its impact on the data misfit measure E. This approach increases the number of models that fit the data, but allows the inversion to weight badly determined data points less without completely deleting subjectively identified outliers.

There are further measures, which are very useful to assess the reliability and value of the solutions and estimate the reliability of the model determined by inversion. The most important one is the covariance allowing to assign an uncertainty to the model **m** on the basis of error estimates of the measured data. Assuming a simplified error for data **d** i.e. that all data is not correlated and has same variance σ^2, the covariance for **m** is

$$[\text{cov}\,\mathbf{m}] = \sigma^2[\mathbf{G}^T\mathbf{G}]^{-1} \tag{10}$$

for Least Square

$$[\text{cov}\,\mathbf{m}] = \sigma^2\mathbf{G}^T[\mathbf{G}\mathbf{G}^T]^{-2}\mathbf{G} \tag{11}$$

for Minimum Length.

Two most valuable measures in the inversion of geophysical data are the data resolution and model resolution matrices, which allow the assessment of the relation and dependences between observed and predicted data as well as between estimated and true model parameter. Introducing a generalized inverse $\mathbf{G}^{-g}$ relating observed data to the best estimation of model parameter (for various criteria)

$$\mathbf{m}^{est} = \mathbf{G}^{-g}\mathbf{d}^{obs} \tag{12}$$

and with $\mathbf{d}^{obs} = \mathbf{G}\,\mathbf{m}^{est}$ the data resolution **N** is given by

$$\mathbf{d}^{pre} = \mathbf{N}\mathbf{d}^{obs} \qquad \mathbf{N} = \mathbf{G}\mathbf{G}^{-g} \tag{13}$$

and with $\mathbf{d}^{obs} = \mathbf{G}\,\mathbf{m}^{true}$ model resolution **R** is given by

$$\mathbf{m}^{est} = \mathbf{R}\mathbf{m}^{true} \qquad \mathbf{R} = \mathbf{G}^{-g}\mathbf{G} \tag{14}$$

Using N and R provides measures on how good individual model cells are resolved by the given data and how important data are for the determination of the model. Careful investigation of these matrices allows optimum survey design and model discretization

Basic equations for MRS modelling and inversion

The measurements in MRS are conducted using a fixed layout of loops with specific location, loop size, loop separation etc. for various excitation intensities (see Plata and Rubio, 2007, this Issue, and Bernard, 2007, this Issue). The increase of excitation intensity (pulse moment) allows that deeper regions are covered subsequently and effects from shallower regions are damped or even cancelled. The actual set of data achieved by the "sounding" consists of amplitude, decay time (or decay spectra) and phase versus excitation intensity (Figure 2). The relation of measured

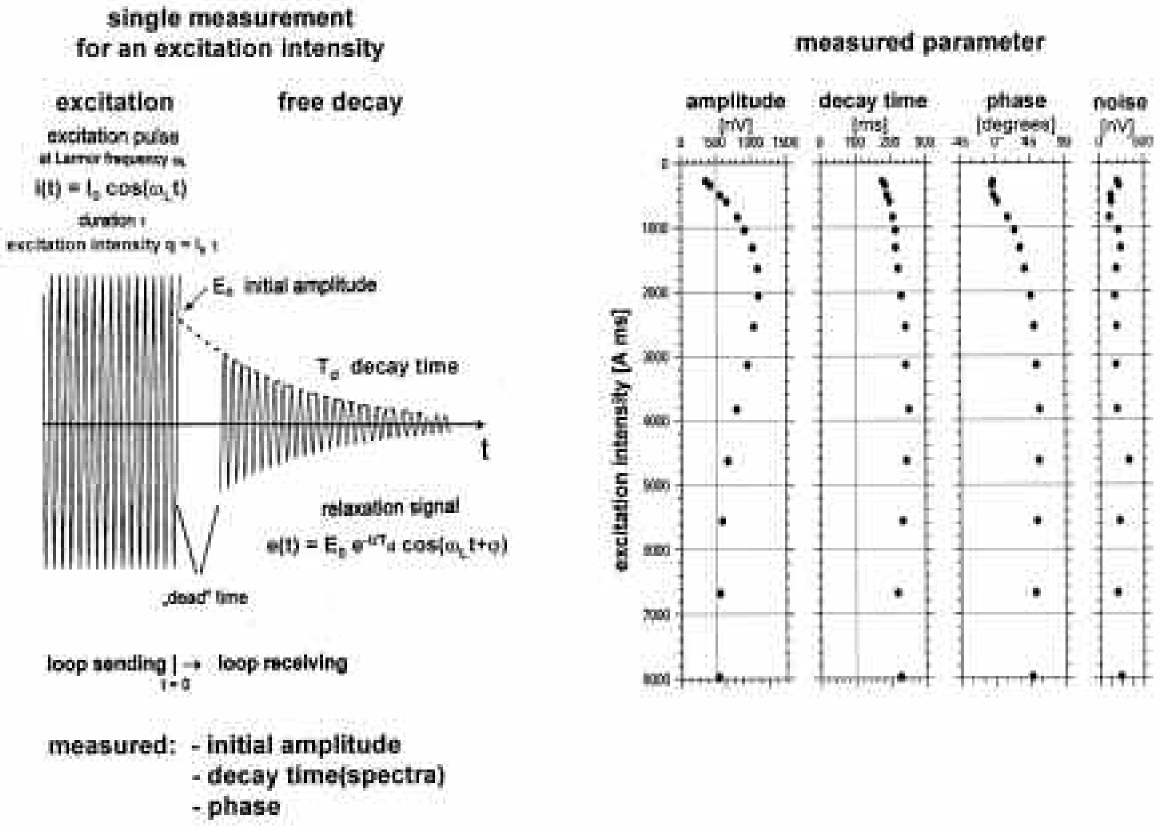


Fig. 2. Principle of a MRS measurement and sounding
Fig. 2. Principio de medición de un SRM y resultado del sondeo

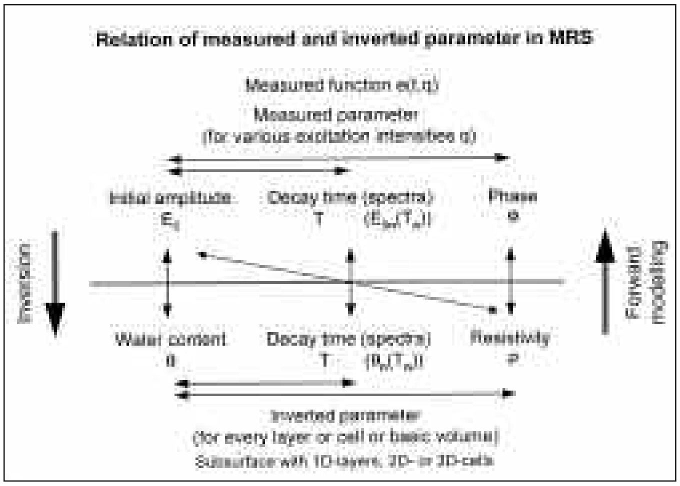


Fig. 3. Relation of measured data and inverted parameter in MRS
Fig. 3. Esquema de la relación entre los datos medidos y los parámetros obtenidos en la inversión de un SRM

data and inverted parameter can be multifold (Figure 3). The spatially selective pattern, i.e. depth penetration as well as resolution, for 1D or 2D investigations, can be achieved by variation of the excitation intensity as well as with variation of the loop layout of transmitter and receiver.

The imaging equation of the response amplitude of a single measurement is given by:

$$e(q,t) = \omega_L M_0 \frac{2}{I_0} \int_V \left|B_R^{-}(r)\right|$$
$$\sin\left(\frac{\gamma \cdot q}{I_0}\left|B_T^{+}(r)\right|\right) e^{i[\varphi_T(r)+\varphi_R(r)]}$$
$$\left[b_R^{\perp}(r) \cdot b_R^{\perp}(r) + i b_0 \cdot b_R^{\perp}(r) x b_R^{\perp}(r)\right]$$
$$\int_{T_s} w_s(r, T_s') e^{\frac{-t}{T_s'(r)}} dT_s' dr \qquad [15]$$

where:

e(q,t)= Envelope of the voltage in the receiving loop
q = Excitation intensity (Pulse moment) = $I_0 \tau$
I_0= Current through the transmitter loop
τ = Pulse duration
t =Time
ω_L= Larmor frequency = γ B_0
γ = Gyromagnetic ratio of hydrogen nuclei
B_0= Local Earth magnetic field
M_0 =Specific nuclear magnetization of water
B_R^-, B_T+ = Co- and counter-rotating components of the excitation
r = Location
φ = Phase shift due to resistivity = [φ_T(r)+ φ_R(r)]
$b_T^{\perp}$(r)= Unit direction of transmitter field perpendicular to b_0
$b_R^{\perp}$(r)= Unit direction of virtual receiver field perpendicular to b_0
b_0= Unit direction of Earth magnetic field
$w_s(r,T_s')$= Partial water contents in decay time classes
T_S'=Decay times (relaxation constants) classes

The first and second lines of the equation describes basically the excitation field in strength and in spatial distribution. It depends mainly on the excitation strength q and deflection of protons from equilibrium in the sin term. The influence of local electrical conductivity on the spatial distribution of the loop fields by electromagnetic induction shows in attenuation of B_R^- and B_T^+ and in the phase shift φ.

The third line accounts for the loop layout geometry with $b_T^{\perp}$ and $b_R^{\perp}$ the unit direction vectors of transmitter and virtual receiver field perpendicular to the Earth's field direction b_0. All contributions of the loop electromagnetic fields are only the components locally perpendicular to the static Earth's field B_0 since only these are physically acting on the Spin system.

The fourth line contains the actual effect of hydrogen protons in form of water content and relaxation. For pore structures with continuous distribution (spectra) of decay times T_s', corresponding to a pore size distribution, the respective partial water contents $w_s(r, T_s')$ in pore classes contribute with their individual decay times T_s'. Thus, this accounts for such continuous pore size geometry. The total water content per volume element w(r) is accordingly given by

$$w(r) = \int_{T_s'} f_s(r, T_s') dT_s' \qquad [16]$$

which is the main property looked for in MRS. Note that decay times in subsurface volumes are denoted by primes, while measured decay times are denoted without. Since water in very fine pores, having very small decay times, is not detectable with existing MRS equipment, the MRS determined water content is closely related to mobile water (see Plata and Rubio, 2007, this Issue).

In case of 2D or 1D conditions, the formulation is commonly simplified by reducing the kernel function to the necessary dimension by integrating the general kernel in direction of the respective Cartesian dimension. Simplifying the time dependent signal e(q,t) to its initial amplitude (at t=t_0) after pulse cut-off

$E_0(q)$, and rewriting equation [15] using the kernel function, which at the same time give the sensitivities, the expression for 3D is then

$$E_0(q) = \int_0^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty w(x,y,z) K_{3D}(q;x,y,z)\,dx\,dy\,dz \qquad [17]$$

and can be reduced to 2D as a section in depth and profile direction as

$$E_0(q) = \int_0^\infty \int_{-\infty}^\infty w(x,z) K_{2D}(q;x,z)\,dx\,dz$$

$$K_{2D}(q;x,z) = \int_{-\infty}^\infty K_{3D}(q;x,y,z)\,dy;$$

$$\partial w(x,y,z)/\partial y = 0 \qquad [18]$$

Reducing the kernel to 1D allows only a water content variation in depth

$$E_0(q) = \int_0^\infty w(z) K_{1D}(q;z)\,dz$$

$$K_{1D}(q;z) = \int_{-\infty}^\infty \int_{-\infty}^\infty K_{3D}(q;x,y,z)\,dx\,dy;$$

$$\partial w(x,y,z)/\partial x = \partial w(x,y,z)/\partial y = 0 \qquad [19]$$

A synthetic sounding is then obtained by the multiplication of a kernel function and a water content distribution of the respective dimension (Legchenko and Valla, 2002; Yaramanci *et al.,* 2005). This forward operator is the basis for the inversion to determine a water content distribution in the subsurface from measured data.

For 1D condition, the kernel function can be represented by a contour plot, demonstrating the sensitivity with depth in dependency of the excitation intensity q. The characteristics of the kernel function regarding the depth sensitivity are significantly determined by the loop size. Figure 4 shows the kernels for loop sizes of 100 m, 50 m and 20 m above an insulating half-space as contour plots. The characteristic depth focus changes to shallow depths for smaller loops. However, it is visible that the penetration depth cannot be arbitrarily increased by only increasing the

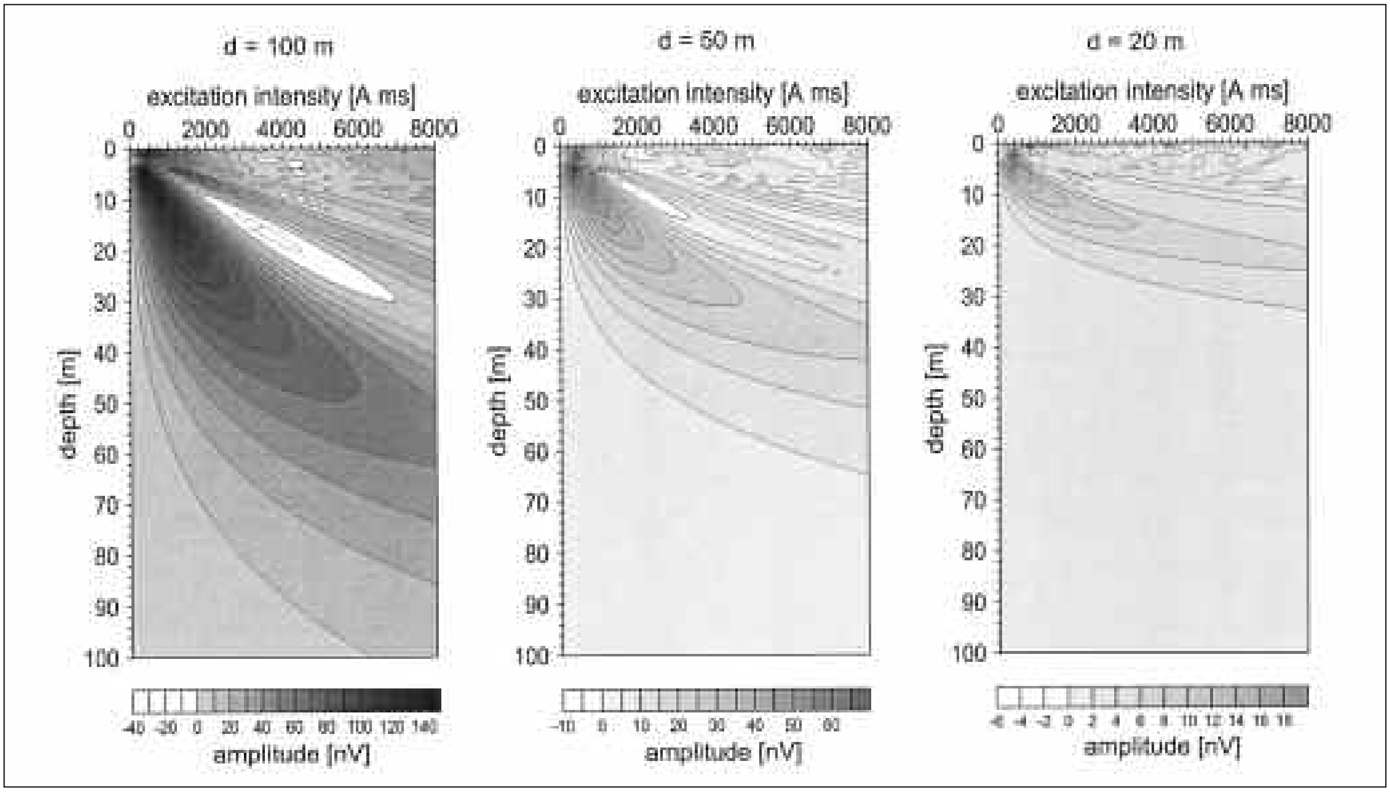


Fig. 4. Kernel functions (for 1D soundings) for different loop diameters d
Fig. 4. Funciones Kernel (en sondeos 1D) para diferentes diámetros d de la antena

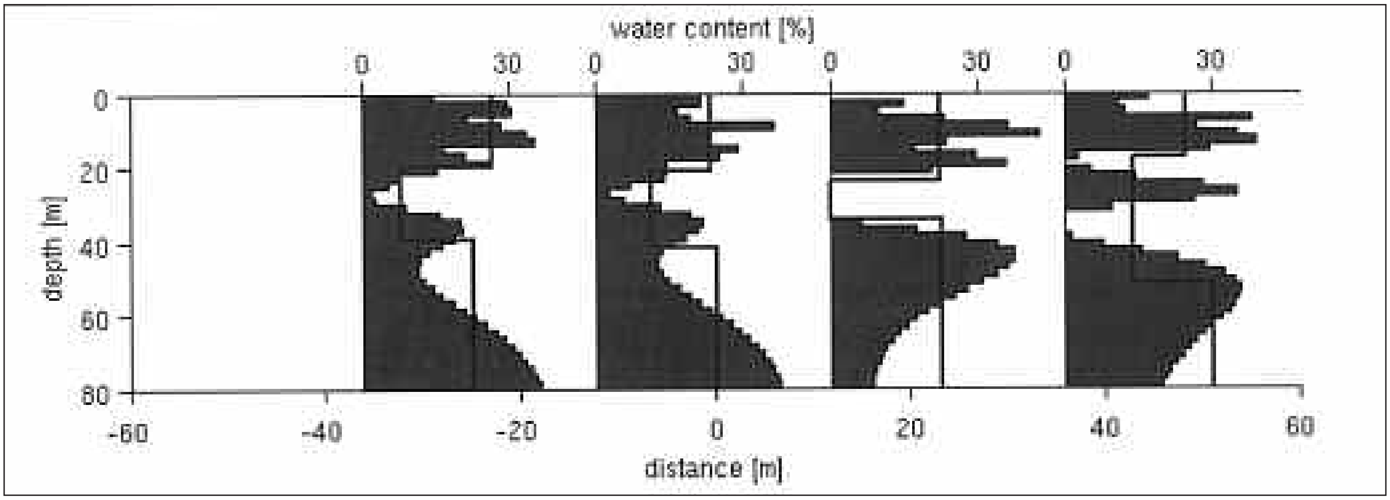


Fig. 5. Comparison of block and smooth inversion of adjacent MRS measurements at the test site Nauen/Germany. Patch plots show the smooth inversion result for a constant basic layer thickness of 1 m and moderate smoothing constraint. Line plots show the block inversion result

Fig. 5. Comparación entre los resultados de la inversión por bloques y suavizada de SRM adyacentes medidos en el lugar de ensayo de Nauen-Alemania. El gráfico sombreado muestra el resultado de la inversión suavizada adoptando como potencia básica de capa 1 m y utilizando un suavizado moderado. El diagrama de línea es el resultado de la inversión por bloques

excitation intensity since the focus depth converges to a maximum depth. Due to the reduced investigated volume for smaller loops the magnitudes of the kernels and consequently the maximum possible response signals decrease with loop size and currently limit the method for very shallow applications in the range of the usually observed natural noise.

The basic equations [15] – [19] for MRS are to be converted into the form of **d** = **G m** as to apply the schemes and principles of inversion shown for the general case.

Block and smooth inversion of MRS data

The model of subsurface water content distribution from field data is obtained by inversion. Such inverse problem is in general ill-posed for the amount of available data and limited data quality. Inversion has therefore to be constrained by reducing the number of degrees of freedom either by reducing the number of model parameters or by constraining the model parameters by sensible means. The first method, the block inversion as a result of damped least square, is achieved by allowing only a small number of discrete layers to have individual water contents and arbitrary boundary depths, the latter method, smooth inversion, is realized by a larger number of layers with fixed boundaries but variation of water content between adjacent blocks is additionally minimized during inversion and provides a smooth model of water content distribution with depth. Both methods are commonly used in interpretation of MRS data and several authors describe advantages and limitations of both approaches (Legchenko and Shushakov, 1998; Mohnke and Yaramanci, 2002; Guillen and Legchenko, 2002a, b; Weichmann *et al.,* 2002).

Figure 5 shows the comparison of smooth and block 1D inversion of four MRS measurements, recorded at the test site in Nauen/Germany. Inversion results indicate a top aquifer between 2 m and 20 m and a second aquifer below 35 m. Left of the profile both inversion results represent the aquifer structure accurately but block inversion gives a sharper estimation of aquifer boundaries. The measurement at right on the other hand indicates a more differentiated subsurface structure having an additional water bearing layer between the upper and the lower aquifer. The model of a three layer case as assumed for block inversion is consequently not capable to render this structure due to the underestimated layering at this point. From the interpretation point of view none of the two methods is objectively more precise and superior. For an accurate interpretation the most preferable way is to perform both inversion schemes in combination, deriving the necessary number of layers for block inversion from the smooth inversion result and plotting both derived models together to obtain a reliable measure of the subsurface aquifer structure.

2D MRS measurements and inversion

In extension to the conventional MRS depth soundings using coincident surface loops, the method is recently extended to allow interpretation of measurements with individual loops for transmitter and receiver (Hertrich *et al.,* 2005; Hertrich, 2005). Such measurement scheme conducted along a profile with a small number of loop positions but performing all possible permutations of transmitter and receiver finally provides a significantly improved subsurface coverage and consequently a reliable sensitivity for 2D inversion (Hertrich, 2005; Hertrich *et al.,* 2006). Figure 6 shows a survey of four loop positions along a profile covering a two dimensional water content distribution. The individual 1D inversion is the one shown in Figure 5. Obviously, the 2D inversion of all possible soundings provides a high resolution rendering of the 2D structure. Automation of such surveys by a multi-channel recording system then provides superior 2D investigations at feasible survey speed.

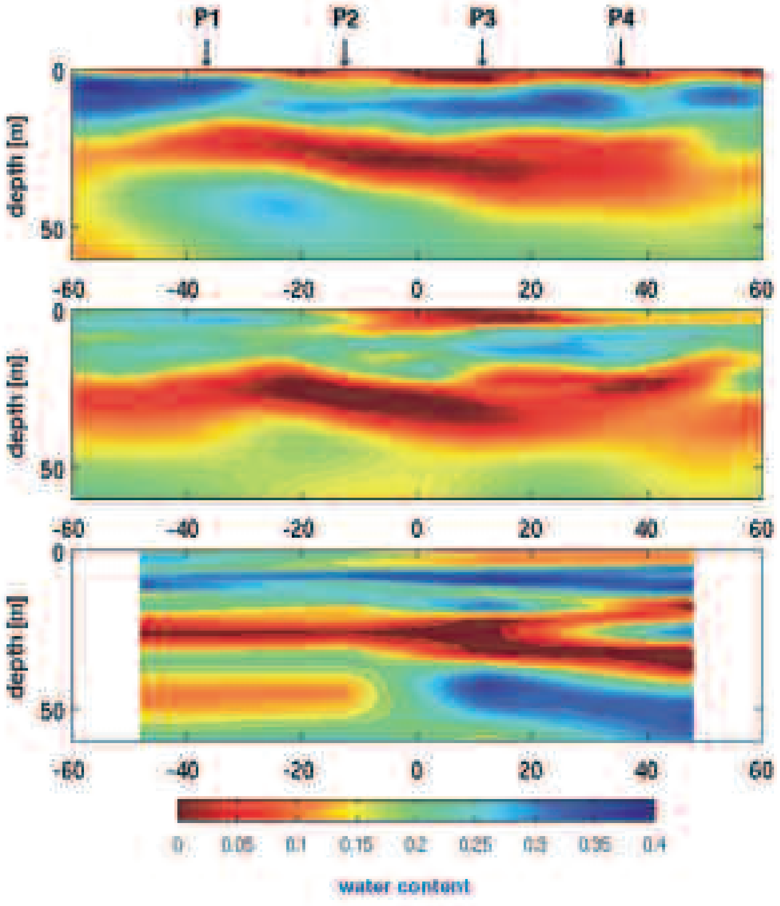


Fig. 6. 2D inversion of MRS data (Nauen/Germany). Comparison of different inversion approaches. Top: 2D inversion of the complete dataset using the four coincident loop soundings at P1-P4 and additionally the twelve separated loop soundings. Middle: 2D inversion of the four coincident loop soundings only. Bottom: Individual 1D inversion of coincident loop soundings (from Figure 5) countered to 2D

Fig. 6. Inversión 2D de datos de SRM (Nauen/Alemania). Comparación de diferentes sistemas de inversión. Parte superior: inversión 2D del conjunto de datos, utilizando los cuatro sondeos medidos con bucle coincidente en P1-P4 junto con los doce sondeos de bucles separados. Centro: inversión 2D tomando solamente los cuatro sondeos de bucle coincidente. Parte inferior: resultado de la inversión 1D para los sondeos de bucle coincidente (Figura 5) representado en 2D

Resistivity inversion from MRS measurements

The MRS signal on a conductive subsurface is given by the volume integral in equation [15]. The distribution of the electromagnetic field generated by the transmitter and received with the surface loop controls the response signal beside the water content distribution. The spatial distribution of these fields is according to electromagnetic theory dependent on the subsurface electrical conductivity, its stratification and the frequency of the inducing current. Due to electromagnetic induction, these fields are in general complex valued and possess elliptical polarization. Consequently, the recorded NMR signal is also complex valued (Shushakov, 1996; Valla and Legchenko, 2002; Weichmann *et al.,* 2000; Braun *et al.,* 2005). Here, the contribution of the phase lag of a subsurface point is scaled by its induced magnetization and the water content. Performing a conventional depth sounding then leads to complex amplitudes in dependency of the excitation intensity.

Some previous work already showed that a joint inversion of MRS and Vertical Electrical Sounding (VES) considering only the amplitudes is possible and capable to improve on estimation of aquifer characteristics (Hertrich and Yaramanci, 2002). In a recent research project investigations are conducted to invert for the resistivity from the complex valued

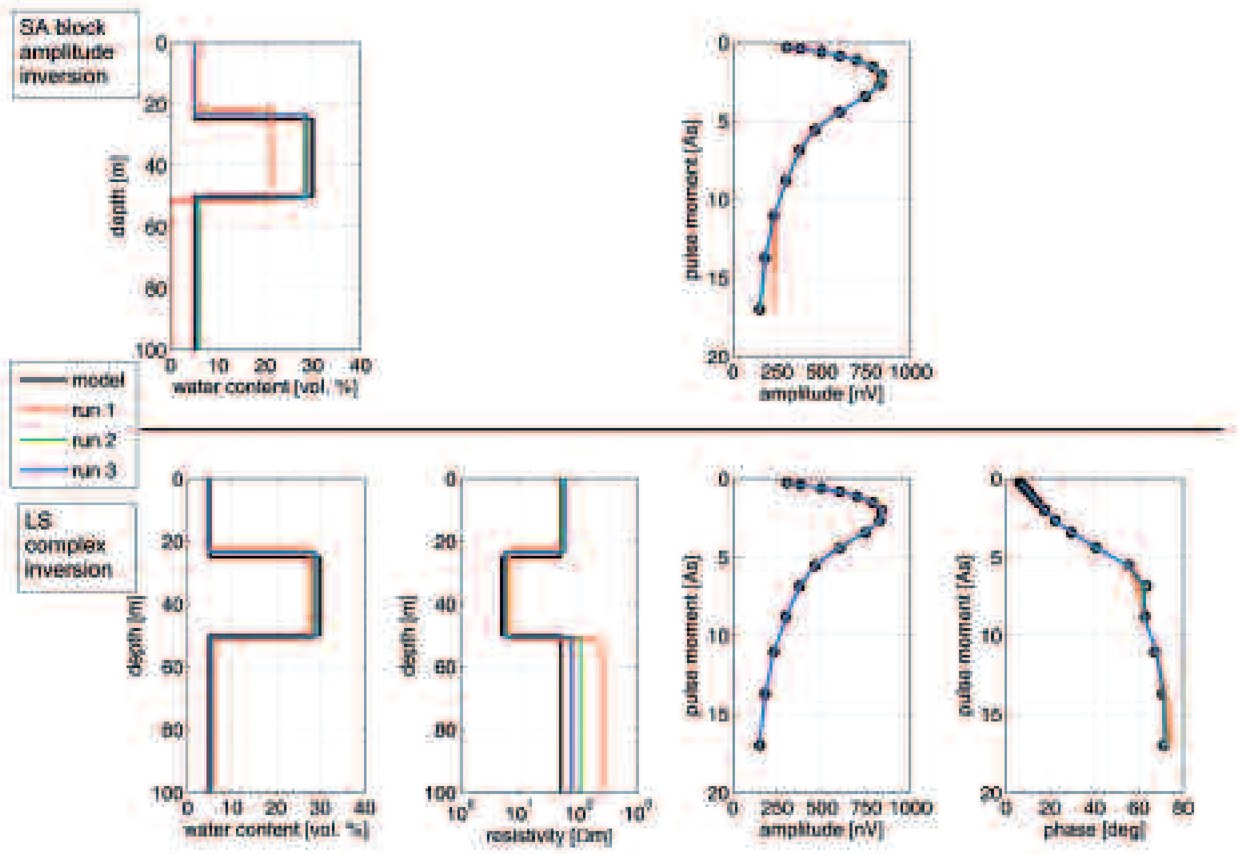


Fig. 7. Inversion for resistivity from MRS data. Top: Inversion of water content and layer boundaries from amplitudes using the SA block inversion. The resistivity must be given as initial for 1. iteration and used from previous LS inversion otherwise. Bottom: Inversion for water content and resistivity from amplitudes and phases using the LS complex inversion. The layer thickness is fixed according the result of previous SA inversion

Fig. 7. Inversión de resistividad a partir de datos de SRM. Parte superior: Inversión obteniendo el contenido en agua y los límites de capa a partir de las amplitudes de la señal SRM, utilizando el método de inversión por bloques SA. La resistividad debe introducirse para la primera iteración, utilizándose la obtenida en la inversión por LS para las siguientes. Parte inferior: inversión obteniendo el contenido en agua y la resistividad a partir de las amplitudes y fases de la señal SRM, utilizando la inversión compleja por LS. La potencia de las capas utilizada en esta fase es la obtenida en la fase previa de inversión SA

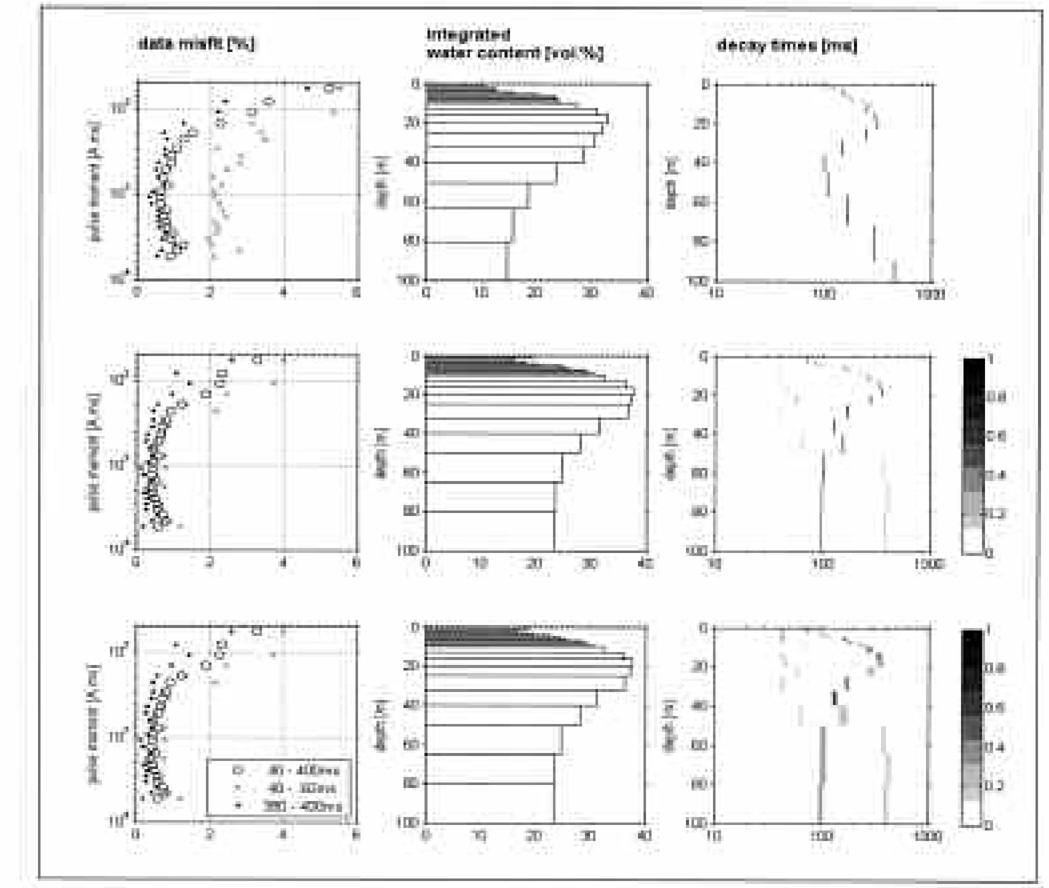


Fig. 8. Inversions of decay time distributions from MRS data (Waalwijk-2). Left column: Percentage data misfit for time windows. Center column: Water content. Right column: Decay time distribution. (Gray scale denote amount of partial water content). Different kind of inversions are shown with (a) at top: Conventional mono-exponential, (b) at middle: Using two free decay times, (c) at bottom: Using 100 fixed decay times

Fig. 8. Inversión para obtener la distribución de los tiempos de decaimiento para datos SRM (Waalwijk-2). Columna izquierda: errores de ajuste para las diferentes ventanas de tiempo. Centro: contenido en agua. Derecha: distribución de la constante de decaimiento. (la escala de tonos grises indica la cantidad parcial de contenido en agua). Se han utilizado diferentes sistemas de inversión. (a) fila superior: método convencional mono-exponencial; (b) fila media: utilizando dos valores de la constante de tiempo; (c) fila inferior: utilizando 100 valores fijos para la constante de tiempo

MRS including not only the real part but also the imaginary part of the signal (Braun et al., 2005; Braun, 2007). An inversion algorithm based on both Least Square (LS) and random search with Simulated Annealing (SA) (Mohnke and Yaramanci, 1999) has been developed to determine both the water content distribution and the layer resistivity for a 1D stratified Earth and conventional coincident sounding. The crucial point is that the acting magnetic field depends on the electrical conductivity and the complete forward problem must be recalculated in each iteration. Therefore, an inversion scheme has been developed that comprises the stability of the SA inversion and the fast convergence of the LS algorithm. Figure 7 shows the results for synthetic data using this new approach. First inversion of amplitudes (using a guess for resistivity) with SA yields a first estimate of the water content and the thickness of the layers. Using this estimated layer thickness, the LS complex inversion of amplitude and phase yields new water content and also a resistivity distribution. Run 2 of the SA inversion uses the electrical resistivity distribution of the LS inversion run 1. The procedure then is used iteratively.

Inversion of decay times spectra

The MRS signal exhibits basically an exponential decay for each excitation intensity. Whereas the initial amplitudes are proportional to the amount of water in the subsurface, the decay times are a function of pore sizes (e.g. Kenyon, 1992). While small pores correspond to small decay times large pores will exhibit long decay times. In general the MRS signals exhibit a multi-exponential relaxation behavior due to a signal superposition of layers or volume units having different decay times and due to a possibly multimodal decay time distribution within layers or volume units.

While the conventional inversion approaches assume mono-exponential relaxation, a new comprehensive inversion scheme allows taking into account the multi-exponential features (Mohnke and Yaramanci, 2005). Such sophisticated data analysis can yield a more realistic decay time distribution with depth. Moreover, since the initial signal amplitudes are proportional to water content, improvement of data fitting by multi-exponentials obviously improves the estimated water content. So far the water contents are usually underestimated by the conventional approach.

An example is shown with conventional mono-exponential inversion (Figure 8 a) and the multi-exponential inversion (COIN) using free and fixed decay times (Figure 8 b and 8 c). Conventional inversion

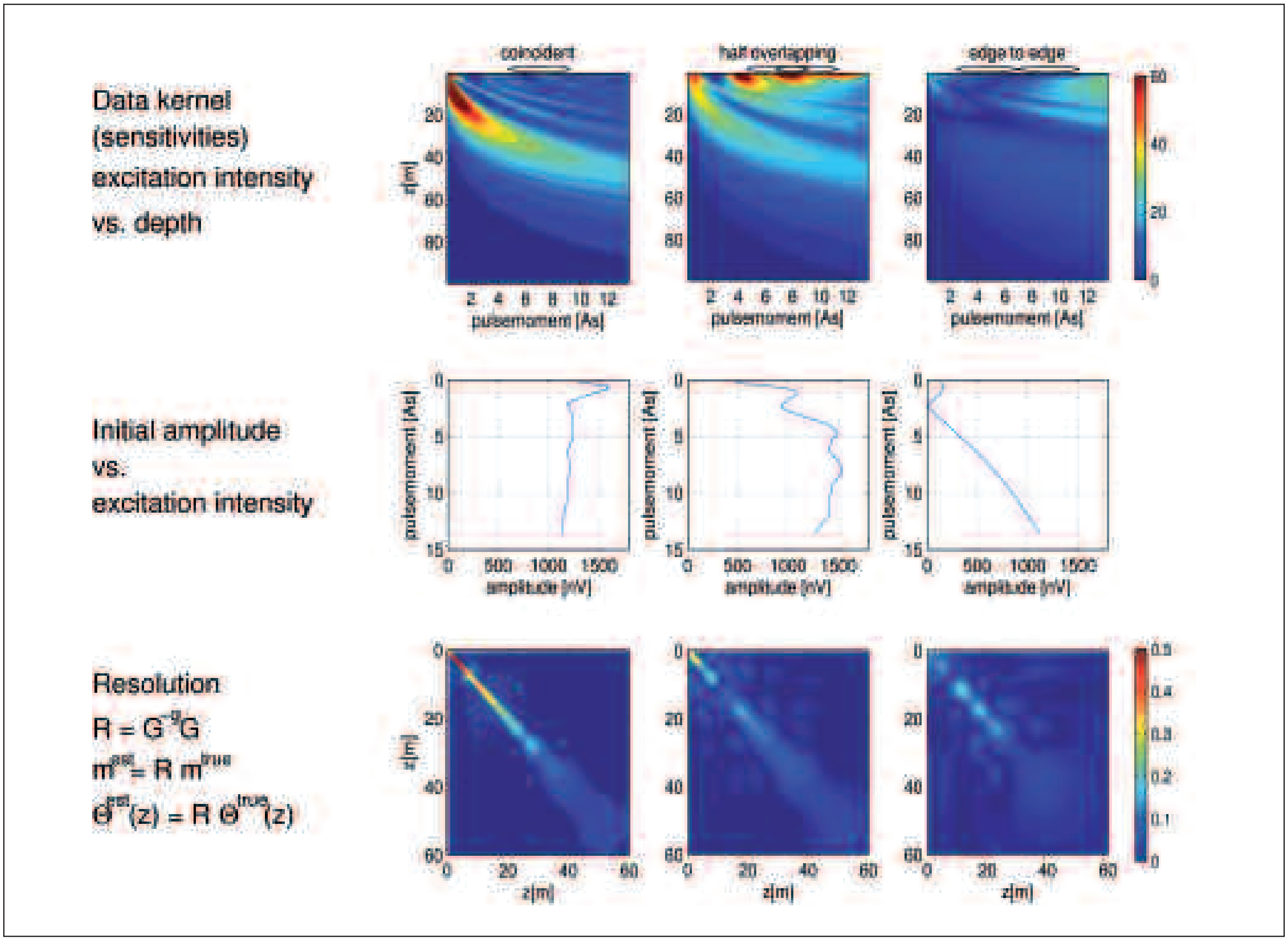


Fig. 9. Sensitivities, initial amplitudes and model resolutions for different loop lay-outs with 24 m loop radius, 100 ohm.m Wm halfspace resitivity (normalised water content to 100%)

Fig. 9. Sensibilidad, amplitud inicial y resolución para diferentes configuraciones de antenas de 24 m de radio y terreno de 100 ohm.m de resistividad

	Measured Parameter				Inverted Parameter				Modelling [references]	Modelling and Inversion [references]	year
	Initial amplitude	Decay time	Decay time spectra	Phase	Water content	Decay time	Decay time spectra	Resistivity			
1D	x				x				[1],[2],[3]	[1],[2],[3]	1989
	x	x	--		x	x	--		[4]	[4]	1991
	x	--	x		x	--	x		[9],[15],[16]	[9],[15],[16]	2001, 2005
	x			x	x			x	[5],[6],[7],[10]	[13]	1992, 2005
	x	x	--	x	x	x	--	x			In prep.
	x	--	x	x	x	--	x	x			In prep.
2D	x				x				[8]	[11],[12]	2000
	x	x	--		x	x	--		[11]	[11]	2002
	x	--	x		x	--	x		[14]		In prep.
	x	x	--	x	x	x	--	x			In prep.
	x	--	x	x	x	--	x	x			?
3D	x	--	x	x	x	--	x	x	[11]		?

Table 3 Overview about the current state of inversion for MRS
[1] Semenov, 1987 [2] Semenov *et al.,* 1989 [3] Legchenko *et al.,* 1990 [4] Shirov *et al.,* 1991 [5] Shushakov and Legchenko ,1992 [6] Trushkin *et al.,* 1995 [7] Weichman *et al.,* 1999 [8] Eikam ,2000 [9] Mohnke, *et al.,* 2001 [10] Braun *et al.,* 2002 [11] Warsa *et al.,* 2002 [12] Hertrich *et al.,* 2004 [13] Braun, 2007 [14] Braun *et al.,* 2005 [15] Mohnke and Yaramanci, 2005 [16] Roy and Lubczynski, 2005.

Tabla 3. Esquema de la situación actual de los sistemas de inversión de SRM. [1] Semenov, 1987 [2] Semenov et al., *1989 [3] Legchenko* et al., *1990 [4] Shirov* et al., *1991 [5] Shushakov and Legchenko,1992 [6] Trushkin* et al., *1995 [7] Weichman* et al., *1999 [8] Eikam, 2000 [9] Mohnke,* et al., *2001 [10] Braun* et al., *2002 [11] Warsa* et al., *2002 [12] Hertrich* et al., *2004 [13] Braun, 2007 [14] Braun* et al., *2005 [15] Mohnke and Yaramanci, 2005 [16] Roy and Lubczynski, 2005.*

shows a shallow aquifer in 6-50 m with maximum water content of about 33 %, which is underestimated. The decay times range in 200-300 ms for the aquifer layer and in 100-150 ms for neighboring layers. For depths greater than 50 m the decay times are about 400 ms with an increase of data misfit and do not comply with the fine grained material found in borehole data. The multi-exponential inversion, on contrast, shows higher water contents and appropriate decay times, which considerably improves the subsequent estimation of pore sizes i.e. hydraulic conductivities and transmissivities.

Model resolution matrix for the inversion

A very useful exercise by inversion is the investigation of the model resolution matrix, which will give an insight about the estimated model parameter to which degree and in which way they depend on the true values of the model parameter. In extreme favorable case the model resolution matrix will have only nonzero elements in the diagonal meaning that an estimated model parameter depends only on the true value of this parameter and not on other model parameters (Mueller-Petke et al., 2006). In Figure 9 an assessment of different loop layout are given showing that separated loops do have only a small depth sensitivity but a higher resolution.

Outlook

The inversion of MRS data is subject of ongoing research with newly introduced improvements for which some examples are shown previously. A comprehensive account on the state of art of MRS inversion is given in Table 3 showing the possibilities currently available, i.e. that what can be measured and inverted and in particular the dimensionality of the inversion. The higher dimensionalities obviously require adequate data collection, which have appropriate sensitivities and justifiable afford of field logistics in particular measurement times.

The basic equation of MRS shown in this paper presents the most sophisticated and complete formulation of the underlying physics and mathematical description in the state of the art in MRS methodology. It covers the resistivity influence on the electromagnetic fields, spectral nature of MRS relaxation and the general formulation of measurements using separated transmitter and receiver loops. The given examples and case histories underline the improvement in application of MRS in challenging new approaches in geophysical groundwater investigation.

The obtained results prove the establishment of this new technology of MRS in hydrogeophysical applications. The capability of this technique to determine quantitative measures of water content distribution and pore space properties provides unique parameters in hydrogeological interpretation quite different from other surface geophysical investigations. Complementary to conventional geophysical methods, in particular to electrical an electromagnetic methods the application of MRS gives essential information of aquifer structure and characteristics. The method is in its current state of the art already capable to meet new challenges in hydrogeophysical investigation.

The reliable inversion is crucial for the success of MRS. Improved inversion is not only needed for having better estimates of the subsurface properties. It also serves as a guide to design measurements, layouts and defines technical requirements for new hardware capable to measure physical properties, which have been shown to exist in the data and can therefore be extracted.

For a reliable and appropriate inversion, we do need to asses the requirements and the possibilities. Some of the questions arise, which need to be answered may serve as a guide:

- 1D or 2D or 3D?
- Which data to be used? How to conduct the measurements? Coincident loop, separated loop, etc.?
- Which subsurface parameter to be inverted? Water content, decay time, decay time spectra, resistivity?
- Which scheme? Smooth or block? Sharpness? How much of it? Which assumptions and simplifications are actually made? (Implicit and explicit) by the choice of the kind of solution (inversion scheme)?
- Layer (or cell) size?
- Fixed layer boundaries? Free layer boundaries?
- Including priory knowledge? Conditioning inversion? (layer boundaries, resistivities, water contents, by borehole, core samples, other geophysical measurements, ...)

Beyond current conventional application of MRS on detection and characterization of aquifers, future work shall focus also for example on contamination detection and preferential migration prediction, monitoring of variations in water content in the saturated as well in the vadose zone and application of the technology on targets with very low porosity or complex fractured porosity. The inversion schemes to be developed need to take account on this.

The technique in its current state of development is designed for target depths between 5 to 150 m. Oncoming research focus will evaluate the applicability and limitations of the technique both to larger and smaller scales.

Implementing currently developed new numerical approaches allowing for arbitrary 2D and 3D topography and internal structure a variety of new challenges in environmental and engineering problems can then be focused.

Beside the basic research on MRS itself additional effort shall be taken in determination of reliable correlation of physical parameters determined in the field to petrophysical and hydrogeological parameters. Implementation of comprehensive laboratory work to understand the processes in the pore space scale and to validate field results is being realized in supplementary projects.

Emerging new aspects and possibilities in numerical modelling, data processing, physical understanding and mathematical foundation, data inversion and interpretation as well as technical advance of measurement equipment will provide further development of MRS technology and an active research environment for hydrogeophysical research.

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