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Use of MRS for hydrogeological system parameterization and modeling

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ABSTRACT

In this paper, first, a revision of those hydrogeological parameters that can be derived with MRS is presented followed by explanation on how those parameters can be derived from the MRS data and what are the limitations. In this manner, the aquifer storage and flow parameters are presented with emphasis on practicality of MRS use in aquifer system parameterization and on limitations of the conversion of MRS output into hydrogeological data. Next, the integrated use of storage and flow parameters is discussed in subsurface hydrostratigraphy applications. This is followed by discussion on the potential of MRS for vadose zone investigation with emphasis on suitability for depth-wise evaluation of unsaturated zone moisture. Finally, the MRS-specific ability of large volume data integration is discussed in the context of hydrogeological data integration and as input data provider for distributed groundwater models.

Key words: groundwater, hydrogeological parameterization, MRS, saturated zone, unsaturated zone

Utilización de los SRM en la obtención de parámetros y en la preparación de modelos de sistemas hidrogeológicos

RESUMEN

En este trabajo se presenta, en primer lugar, una revisión de los parámetros hidrogeológicos que pueden obtenerse a partir de los SRM, explicando seguidamente la forma en que pueden utilizarse los datos de SRM para su cálculo, así como las limitaciones existentes. En este sentido, se presentan los parámetros de almacenamiento y flujo de los acuíferos, enfatizando la viabilidad de la utilización de los SRM en su obtención, y los límites existentes en la conversión de los valores obtenidos en un SRM en datos hidrogeológicos. En segundo lugar, se analiza el uso integrado de los parámetros de almacenamiento y flujo en aplicaciones de hidroestratigrafía del subsuelo, pasando seguidamente a discutir el valor potencial que tienen los SRM para la investigación de la zona vadosa, con especial énfasis en su adecuación para la evaluación de las variaciones de la humedad con la profundidad en la zona no saturada. Finalmente, se analiza la capacidad específica del método SRM, que proporciona valores integrados provenientes de un gran volumen del subsuelo, en el contexto de integración de datos hidrogeológicos y su aplicabilidad como método para proporcionar datos para modelos de distribución de agua subterránea.

Palabras clave: agua subterránea, evaluación de parámetros hidrogeológicos, SRM, zona no saturada, zona saturada

Introduction

Groundwater engineering has approximately 150 years of experience since Darcy's publication on Dijon's water supply. By contrast, the geophysical MRS technique is commercially available only for last approximately 10 years. MRS is adding new ways to explore, quantify, monitor and manage groundwater resources being able to contribute to aquifer system parameterization and modeling. It supplies however information in different ways than classical hydrogeological mapping and borehole testing, using also different physical principles.

MRS supplies a depth-wise in-situ NMR water content characteristic that is convertible into hydrogeological parameters of saturated and unsaturated zones. In special cases now, and likely in normal cases in the future, it also supplies the pore-size distribution as a function of depth, which together with water content provides a much more detailed evaluation of aquifer storage and flow property than what is offered by classical geophysical techniques.

There are solid physics foundations on the use of MRS to determine both groundwater storage and flow properties. Therefore in hydrogeological system parameterization, MRS is less ambiguous than any other geophysical method. MRS has advantages not only as compared to other geophysical methods but even as compared to standard hydrogeological pumping test parameterization method considered widely as reference in that field. In contrast to pumping test, MRS data is acquired non-invasively, i.e. through a series of measurements made from the surface without need of expensive and time consuming drilling boreholes and pump testing. As it is a sounding method, it supplies information as a function of depth. Boring a hole also supplies information from cuttings discriminated as a function of depth while most pump tests supply information on a 'bulk' volume, without depth-wise discrimination of the horizons contributing to the test, except when several tests are run with packers. Besides pump tests provide information without lateral heterogeneity of the area adjacent to the well. Such depth-wise and lateral aquifer heterogeneity can be resolved with MRS. Finally, for a pump test, the time, cost, resources, and environmental impact are significantly larger than for an MRS test.

As compared to MRS, pump tests have however one fundamental advantage; the information supplied originates from dynamic test where aquifer is exposed to a hydraulic stress originated from borehole yield. In such test, the aquifer i.e. groundwater table (or potentiometric surface in case of confined aquifers) is 'observed' in situ as function of time. This is mainly why, despite MRS efficiency and convenience, the pump test method is considered as reference in hydrogeology and as such is also considered in this study.

MRS is a relatively new method so it is quite normal it still has some problems. For example there are still locations with low signal-to-noise ratio or with high magnetic gradient where MRS surveys are likely unsuccessful. Besides, 3D or even 2D MRS surveys are not yet operational. Finally it is still difficult to define one-to-one correspondence between information supplied by MRS and pump tests or grids of numerical groundwater models. MRS technology has however large potential and is in rapid development so the remaining problems will most likely be solved soon. Once it is done it will enhance the hydrogeological applicability of that already well performing method and consolidate its position in hydrogeology.

Storage related parameters

A basic definition of the parameters used to characterize an aquifer has been presented in Mejias and Plata (2007, this Issue). In MRS applications, all the storage related parameters are derived from MRS parameter called MRS water content (θ_{MRS}). θ_{MRS} is defined as percentage of water with depth derived from the MRS inversion of the initial signal amplitude, as described in Plata and Rubio (2007, this Issue) and Yaramanci and Hertrich (2007, this Issue). The subsurface hydrogeological parameterization with MRS is based on the assumption that the θ_{MRS} is comparable with the free water content (θ_f) defined in hydrology as the percentage of water that is outside the field of molecular forces of attraction of the solid particles that can be displaced by gravity or hydraulic head gradient, with respect to the total rock volume (Lubczynski and Roy, 2003). Based on that assumption $\theta_{MRS} \approx \theta_f$, the MRS technique can contribute to the evaluation of the following storage-related parameters: effective porosity, total porosity, specific yield, specific storage, elastic storativity, specific drainage, specific retention and hydrostatic water column.

Overview of the selected storage-related parameters

Conversion between MRS output and storage-related parameters requires not only a good knowledge of MRS technique but also a good hydrogeological knowledge of the storage parameters to be defined with MRS. Besides, there are differences in terminology between the disciplines of hydrology, soil science and geophysics, particularly with respect to the least-defined microscopic processes at gas-liquid-solid interfaces at the pore level. Therefore, before discussing the conversion of the MRS signal into hydrogeological parameters, in the following section, the hydrogeological parameters, most relevant to MRS, are discussed and the appropriate terminology is harmonized.

Effective porosity, total porosity

Effective porosity (n_e), also known as kinematic porosity (Marsily, 1986), is generally defined as the portion of a medium that contributes to flow (Domenico and Schwartz, 1990; Fetter, 2001) or in solute transport studies as that portion of the soil or rock through which chemicals move (Stephens *et al.,* 1998). The most appropriate definition, however, seems to be that the effective porosity represents the portion of a medium that contributes to the flow and advective transport (transport according to the velocity vector due to the presence of a hydraulic gradient). The main application field of n_e is contaminant-transport modeling according to the advective-dispersive equation (Zheng and Bennett, 1995), in which n_e, is the parameter that characterizes advective solute transport. n_e refers to the motion of water through flow and transport processes therefore water content involved in this motion is called mobile water content (θ_m) as presented in Figure 1.

The total porosity (n) also known as porosity, is defined as the percentage of rock or soil that is void of material (Fetter, 2001). The n is greater than n_e (Figure 1) because, firstly, part of n corresponds to bound water θ_b, i.e. water attached to the surface of the grains due to the forces of molecular attraction and, secondly, because another part of n can be occupied by unconnected and dead-end porosity.

The pores that are not interconnected, as it is typical in volcanic and karstic rocks, are defined in hydrogeology as an unconnected porosity. Dead-end porosity (fractures and micro-joints but also non-flowing karstic cavities, etc.) is represented by "blind" pore channels. Dead-end porosity is abundant in karstic and hard-rock aquifers. Unconnected and dead-end porosity that does not contribute to groundwater flow and solute transport are referred together as trapped porosity (n_t). In unconsolidated sediments and in sandstones, the role of n_t is negligible and can usually be disregarded. In rocks with considerable n_t, e.g. karstic rocks, the θ_t in unsaturated zone can vary with time because of variable θ_t in dead-end pore channels, and in saturated zone is equal to n_t (Figure 1).

Effective porosity (n_e) is dependent on rock type. It is high in well-sorted sands or gravels, but also in clayey rock types (Table 1) and low in poorly sorted deposits, such as glacial tills. High effective porosity in clayey rock types is due to the large contribution of water that is not drainable by gravity but that can move and carry solutes due to advection. Groundwater flow occurs only in the portion of rock defined through effective porosity and in microscopic processes, it refers to the continual exchange of molecules from one phase to the other through molecular Brownian motion. For example, a circulating molecule may become immobilized in the course of its progress, while another one that was originally immobile may be set in motion (Marsilly, 1986). Brownian motion occurs also in clays therefore clayey fractions of rocks contribute to effective porosity as well (in contrast to specific yield). In contaminant-transport modeling, it is common practice to make an initial guess of effective porosity from the laboratory estimates of the total porosity or from the standard literature as shown in Table 1. Tracer methods (laboratory and field) are more sophisticated but

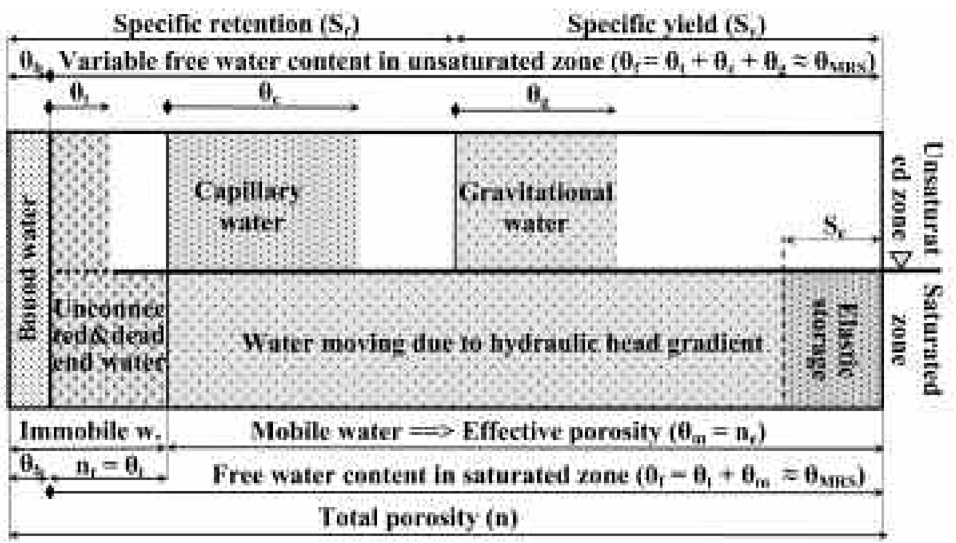

Fig. 1. Aquifer storage concept (Modified after Lubczynski and Roy, 2005)
Fig. 1 Esquema conceptual de almacenamiento de agua en un acuífero (Modificado de Lubczynski and Roy, 2005)

are quite seldom used because of their cost, duration and the possible impact of the tracer upon the aquifer, which often leads the regulators to forbid tracer application. The most reliable but also the most time- and data-demanding n_e method, is calibration of a distributed, solute transport model, based on spatio-temporal distribution of a concentration of natural tracer, artificial tracer (e.g. NaCl) or even contaminant. The advantages of using distributed groundwater models for n_e assessment are that various sources of information can be integrated in the model calibration against n_e, and that models can well depict spatial aquifer heterogeneity, providing n_e output spatially.

The media heterogeneity and the scale-effect problem (Sanchez-Vila, *et al.,* 1996) result in substantial differences between n_e derived using various methods (Stephens *et al.,* 1998). The lack of a universal, efficient and accurate n_e evaluation method in hydrogeology, creates a unique opportunity for MRS because, firstly, MRS experiment is much cheaper and less time consuming than tracer test, secondly, MRS survey provides output from a large investigated volume up to approximately 10^6 m^3, depending on loop size (Lubczynski and Roy, 2003) so it well handles the heterogeneity problem and thirdly, MRS has a solid scientific, NMR background, particularly suitable for quantitative assessment of water in the subsurface.

Storativity, specific yield, specific drainage and elastic storativity

The storage of aquifers is typically described by a storativity parameter (Fetter, 2001), which consists of a gravitational component, representing water that can be removed from a rock due to the forces of gravity, and of an elastic component, representing water that can be removed from a rock due to the water expansion and aquifer compaction attributed to aquifer pressure changes.

Storage of unconfined aquifers is described by unconfined storativity term (S_u). S_u consists of dominant gravitational storage represented by specific yield (S_y) and negligible elastic storage. Therefore often the assumption is made that $S_u \cong S_y$. The S_y of a rock/aquifer is the ratio of the volume of water a rock/aquifer releases from storage by gravity forces, to the total dewatered rock/aquifer volume. In the hydrological literature, specific yield is often confused with effective porosity despite they represent two different parameters. These two parameters do have in fact comparable values for coarse rock materials where $S_y \cong n_e$. However, in fine-grained rocks and particularly in clayey materials, S_y is low while n_e is high so the S_y differs substantially from n_e (Table 1).

S_y has critical importance in groundwater resources evaluation. For example, the process of dewatering of an aquifer, geometrically defined by a cone of depression (Figure 2), is governed by gravity-based drainage of groundwater to a pump or groundwater drain. Therefore in any aquifer, S_y provides a direct estimate of the quantity of potentially extractable water for water resources development projects. Not only dewatering but also replenishment of unconfined aquifers is governed by S_y. In such application S_y allows for estimation of aquifer recharge using groundwater table fluctuation monitoring (Lubczynski and Gurwin, 2005). In large water resources evaluation scales, S_y estimates are also used as input for calibration of transient groundwater models and for model prediction scenarios commonly applied in groundwater management. S_y depends upon rock type, pore-size, texture and sorting. The nature of this dependence is generally known (Figure 3 and Table 1). S_y can be estimated from literature sources but it can also be determined experimentally by gravitational dewatering of a fully saturated rock. For example, by dewatering a vertical column filled in with water-saturated sand, King (1899) successfully determined S_y as equal to 0.20 although it took him two-and-half years to obtain that particular result. Conveniently and reliably but expensively, S_y can be determined by field experiments called piezometric pumping tests (Kruseman and de Ridder, 1990). Piezometric pumping tests in contrast to single well pumping tests consist of well and at least one observation piezometer recording behavior of an aquifer in response to the well abstraction. In large scale water resources projects, specific yield can also be accurately determined by transient model calibration (Lubczynski and Gurwin, 2005).

Storage of confined aquifers is described by confined storativity term (S_c) consisting of elastic storage represented by elastic storativity (S_e) and gravitational storage. The elastic storage is the volume of water that can be released from confined aquifers owing to the compressibility of the rock skeleton and compressibility of pore water. Therefore S_e is not an extra volume of water but rather part of the overall water content in the aquifer (Figure1). When the groundwater potentiometric surface remains above the bottom of the confining layers (Figure 3), the S_e is dominant and gravitational storage negligible, therefore often the assumption is made that $S_c \cong S_e$. This assumption however becomes invalid when potentiometric surface starts falling below the bottom of the confining layer, for example due to the well abstraction; this

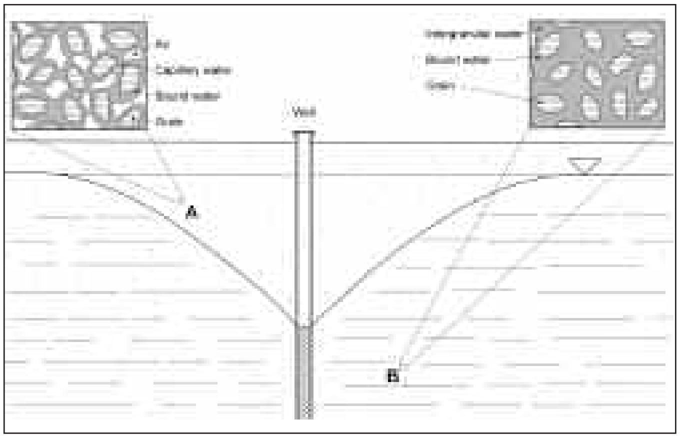

Fig. 2. Dewatering of an unconfined aquifer in macroscopic and microscopic views of: (A) an unsaturated zone and (B) a saturated zone (after Lubczynski and Roy, 2005)

Fig. 2. Esquemas general y de detalle de un acuífero libre durante la extracción de agua: (A) en la zona no saturada, y (B) en la zona saturada (según Lubczynski and Roy, 2005)

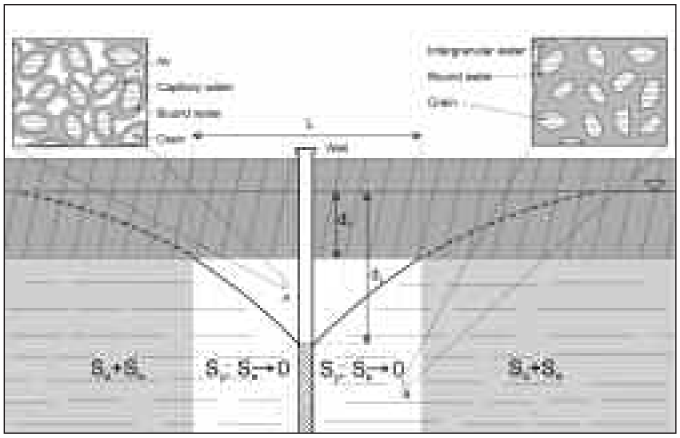

Fig. 3. Dewatering of confined aquifer in macroscopic and microscopic views; dark shaded – confining layer; light shaded – confined part of the aquifer; white – unconfined part of the aquifer with macroscopic views of: A – an unsaturated zone; B – a saturated zone

Fig. 3. Esquemas general y de detalle de un acuífero confinado durante la extracción de agua; en gris oscuro se representa la capa impermeable superior; en gris claro, la porción confinada del acuífero; en blanco, la parte no confinada del acuífero, con esquema de detalle de la zona no saturada (A) y saturada (B)

creates then a local unconfined conditions from which water is released by action of gravity according to the specific drainage (S_d).

The elastic storativity (S_e) is defined as

$$S_e = S_s \Delta z \qquad [1]$$

where Δz is the aquifer thickness and S_s-specific storage (aquifer-specific coefficient) defined as

$$S_s = \rho g(\alpha + n\beta) \qquad [2]$$

where ρ – density of water; g – acceleration of gravity; α – compressibility of the aquifer skeleton; n – aquifer porosity; and β – compressibility of the water. The specific drainage (S_d), as defined by Lubczynski and Roy (2004), is the ratio of the volume of water that could potentially be released from the confined aquifer by gravity forces if the piezometric surface falls below the bottom of the confining layer, thus creating unconfined conditions, to the total confined aquifer volume. S_d quantifies a virtual gravitational storage of the confined aquifers that would equal to S_y if aquifer conditions changed into unconfined, e.g. by physical depressing of the potentiometric surface below the bottom of the confining layer by action of pump. Thus the term S_d, was implemented to describe gravitational storage of confined aquifers in non-invasive way (e.g. of an aquifer under thick layer of clay). Before introducing MRS, this was not possible.

In well abstraction of confined aquifers, two storativity types are involved in the dewatering process, elastic storativity (S_e) and gravitational storativity called specific drainage (S_d) according to $S_c = S_e + S_d$. In that process reflected by expansion of a cone of depression, at the beginning of pumping $S_c \cong S_e$; this remains until the cone of depression reaches the bottom of the confining layer; from that moment continuous expansion of the cone of depression, is associated with increase of S_d and decrease of S_e, so the S_d cannot be anymore neglected in calculation of S_c.

Specific retention

Specific retention (S_r), in soil science also known as field capacity, is the ratio of the maximum volume of water a rock can retain against gravity drainage, to the volume of that rock. The sum of S_r and S_y is equal to the total porosity (n) in unconfined aquifers, so the higher the value of S_r for a given rock type, the lower the value of S_y (Figure 4).

Clays, for example, have high S_r and negligible S_y in contrast to coarse sands, which are characterized by low S_r and high S_y. S_r is a measure of how much water has to be supplied to the unsaturated zone stor-

Texture class	Sample size [cm^3]	Total porosity n [cm^3/cm^3]	Residual (bound) water-content θ_b [cm^3/cm^3]	Effective porosity n_e [cm^3/cm^3]	Pore-size Distribution; Arithmetic mean	Specific retention (S_r) water retained at 33 kPa) [cm^3/cm^3]	Wilting point (water retained at 1500 kPa) [cm^3/cm^3]	Specific yield estimated from $S_y = n - S_r$ [cm^3/cm^3]	Saturated hydraulic conductivity K [cm/h]
Sand	762	0.437 (0/374-0/500)	0.020 (0.001-0.039)	0.417 (0.354-0.480)	0.694 (0.298-1.090)	0.091 (0.018-0.164)	0.033 (0.007-0.059)	0.346	23.56
Loamy sand	338	0.437 (0.368-0.506)	0.035 (0.003-0.067)	0.401 (0.329-0.473)	0.553 (0.234-0.872)	0.125 (0.060-0.190)	0.055 (0.019-0.091)	0.312	5.98
Sandy loam	666	0.453 (0.351-0.555)	0.041 (-0.024-0.106)	0.412 (0.283-0.541)	0.378 (0.140-0.616)	0.207 (0.126-0.288)	0.095 (0.031-0.159)	0.246	2.18
Loam	383	0.463 (0.375-0.551)	0.027 (-0.020-0.074)	0.434 (0.334-0.534)	0.252 (0.086-0.418)	0.270 (0.195-0.345)	0.117 (0.069-0.165)	0.193	1.32
Silt Loam	1206	0.501 (0.420-0.582)	0.015 (-0.028-0.058)	0.486 (0.394-0.578)	0.234 (0.105-0.363)	0.330 (0.258-0.402)	0.133 (0.078-0.188)	0.171	0.68
Sandy clay loam	498	0.398 (0.332-0.464)	0.068 (-0.001-0.137)	0.330 (0.235-0.425)	0.319 (0.079-0.559)	0.255 (0.186-0.324)	0.148 (0.085-0.211)	0.143	0.30
Clay loam	366	0.464 (0.409-0.519)	0.075 (-0.024-0.174)	0.390 (0.279-0.501)	0.242 (0.070-0.414)	0.318 (0.250-0.386)	0.197 (0.115-0.279)	0.146	0.20
Silty clay loam	689	0.471 (0.418-0.524)	0.040 (-0.038-0.118)	0.432 (0.347-0.517)	0.177 (0.039-0.315)	0.366 (0.304-0.428)	0.208 (0.138-0.278)	0.105	0.20
Sandy clay	45	0.430 (0.370-0.490)	0.109 (0.013-0.205)	0.321 (0.207-0.435)	0.223 (0.048-0.398)	0.339 (0.245-0.433)	0.239 (0.162-0.316)	0.091	0.12
Silty clay	127	0.479 (0.425-0.533)	0.056 (-0.024-0.136)	0.423 (0.334-0.512)	0.150 (0.040-0.260)	0.387 (0.332-0.442)	0.250 (0.193-0.307)	0.092	0.10
Clay	291	0.475 (0.427-0.523)	0.090 (-0.015-0.195)	0.385 (0.269-0.501)	0.165 (0.037-0.293)	0.396 (0.326-0.466)	0.272 (0.208-0.336)	0.079	0.06

Table 1. Water retention properties classified by soil texture, after Rawls and Brakensiek (1983) in Maidment (1993) table 5.3.2 and hydraulic conductivity from table 5.5.5. First line is the mean value. Second line is +/- one standard deviation about the mean.

Tabla 1. Propiedades referentes a la retención de agua, clasificadas según el tipo de suelos (según Rawls y Brakensiek (1983) en Maidment (1993) tabla 5.3.2), y conductividad hidráulica (tomada de la tabla 5.5.5). La primera cifra indica el valor medio. Los valores entre paréntesis indican la desviación standard entorno a la media.

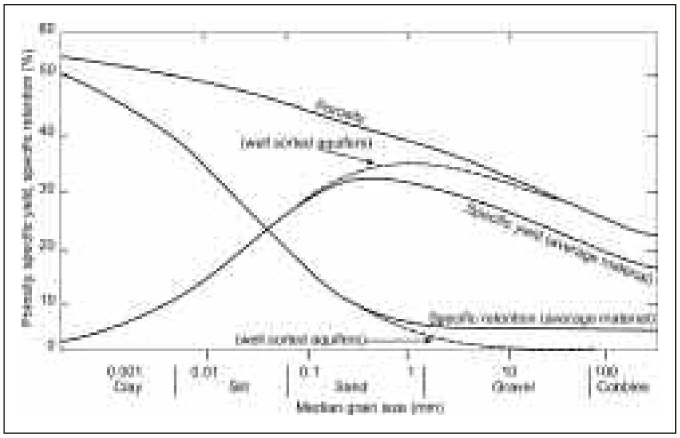

Fig. 4. Relation between specific yield, specific retention and porosity (Stephens *et al.,* 1998)
Fig. 4. Relación entre rendimiento específico, retención específica y porosidad (Stephens et al., *1998)*

age before any downward flow can take place, unless so-called bypass gravity flow through large cracks and/or open fractures takes place.

S_r represents maximum water content (moisture status) that can be held in unsaturated zone against gravity. In many rock types, e.g. in unconsolidated deposits, θ_b and θ_t can be neglected, so then S_r is represented by maximum capillarity water content (θ_c) that can be held against gravity. Larger than that water content will result in gravitational dewatering.

The S_r moisture status can be achieved, not only by adding water to the dry, unsaturated zone (e.g. rainfall), but also by releasing water from a saturated zone either by natural groundwater table decline or by dewatering of part of an aquifer through a well-abstraction. In such a case, immediately after gravitational water release, soil moisture is at the specific retention (field capacity) status.

In the unsaturated zone, water is held against gravity due to the tension pressure (sometimes also called suction pressure). This pressure is negative, relatively to the atmospheric pressure, in contrast to the saturated zone where the pressure is positive. The groundwater table at the intermediate surface between saturated and unsaturated zones represents then a relative tension pressure of zero. The unsaturated zone tension originates from adsorption, capillary and osmotic forces (Ward and Robinson, 1989). Adsorption forces are the molecular electrostatic forces, which bind water to the charged faces of solids (Marshall and Holmes, 1979). The strength of the adsorption forces increases with the increase in the specific surface of the soil particles, which is larger for the smaller and flatter soil particles, and also depends on the mineral type (Grabowska-Olszewska and Siergiejew, 1977; Coates *et al.,* 1998). Capillary forces result from surface tension at the interface between the soil, water and air (Ward and Robinson, 1989). The strength of the capillary forces is higher for fine rocks with small pore-sizes than for coarse rocks with large pore-sizes, and it increases with decreasing water content. The interdependent adsorption and capillary forces are of similar nature, and in practice, it is not possible to measure them separately. Therefore their combined effect is often referred to as matric pressure (Marshall and Holmes, 1979). A third force that contributes to tension pressure originates from osmotic pressure exerted by plant roots. It depends on the type of plant, the root density and the plant moisture stress. The tension pressure of a soil is an indication of the moisture status of the soil. The drier the soil, the higher is the tension pressure, and vice versa. In practice, hydrological determination of S_r is linked to the tension pressure. In that respect very important is an experimental observation that different soil/rock types reach S_r at the same tension pressure, i.e. at approximately –340 mBar (Dingman, 1994). Based on that observation the S_r is defined in hydrology by: (i) laboratory analyze of soil/rock samples obtained in the field by exposing them to various matric pressures and simultaneous recording their corresponding soil moisture; the resultant from that experiment pF curve, representing relation between soil moisture and matric pressure, is specific for the analyzed soil/rock sample so its moisture corresponding with the matric pressure of approximately -340 mBar can be considered as S_r; (ii) simultaneous measurement of matric pressure (e.g. by matric potential sensors or tensiometers) and soil moisture in orden to determine the specific retention moisture status i.e. when matric pressure is ~-340 mBar, for example using TDR (time domain reflectometry), GPR (ground penetrating radar), neutron logs (if boreholes available) or by using MRS. The main disadvantage of using hydrological methods for S_r determination is their weakness with regard to the scale effect related to spatial heterogeneity because standard hydrological sensors can measure only very small volumes of less than 1 m^3 in contrast to MRS that can measure volumes up to 10^6 m^3.

Free-water content

The term, free-water content (θ_f), is not commonly used in hydrogeology but it is very useful for the purpose of MRS signal interpretation (Figure 1). θ_f is the percentage of water that is outside the field of molecular forces of attraction of the solid particles that can be displaced by gravity or hydraulic head gradient, with respect to the total rock volume (Lubczynski and Roy, 2003). This means that, in the saturated zone, the free water content (θ_f) is at its maximum as well as each of its components i.e. θ_m and θ_t. This implies that

$$\theta_f = \theta_m + \theta_t = n - \theta_b \qquad [3]$$

In unsaturated zone θ_t, θ_c, θ_g are variable so the θ_f is variable as well and lower than in saturated zone

$$\theta_f = \theta_t + \theta_c + \theta_g < n - \theta_b \qquad [4]$$

as can be seen in Figure 1.

Physical foundation: storage from MRS data

As explained in Plata and Rubio (2007, this Issue):

(1) MRS uses NMR to selectively excite, detect, quantify and characterize hydrogen nuclei ($^1H^+$) of the in-situ groundwater;

(2) In MRS, an effective volume of investigation is determined by: (i) the loop size and shape; (ii) the actual excitation moment i.e. by q value; (iii) the local Earth's magnetic field i.e. by magnitude and dip; and (iv) the subsurface electric conductivity;

(3) Taking into account the constraints listed in (2), the initial value of the MRS signal amplitude (E_0) is directly proportional to the in-situ water content (θ_{MRS}), in the investigated volume;

(4) The θ_{MRS} represents all the measurable by MRS in-situ water above a given threshold water 'size';

(5) The threshold water 'size' is roughly defined as the smallest dimension characterizing the water-bearing pore, interstice etc. that can be measured by MRS. For a cylindrical pore the 'size' is typically the cylinder radius;

(6) The threshold water 'size' is rock dependent: for clastics, the size is roughly 3 times larger than for carbonates;

(7) The detectability of the lower threshold water 'size' is instrumentally dependent. For MRS NUMIS instrument it is in the micron range (μm), which corresponds to mobile water;

(8) There is no upper threshold on water 'size' detectability: MRS done on frozen lake or river can easily detect the bulk water under the ice crust.

Deriving storage related parameters with MRS

The principle of evaluating storage related parameters is based on the evaluation of the free-water content (θ_f) from the MRS-measured water content (θ_{MRS}) assuming that $\theta_f \cong \theta_{MRS}$. As mentioned θ_f represents water content that can move within the rock matrix either by gravity (e.g. aquifer dewatering) or by pressure gradients (e.g. groundwater flow but also unsaturated water flow). This statement does not apply to bound water (θ_b) which is a volume of water bound to the rock matrix by the molecular forces of attraction (not by capillary surface tension forces). Bound water in contrast to free water is removable only by much stronger than gravity and/or pressure gradient forces of centrifugal action (Polubarinova-Kochina, 1962). In saturated media, free water content (θ_f) plus bound water content (θ_b) represents the total porosity ($n = \theta_f + \theta_b$) as indicated in Figure1. In productive aquifers the bound water content is negligible therefore the assumption $n \cong \theta_f$ is justified.

With current MRS technology, the very short signals (undetected due to instrumental dead-time) that likely reflect bound water content are not measured yet, so the reliable division between bound water and free water content is not possible yet. In most of MRS applications, this is however not a big problem because bound water content is typically very low, especially in aquifers with coarse structure, that are the focus of primary interest of groundwater exploration and management. This leads to the fundamental and permissible in hydrogeological applications assumption that the measured by MRS water content represents free water content, i.e. $\theta_{MRS} \cong \theta_f$. This assumption implies the following: (i) the water contents from full saturation to approximately 1% can be detected by MRS (under low noise conditions), although the very low moisture estimates particularly those below 1% have not yet been verified; (ii) the accuracy of the assumption is rock-dependent i.e. is reasonable for sandstones and quartz-rich clastics but is likely to be less accurate for carbonates where θ_{MRS} likely covers part of θ_b. More information in that respect can be found in Vouillamoz (2003).

The hydrogeological system introduced schematically in Figure 1 consists of the saturated zone (aquifer), showed in the lower part of the graph and of the unsaturated zone (vadose zone) showed in the upper part of the graph. In the saturated zone, the total porosity (n) consists of free water (θ_f) and bound water (θ_b) so assuming that $\theta_f \cong \theta_{MRS}$, the n can be estimated from $n = \theta_{MRS} + \theta_b$ or from $n \cong \theta_{MRS}$ if assumption $\theta_b \to 0$ can be made. In the saturated zone, the free water content (θ_f) consists of the effective porosity (n_e)

and trapped porosity (n_t). The n_t does not contribute to groundwater flow but it is a part of free water content and therefore it contributes to the measured θ_{MRS}. If however an MRS sounding is performed over the rocks where n_t can be neglected and θ_{MRS} can be assumed as equal to θ_f, then the assumption $n_e \cong \theta_{MRS}$ is justified as shown for the lower part (saturated zone) of the Figure 1. If also another assumption $\theta_b = 0$ can be made (valid for most of the productive aquifers with medium to coarse grains or fractures), than $\theta_{MRS} \cong n_e \cong n$.

Under the assumptions that $\theta_{MRS} \cong n$, the S_y can be calculated from (Figure 1)

$$S_y = \theta_{MRS} - S_r \quad [5]$$

Evaluation of S_y requires then S_r which can be derived with standard hydrological methods (see above) but also with MRS by measuring θ_{MRS} before ($\theta_{MRS}{}^b$) and immediately after ($\theta_{MRS}{}^a$) dewatering of an unconfined aquifer (Figure 2) at the scale comparable with the volume investigated by MRS. The θ_{MRS} measured within the cone of depression after its dewatering, would then equal to S_r ($\theta_{MRS}{}^a = S_r$) so the S_y could be then calculated from

$$S_y = \theta_{MRS}{}^b - \theta_{MRS}{}^a \quad [6]$$

Difficulty and potential uncertainty of that approach is in making sure that the MRS investigated volume corresponds with the volume of the "freshly" desaturated part of an aquifer and that the MRS investigated volume is representative for the entire aquifer.

Whenever S_r is not available and cannot be estimated, Vouillamoz *et al.,* 2006 (see also Vouillamoz *et al.,* 2007, this Issue) propose to use simplified formula $S_y = C_y\ \theta_{MRS}$, where C_y (proportionality factor) is derived from several data pairs of S_y from pumping tests and θ_{MRS} from MRS soundings. The relation between the two is then linear, therefore once C_y is established, it can be then used to derive S_y from MRS measurements of θ_{MRS} but only for the same type of rocks and the same hydrogeological conditions as those for which the C_y factor was determined.

In confined aquifers, the elastic storativity is not directly detectable by MRS but can be calculated from

$$S_e = \rho g(\alpha + n\beta)\Delta z \quad [7]$$

Using equation 7, not only n but also Δz can be estimated by MRS from

$$S_e = \rho g(\alpha + \theta_{MRS}\beta)\Delta z_{MRS} \quad [8]$$

where Δz_{MRS} is the layer thickness obtained with MRS; other parameters such as ρ, g, α, β can be estimated from other data sources such as Fetter (2001).

The specific drainage (S_d) is detectable by MRS in the same way as S_y so it can be estimated from the formula

$$S_d = \theta_{MRS} - S_r \quad [9]$$

applying the same assumptions as in S_y determination. It should be noticed that the S_d water volume cannot be directly referred as the quantity of extractable water for utilization because in order to use this storage, first the potentiometric surface of the confined aquifer has to drop below the bottom of the exploited aquifer which is not always possible for various reasons.

The most reliable (because of the lowest impact of equivalence error), but also not very popular in hydrogeological applications is the storage related parameter called free hydrostatic column of water

$$H_w = \theta_f \Delta z \quad [10]$$

Applying MRS, H_w can be obtained from

$$H_w = \theta_{MRS}\Delta z_{MRS} \quad [11]$$

(Lubczynski and Roy, 2003; 2004). The H_w provides volumetric estimate of the free water content with depth and can be estimated for single layers of interest like aquifers but also for the arbitrary depth intervals (Lubczynski and Roy, 2004). H_w is particularly useful and reliable in evaluation of a potential of aquifers and in comparing them.

Verifying storage related parameters derived with MRS

MRS storage related parameters are typically verified against hydrogeological data, firstly by checking whether they are realistic (check if they are in the realistic range) and secondly, (if the first condition fulfilled) whether they are correct (accuracy estimates). The MRS based storage related parameters can be classified in two groups with respect to such verification: (1) parameters that can be estimated (in some cases roughly) directly from the MRS signal inversion using θ_{MRS} or θ_{MRS} coupled with Δz_{MRS}; these are: porosity (n), effective porosity (n_e), specific storage (S_s), elastic storage (S_e) and free hydrostatic water column (H_w); (2) parameters that cannot be estimated directly from the standard MRS survey; these are: specific yield (S_y) in case of unconfined aquifers and specific drainage (S_d) in case of confined aquifers; determination of these two parameters, requires additional parameter of specific retention (S_r) as explained above.

The verification of the MRS storage related parameters of the group 1 is straightforward and quick. The principle of this verification is to test the correctness of $\theta_{MRS} \cong n_e$ (which itself also is an approximate estimate (Lubczynski and Roy, 2003) by comparing MRS output with n_e determined in hydrogeological manner). In the simplest verification, θ_{MRS} can be compared with literature values of n_e, e.g. from the Table 1. Such verification is considered as the first and the quickest but not accurate data quality check confirming that the acquired θ_{MRS} is in the realistic range. This is quite relevant because there is always a risk that for example in fine deposits, large part of the overall water content might be not seen by MRS due to the dead-time technological constrains. The simplest experiments to verify MRS effective porosity estimates are based on the field collection of the soil/rock samples from the investigated by MRS rock volume and their laboratory analyze with regard to n_e. Such verification however is always affected by scale effect problem resulted by the rock heterogeneity within the volume of the MRS survey i.e. the variability of the collected field samples of n_e, may not well represent the n_e of the MRS surveyed volume. Better way of θ_{MRS} verification can be done by field tracer test (e.g. Vandenbohede and Lebbe, 2006) because the scale of such experiment is comparable with the scale of MRS survey so less vulnerable to the scale effect problem. Tracer tests can also be performed in the laboratory conditions but they are less accurate mainly because they are more affected by scale effect problem and because in laboratory conditions tracer tests can only be carried out on disturbed rock samples. The most appropriate and the most reliable way of determining n_e for verifying θ_{MRS}, is combination of field tracer tests with calibration of an advective-dispersive transport model (e.g. Ptak *et al.,* 2004). In such solution all the hydrogeological complications can be taken into account.

The verification of the storage related parameters of the group 2, i.e. S_y, S_d, S_r, is by far more complicated than of the group 1. Assuming that the surveyed θ_{MRS} represents the entire free water content of an aquifer, only part of it (extractable by gravity part) is represented by S_y (or S_d). The other non-extractable part of the total water content is defined by S_r (Figure 4) The strategy of the S_y verification will rely then on the separate definitions of S_y (or S_d) and S_r and comparing their sum with the surveyed θ_{MRS} value.

Hydrogeological methods applied to derive S_y (or S_d) for verification of θ_{MRS} differ with regard to their accuracy and their vulnerability to scale effect. The most inaccurate is the sampling of the rock volume investigated by MRS combined with laboratory determination of S_y (or S_d); this is because that method is based on disturbed samples and is affected also by scale effect resulted by rock heterogeneity within volume of the MRS survey; this means that S_y of the collected in the field samples do not always represent the S_y of the entire volume of MRS survey. More reliable is piezometric pumping test. This method is considered as accurate in hydrogeology and also the scale of the experiment is comparable with the scale of MRS survey so less vulnerable to the scale effect problem. The most accurate however, seems to be the S_y obtained from a calibrated transient numerical groundwater model based on reliable transient input data including pumping tests; this is because models can integrate data from various sources and because they handle best spatial heterogeneity of a hydrogeological system.

Hydrogeological methods for determination of S_r are quite poor, mainly restricted either to rock sampling and laboratory testing, or to in-situ measurements using sensors (see above). Both are small scale measurements largely vulnerable to heterogeneity effect particularly when comparing with large volume surveyed by MRS. The scale difference creates a potential problem (larger in case of heterogeneous medium) in verification of S_r derived by θ_{MRS} (e.g. through measurement of a freshly dewatered part of the aquifer as explained above). However, such protocol of deriving S_r using MRS has not been experimentally confirmed yet.

Only few case examples of field verification of storage related parameters obtained with MRS are known so far. This is because piezometric pumping tests and transient numerical models, both particularly suitable for extraction of valid S_y, are quite rare due to the large costs involved. First attempts of verification of storage related parameters were made by Lubczynski and Roy (2003) and Lubczynski and Roy (2004) where S_y and S_r were estimated separately and their sum was compared with θ_{MRS}. Also Vouillamoz (2003) compared storage coefficients evaluated from pumping tests with MRS storage coefficients adapted to cases of unconfined, mixed and confined aquifers. More verification cases, though without separate definition of S_r, but at various hydrogeological conditions, using many piezometric pumping tests and with transient numerical groundwater model, were carried out in Myanmar by Vouillamoz *et al.* (2007)

and in Niger by Vouillamoz *et al.* (2006), both summarized in Vouillamoz *et al.* (2007, this Issue).

Caveats

On well-known lithology, MRS supplies reliable and quantitative groundwater storage estimates. This means that geometric parameters of saturated zone (depth, thickness) have determinable tolerances; θ_{MRS} supply good estimate of θ_f, which for most types of rocks provides quick and reliable estimate of n_e, S_y (if S_r can be estimated) and eventually any other parameter that can be deduced from θ_f. The accuracy of the n_e assessment will depend on the validity of the two assumptions: (i) $\theta_f = \theta_{MRS}$ and (ii) $n_t = 0$. The quality of the S_y assessment with MRS will depend on the validity of $\theta_f = \theta_{MRS} = n$ and on the accuracy of S_r determination.

On less known environments however, there are a number of issues the user must keep in mind with respect to storage (but also aquifer flow and unsaturated zone parameterization with MRS) quantification. These issues have been remarked in Plata and Rubio (2007, this Issue), and can be summarized as the following ones:

(1) "S/N" (signal to noise ratio): for reliable interpretation, S/N above 2 after data stacking is needed (see also Legchenko, 2007, this Issue). This means that there are locations where MRS information cannot be reliably acquired. Such locations may include e.g. proximity to power lines or other artifacts, Larmor frequency too near a harmonic of the power line frequency, proximity to a major geo-electrical conductor in a resistive environment e.g. fault, shear zone, banded iron formation, etc.

(2) "T_2 cut-off": in clastics rocks, the boundary between bound and mobile water is considered around 33 ms. This very roughly corresponds to the lower limit of NUMIS aperture window for NMR signals so that the quantity of water detected by MRS is assigned to mobile water. In carbonate environments, including karstic environments, this boundary may be shifted toward longer times. Typically, petrophysicists use 90 ms for this boundary in carbonates. In practice, depending on the decay-time spectra, it may mean that part of the detected water is bound water. In such case, MRS may supply an overestimate of effective porosity.

(3) "magnetic": magnetic effects are everywhere so they are critically important for magnetic resonance applications. Pore-size can be estimated by NMR/MRS because of surface relaxation. Surface relaxation is an enhanced rate of relaxation caused by the precessing $^1H^+$ (hydrogen nuclei) coming on or very near the solid walls of the rock matrix. Groundwater and the solid rock matrix have a magnetic susceptibility contrast. This causes distortion in the $^1H^+$ precession. Such distortion is often magnified by a thin film of magnetic materials (e.g. Fe or Mn oxides) on rock particles, enhancing magnetic susceptibility contrast at the micro-thin layer scale. Such occurrence of thin magnetic film is normal for clastics so the pore-size estimation formula uses the relaxivity ρ parameter (a fluid-matrix interface parameter) to account for such composition. There are, however, other cases, where magnetic gradients exist at the larger scales of the pores' volumes rather than at the scale of micro-thin films. These types of magnetic gradients may be due to: (i) structures, e.g. dykes, faults, etc., the elements of which have a magnetic susceptibility contrast; (ii) dissemination of magnetic minerals (e.g. magnetite with grain size e.g. in the range of 10μm to 1 mm) in the rock. In both cases, because of that magnetic gradient, part of the investigated by MRS water may have such a shortened T_2^* that becomes undetectable with the currently available MRS instruments (NUMIS). In such cases, any MRS-based storage quantification may be highly erroneous.

(4) "phase masking": it is well known to EM users that conductive formations modify the phase of the electromagnetic fields. A practical consequence of this is that in conductive terrains, the NMR fields from a shallow aquifer may completely mask the NMR signals from a deeper water bearing horizon. When such deeper horizon is in or below a conductive horizon, both the NMR excitation and the NMR signal are phase shifted with respect to a surface located sensor. In such case, the phase rotation may be such that the resulting signal from the summation of the shallow and deep MRS responses makes the deep MRS response non-detectable when processed with the classical data inversion software tool. This problem was first addressed by Roy and Lubczynski (2003) and recently by Braun et al. (2006) who used phase shift in the MRS data inversion. Once such inversion tool becomes available to the MRS users the phase masking limitation may disappear.

(5) "Equivalence": this item is of no consequence

with respect to the amount of quantified water but it may have an effect on resolving aquifer geometry. As the ratio of the depth of the target aquifer to the loop dimension is increasing the equivalence phenomena becomes more present. This implies that the free hydrostatic column of water $H_w = \theta_{MRS} \cdot \Delta z_{MRS}$ is more reliable than each of the two components θ_{MRS} and Δz_{MRS} separately.

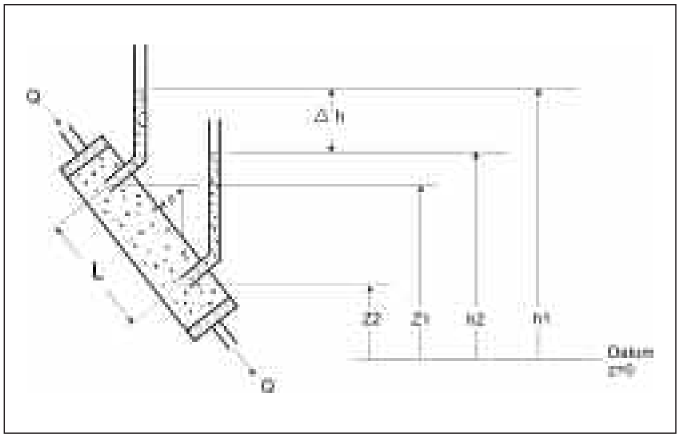

Fig. 5. Hydraulic flow through cylinder, Freeze and Cherry (1979)
Fig. 5. Flujo hidráulico a través de un cilindro, Freeze and Cherry (1979)

Aquifer flow related parameters

Aquifer flow parameters (mainly hydraulic conductivity and aquifer transmissivity) can be deduced from MRS although in less straightforward manner than aquifer storage parameters because they require aquifer system specific calibration, typically done by pumping test method.

Overview of the selected flow-related parameters

Aquifer flow properties are described in terms of hydraulic conductivity following the formulation of Darcy law (Freeze and Cherry, 1979). In order to maintain a constant flow rate Q through a permeable medium, a hydraulic gradient $\Delta h/L$ must be sustained across that medium. For the simple case of a cylinder (Figure 5), with the cross-section A and the porous length investigated L, the Darcy velocity (V) is:

$$V = Q / A = -K\Delta h / L \qquad [12]$$

where the proportionality factor K [L/T] is the hydraulic conductivity and Δh [L] is the hydraulic head drop observed over the length L [L]. K depends not only upon the medium characteristics but also upon the flowing fluid. This is why in petrophysics, another flow parameter called permeability (κ) dependent only upon the medium is used. From measurements over various types of fluids through porous materials made of spherical glass 'grains' with various diameters d, it is known that media-wise Q/A is proportional to d^2, to $1/\mu$ and to the weight density ($j \bullet g$), where g is the Earth's gravity acceleration, j - density and μ - viscosity. This leads to the alternate form of Darcy law:

$$Q / A = -K(j \cdot g / \mu)\Delta h / L \qquad [13]$$

where the contributions of the medium and of the fluid are clearly separated.

Groundwater flow parameters such as K or κ describe groundwater rock medium and eventually also the fluid, but do not provide the characteristic of the size of the flowing area i.e. aquifer. Another hydrogeological parameter, aquifer transmissivity $T = K\ \Delta z$ involves aquifer thickness Δz and gives more complete characteristic of aquifer flow. In the case of 1D MRS survey, the aquifer is seen as a group of parallel strata. The data inversion can supply K estimates of various strata thicknesses within the aquifer. T is then defined as the summation of each water bearing thickness Δz_i as determined from MRS inversion and weighted by hydraulic conductivity, K_i: $T = \sum \Delta z_i\ K_i$.

Physical foundation: flow parameters from MRS data

(1) In the Kozeny-Carman model summarized by Schön (1998) the volumetric flow is evaluated through Poiseuille's law in an elementary cube traversed by a twisted tube of circular cross-section. A shape factor, $1^2/_3 \leq \xi \leq 3$ accounts for cross sections other than circular i.e. from triangular, right up to very thin fracture-like interstices. The main features of the Kozeny-Carman model (e.g. Equation 14) are: (i) κ is proportional to the square of the tube radius r; (ii) the porosity n enter in the equation with an exponent typically between 1 and 3 according to the specific form of the equation; (iii) the narrow range ($1^2/_3$ - 3) ξ shape factor is at exponent -1 while the twisting of the tube, quantified through tortuosity T_{or} is at exponent -2; (iv) one

of the expressions of the Kozeny-Carman model is:

$$k = nr^2 / 4T_{or}^2\xi = n / s_p^2 T_{or}^2 \xi \quad [14]$$

where s_p is the ratio of the tube's area over its volume, the inverse of which is the pore size in NMR context.

The Kozeny-Carman expression of κ is particularly relevant since both n and $1/s_p$ are available from NMR data.

(2) Nelson (1994) developed his model through a compilation of empirical data on sand packs systematically covering a wide range of porosity, grain size and grain sorting. He also observed that κ was proportional to the square of the grain-size and pore-size. Later, Nelson (2005) showed the critical importance of pore-throat size (r_{pt}) in the permeability versus porosity and pore-throat size relationship:

$$k = cr_{pt}^2 n^b \quad [15]$$

where c and b are lithology dependant factors. The r_{pt} in Equation 15 has the linear dimension quantifying the pore interconnection that in the laboratory condition could have been measured with mercury injection pressure whereas n is measured with the NMR signal amplitude.

(3) Following the KST model (Korringa *et al.,* 1962) and the empirical verification by Kenyon et al. (1989), s_p can be derived from NMR decay rate using:

$$1/T_d = \rho s_p \quad [16]$$

where T_d is the surface relaxation component of the NMR decay rate for T_1 or T_2, ρ is the pore surface relaxivity (a material-fluid constant different for T_1 and T_2), s_p is the pore's surface to volume ratio i.e. the inverse of pore-size. This pore-size to NMR decay rate relationship is valid in the so-called fast-diffusion limit; in practice water in pore-size within the range from 3 μm to approximately 1 cm interval should fit this constraint at near surface pressure and temperature.

(4) In practice the permeability can be defined through NMR measurements of n and T_d using formula:

$$k = cn^b T_d^2 \quad [17]$$

where c and b are lithology dependent factors; b is usually between 1 and 4 according to the specific regression model used. c includes the surface relaxivity term to transform decay time into pore-size together with *T* and ξ lithology factors and empirical relationships pore-size and pore-throat size. Similar formula as introduced in NMR for κ is also used in MRS to define hydraulic conductivity through MRS estimates of n and T_d (see below).

(5) Pore connectivity is an important issue in evaluating κ and K using NMR and MRS in various rocks types. Pore connectivity, so far is encountered through the c factor as explained above. Clastic rocks, and sandstones have good and regular pore connectivity which is why investigations over sandstone data sets show a very high correlation coefficient between NMR-derived κ estimates and laboratory determination (0.94) (Sen *et al.,* 1990). In other rock types this relation is not so good and requires more research.

(6) Extracting K from κ estimate is a matter of multiplying by the factor jg/μ. For drinking water this is generally a constant because the salinity effect is low enough to be neglected and the other factor involved in density and viscosity is the subsurface temperature.

Deriving flow related parameters with MRS

Deriving flow parameters involves not only θ_{MRS} but also another MRS output of decay time constant (T_d). In NMR there are three modes of T_d measurements: T_1 (longitudinal relaxation), T_2 (transversal relaxation) and T_2^* (free induction decay time constant). The current MRS implementation – NUMIS^{PLUS} - Iris Instruments (2001) measures T_2^*. The estimation of T_1 is also possible by comparing two T_2^* responses: one at steady state and the other one at a programmed delay following the first one; the delay is selected to be shorter than the time required to reach steady-state in a given environment. Following earlier convention, such estimate will be identified as T_1^* in the remaining part of this contribution. There are the following underlying assumptions and limitations in such T_1^* estimator. In the MRS implementation (NUMIS), the T_1^* estimation is only possible where T_2^* can be measured, i.e. where the magnetic field gradients at various scales are small enough to allow T_2^*

signal detection. It must be kept in mind that only the groundwater components with low enough magnetic gradients, at all scales, to give a measurable free induction decay signal are characterized by such T_1^*. In other words, the T_1^* MRS measurement scheme does not allow to find any additional groundwater as compared to the simpler T_2^* scheme but for that fraction of groundwater it supplies an estimate of the T_1 value which is more reliable than a T_2^*-based estimator as seen below.

From the physical foundations above, it is known that aquifer porosity approximated in MRS by θ_{MRS} (Figure 1) and MRS decay time constant (T_d), are needed to determine permeability (κ) and from there hydraulic conductivity (K) according to the equation:

$$k = C_k \theta_{MRS}{}^a T_d^2 \quad [18]$$

where a, and C_K are the empirical lithology dependent parameters. The selection of the parameter a, according to Legchenko *et al.* (2004), is dependent on the pore-size and pore-throat size (connections between the pores). In most of permeable rocks, for example sands, limestones and chalks, which are characterized by pore-throats as large as the pores themselves, the most reliable K estimates based on Equation 18, can be obtained for a = 1, i.e. for θ_{MRS} T_d^2 estimator (Legchenko *et al.,* 2004). In sandstones, pore-throats are small as compared to pore sizes, so according to laboratory NMR experiments of Sen *et al.* (1990) and field MRS experiments using T_2^* of Vouillamoz (2003) and Legchenko *et al.* (2004), the most reliable K estimates, can be obtained for a = 4, i.e. for $\theta_{MRS}{}^4$ T_d^2 estimator.

Not only hydraulic conductivity (K) but also aquifer transmissivity (T = K Δz) can be derived with MRS. The 1D MRS inversion supplies thickness (Δz_{MRS}) of the water bearing horizons needed to calculate aquifer T. In MRS, the integrated response, i.e. the summation of all water contents times depth intervals is the most reliable information from a water quantity perspective. Transmissivity estimate also represents such integrated response in which next to the depth intervals and water contents also the square of decay time constants are integrated according to:

$$T_{MRS} = C_T \int_{\Delta z} \theta_{MRS}{}^a T_d^2 dz \quad [19]$$

An example is presented through a model with the water content at the power 1 (a=1) after Vouillamoz, (2003):

$$T_{MRS} = C_T \sum_{i=1}^{n} (\Delta z_{MRSi} \theta_{MRSi} T_{di}^2) \quad [20]$$

where Δz_{MRSi}, θ_{MRSi}, T_{di} are the MRS thickness/depth intervals, water contents and decay time constants respectively of each resolved water bearing horizons comprising analyzed aquifer. In such transmissivity estimation the following assumptions are made: (1) the measurement is made in the saturated media so the water content is equal to porosity; (2) porosity is representative of a fluid flow; (3) C_T is available for the decay rate used (T_1^* or T_2^*); (4) empirically calibrated C_T (see below) properly incorporate the lithology/fluid factors such as: relaxivity, pore-size to pore throat size factor, water density and viscosity, allowing the transformation from κ to K, etc.

Calibration of flow related parameters derived with MRS

Deriving T from MRS survey i.e. from T_{MRS} requires calibration. Calibration of T_{MRS} is a process of comparing MRS output $\Delta z_{MRS}\,\theta_{MRS}{}^a\,T_d^2$ with pumping test transmissivities (T_{pt}) to derive area specific C_T from the inverse of the slope of the regression line over the data set as in Figures 6 and 7.

Legchenko *et al.* (2002) calibrated the relationship between MRS derived transmissivity estimators and pump test transmissivity using both T_2^* and T_1^* modes and applying two types of MRS estimators, with a=1 i.e. Δz_{MRS} $\theta_{MRS}{}^1$ T_d^2 (Figure 6-left) and with a=4 i.e. Δz_{MRS} $\theta_{MRS}{}^4$ T_d^2 (Figure 6-right).

Although, the number of data points in Figure 6 was limited, one observes that the correlation between MRS transmissivity estimators and pumping test transmissivities is better while using T_1^* than while using T_2^* and while using a=1 rather than while using a=4 as tested in the environment composed of limestone, sand and clay. However, while using T_2^* in sandstone applications (Legchenko *et al.,* 2004), a=4 gave better results than a=1. Also Vouillamoz (2003) established similar relationships on empirical, field-acquired data sets. His results were compatible with the Legchenko *et al.* (2002) model, however, in addition, he showed that the C_T varied with lithology and was different for granites, sands and chalks (Figure 7, left). Plata and Rubio (2006) reported recently on common for various alluvial aquifers in Spain correlation between C_T and corresponding Δz_{MRS} θ_{MRS} T_1^{*2}.

A comparison of C_T derived using T_1^* and T_2^* in various geological environments is presented in Table 2 assuming the following units: T_{MRS}: [m²/s], C_T:

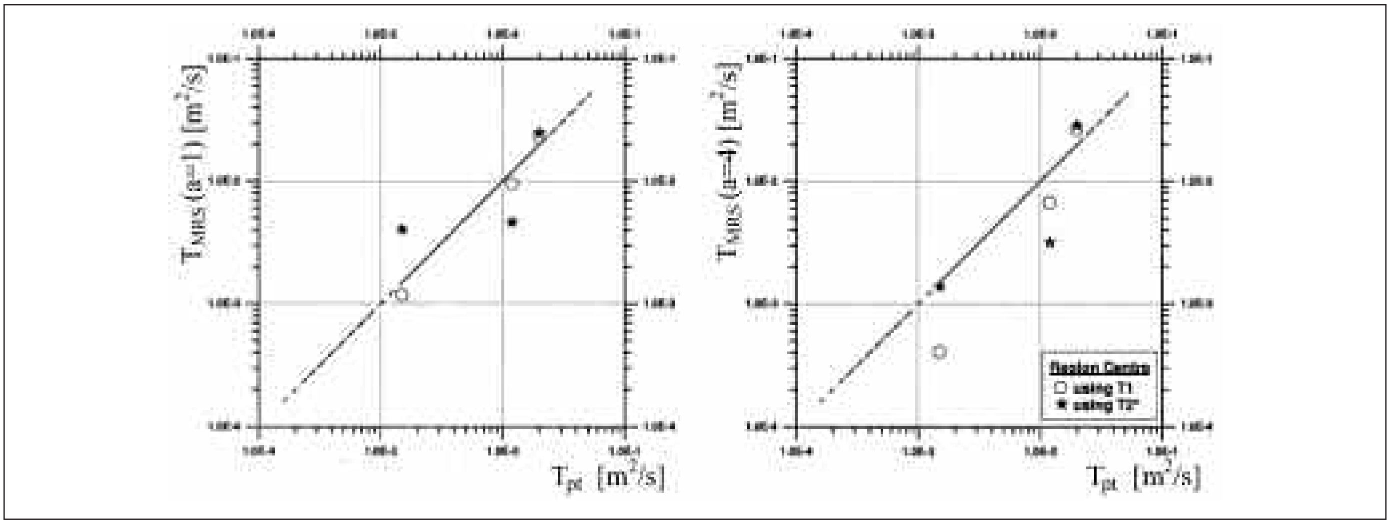

Fig. 6. Comparison of pumping tests transmissivities (T_{pt}) with MRS transmissivities (T_{MRS}) for T_{1^*} (circles) and T_{2^*} (stars) while using a=1 (left) and a=4 (right) in the environment composed of limestone, sand and clay, after Legchenko *et al.,* (2002)

Fig. 6. Comparación entre la transmisividad obtenida mediante ensayos de bombeo (T_{pt}) y la deducida a partir de SRM (T_{MRS}) utilizando la constante de tiempo T_{1^*} (círculos) y T_{2^*} (estrellas), con los valores a=1 (izquierda) y a=4 (derecha), en calizas, arenas y arcillas, según Legchenko et al., *(2002)*

[m/ms•s], T_d: [ms], θ_{MRS}: [%], Δz: [m]. More C_T values are presented in Vouillamoz et al. (2007, this Issue).

As indicated above, field data compilation shows better correlation of pumping test T_{pt} with T_1^* than with T_2^*. One must be careful however in using such observation. In case of “mild enough” magnetic effects, i.e. when all free water is detected by NUMIS, T_1^* as measured with NUMIS gives a suitable estimate of T_1 and thus provide a better than T_2^* parameter to be used for the T estimation. However, in case of severe magnetic gradients the procedure to estimate T_1 by using T_1^* is not valid anymore.

With calibrated at a given lithology and given environment C_T, no other applied geophysical technique

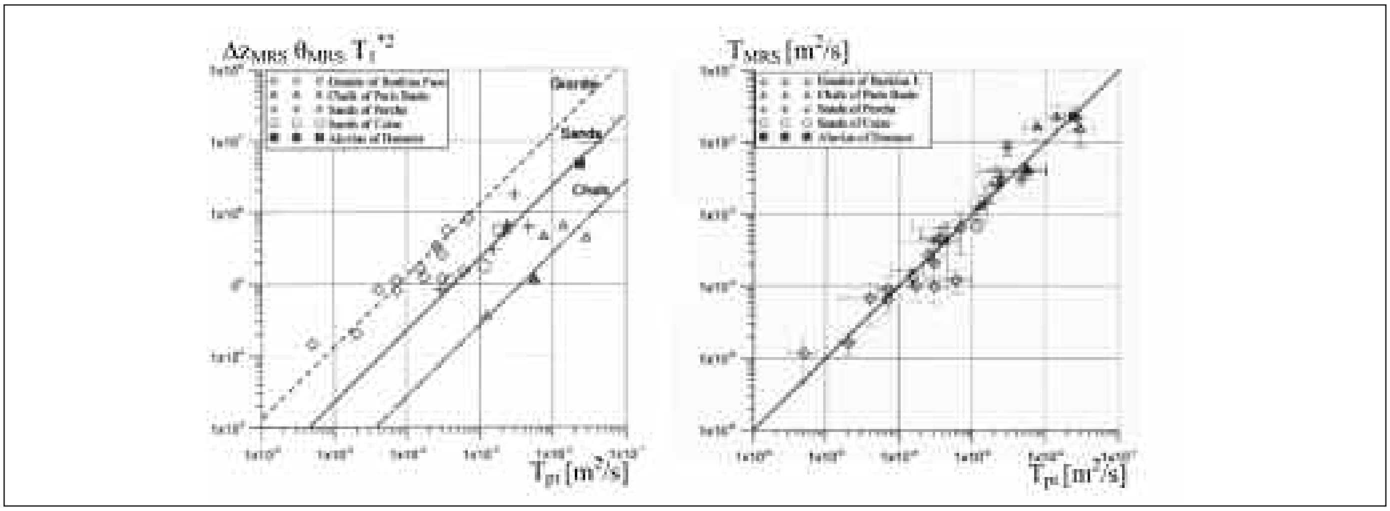

Fig. 7. Pumping test calibration of the flow related parameters: left panel - comparison of MRS estimator $\Delta z_{MRS}\theta_{MRS}T_1^{*2}$ with pumping test transmissivity (T_{pt}) for chalk, sand and granite represented by 3 lines corresponding with three C_T derived using T_{1^*} (Table 2); right panel - correlation between T_{MRS} and T_{pt} after Vouillamoz (2003)

Fig. 7. Calibración de los parámetros de flujo con valores de ensayos de bombeo. Izquierda: comparación del estimador de SRM $\Delta z_{MRS}\theta_{MRS}T_1^{*2}$ con la transmisividad calculada en ensayos de bombeo T_{pt}: cada alineación representa el valor de C_T en creta, arenas y granito respectivamente, utilizando T_{1^*} (Tabla 2). Derecha: correlación entre los valores calculados T_{MRS} y T_{pt}, según Vouillamoz (2003)

Lithology	C_T using T_1^*	C_T using T_2^*
Granites	1.3×10^{-9}	1.1×10^{-8}
Sands	4.9×10^{-9}	2.0×10^{-8}
Chalks	3.5×10^{-8}	6.2×10^{-8}

Table 2. Example of C_T (Vouillamoz, 2003) for the selected rock formations at 12°C

Tabla 2. Ejemplos de valores de C_T (Vouillamoz, 2003) para los tipos de rocas seleccionados, a 12 ºC

can come that close to a 'virtual pump test' as MRS. This is well confirmed by the Vouillamoz (2003) correlation graph as presented in the right panel of the Figure 7 and also by other experiments presented in the following Vouillamoz et al. (2007, this Issue).

Caveats

(1) Nature is more complex than Kozeny-Carman model; however in practice, Kozeny-Carman constitutes a fairly robust solution for aquifer flow parameterization;
(2) Like in storage parameterization there are "difficult" MRS survey locations, where general caveats listed under storage parameterization applies (see above);
(3) The water not detected by NUMIS does not contribute to the K and T evaluation: sometimes this may lead to totally erroneous results.
(4) Under conditions where internal magnetic gradients are negligible, T_1^* data acquisition procedure appears currently to be the most accurate estimator for both K and T.

Subsurface hydrostratigraphy

Hydrostratigraphic units comprise geologic units of similar hydrogeologic properties (Anderson and Woessner, 1992). In simple hydrogeological cases, the lateral and vertical extent of the hydrostratigraphic units (aquifers, aquitards, aquicludes) can be inferred from the combination of borehole data, field cartography and remote sensing mapping techniques. In more complicated cases of complex geology, often important is geometry (i.e. shape and position) of the local hydrogeological bodies (e.g. buried channels). Such bodies are characterized by local change in flow and/or storage properties. MRS can substantially contribute to the evaluation of such bodies because through inversion of signal amplitude and decay time constant it has ability to evaluate rock storage and flow properties.

The MRS data inversion tools, such as various versions of the NUMIS software supplied by IRIS Instruments (e.g. 1997 to present), are essentially 1D MRS inversion tools. In 1D, lateral homogeneity is assumed and vertical layering is determined i.e. water content, θ_{MRS}, and signal decay rate, T_d, as a function of depth. For sedimentary/porous aquifers with sub-horizontal layering, each MRS data set is inverted in terms of subsurface hydrostratigraphy, each unit being characterized by Δz_{MRS}, θ_{MRS} and T_d. The spatial distribution of these soundings' inversions over the area of interest supplies area-wise information on aquifer properties. Thus, the overall geometry of an aquifer is defined with a spatial resolution much coarser area-wise than depth-wise due to practical limitations in the affordable number of MRS stations.

Of course, aquifer lateral heterogeneity is also important information and in some environments, e.g. fractured aquifers, probably the most important information. Weichman et al. (1999, 2000, 2002) and later Hertrich and Yaramanci (2003) made significant contributions in defining the volumetric and lateral sensitivity patterns. These were first steps in the direction of detecting lateral heterogeneity. The most significant step in this direction however is the development of separated excitation and detection loop implementation. Such configuration allows 2D Magnetic Resonance (2DMR) also called Magnetic Resonance Tomography (MRT) e.g. Yaramanci and Hertrich (2006). For MRS it is the equivalent of what happened a few decades ago with Vertical Electric Soundings that moved to 2D resistivity profiling called ERT (electric resistivity tomography) and became affordable due to availability of moderate cost PC and micro-controllers. Hertrich (2003, personal communication), Hertrich and Yaramanci (2003) and Hertrich *et al.* (2005) further worked on the mathematical modeling of the MRT response using coincident and separated loops to bring that concept to an operational status. In parallel with these efforts, IRIS Instruments made available a feature of the NUMIS^{PLUS} where separated loops were supported. Finally, thanks to the support of the BRGM and IRIS, teams from BRGM, TU-Berlin and ITC, field-tested the MRT concept at St-Cyr near Orléans (Hertrich *et al.,* 2005) and at Bulten near Eibergen (Netherlands) where a buried glacial melt channel was mapped by

MRT. An inversion results from this profile is shown in Figure 8.

MRT is a significant step forward in the MRS and hydrogeology fields because it defines both, the vertical and the horizontal boundaries of aquifers. It is expected that MRT will gradually become easier in use regarding both, data acquisition and data inversion. While considering the use of MRT, or even 1D MRS hydrostratigraphy assessment, substantial cost of the MRS survey has always to be considered before deciding to use this technique. From survey time, cost and instrumental availability point of view, whenever possible, for the precise definition of aquifer horizontal or lateral boundaries (but not for quantification of hydrogeological properties) other more efficient geophysical techniques can be used. This is because in most of cases, aquifers have contrasting geophysical properties detectable by those efficient methods. Whenever subsurface hydrostratigraphy has to be combined with quantitative assessment, a combination of carefully selected geophysical techniques including MRS, can be used optimally. For example, in Delta Okavango in Botswana airborne time domain EM was used to map the position and the lateral extent of (low salinity) fresh water buried channel surrounded by saline water while MRS to investigate the depth-wise distribution of fresh water resources, the aquifer storage and the flow property. In that particular task, ground TDEM was less effective than MRS because of lack of contrast between adjacent clay-rich units and the aquifer itself whereas TDEM was advantageous over the MRS in salinity characterization. This was originally notified already in the beginning of 90-ties by Goldman *et al.* (1994).

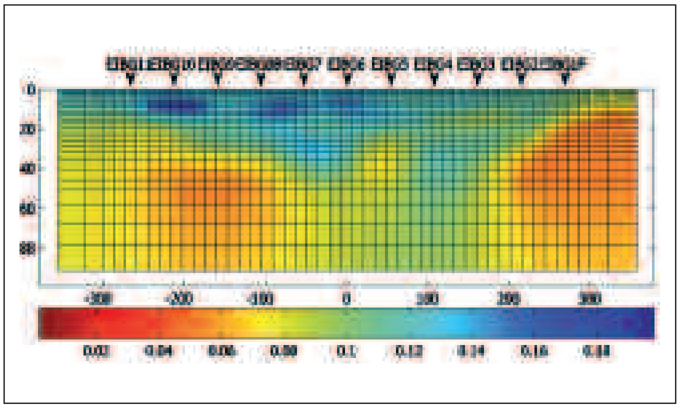

Fig. 8. Separated loop MRT at de Bulten (Eibergen, NL). The color displays the water content. The buried channel is below station 3. Data inversion: Hertrich (2004, personal communication)

Fig. 8. Sección de Tomografía de RM (TRM) obtenida en Bulten (Eibergen, NL). El color indica el contenido en agua. Bajo la estación 3 existe un canal enterrado. Inversión de los datos por Hertrich (2004, comunicación personal)

Currently the MRT technique is available at the cost of more elaborate work in the field and limitations in data inversion. Progress in terms of multichannel hardware and MRT modeling software is expected to bring new capabilities in aquifer geometry definition.

Caveats

(1) The caveats listed under storage parameterization with respect to less known environments (see above), are relevant to subsurface hydrostratigraphy;

(2) The equivalence i.e. loss of reliability on the geometry of the water bearing layers with depth while using the $\theta_{MRS} \cdot \Delta z_{MRS}$ product stays more reliable;

(3) MRS directly maps subsurface water but not always directly the water table; in the case when potentiometric surface is within the impermeable materials there is no water content contrast corresponding to that surface. Also, in permeable materials with fine pore-size, the saturated water is significantly above the water table.

Potential of MRS for vadose zone investigations

As compared to saturated zone, the classical vadose zone characterization techniques are less well established, less direct and less reliable. Typical in-situ vadose zone characterization is done through estimation of water/moisture content (θ) and tension (pressure) head known also as matric potential (ψ). $\theta = \theta_f + \theta_b$ can be measured indirectly through bulk dielectric changes (moisture probe, TDR, GPR for shallow work in resistive formations or in a cross-hole version), neutron probe, etc., while ψ is often measured through tensiometer e.g. manometer reading through a standard membrane or electric resistivity change of a porous standard such as ceramic or gypsum block.

One of the key factors characterizing vadose zone is that it is a three-phase system, such as: rock – water – air (solid-liquid-gas). Water movement in unsaturated zone can be either in liquid or in the gas form. The liquid form of water movement can be either gravitational or capillary. Gravitational downward water movement in unsaturated zone occurs only if soil moisture is above specific retention (field capacity) as indicated in Figure 1, characterized by $\psi \approx 340$ mBar regardless of the soil type (Dingman, 1994). Capillary water movement according to Darcy law is governed by hydraulic gradient and unsaturated hydraulic conductivity that in contrast to saturated zone is moisture dependent. Capillary water movement can take place in any direction (also upward) depending on the hydraulic gradient. Direct unsaturated water flux measurements can be made with lysimeters. Indirectly, unsaturated flux can be estimated through Darcy law i.e. through defining hydraulic gradient and unsaturated hydraulic conductivity. Hydraulic gradient can be defined through matric potential measurements whereas moisture dependent hydraulic conductivity is either defined in the laboratory conditions or estimated from one of the widely used formulas (Maidment, 1993) for the given moisture status. The complication in quantifying water fluxes in unsaturated zone is that its water can move not only in the liquid form but also in the gas form as a vapor, and that it can change state depending on the external conditions (Scanlon *et al.,* 2003). Unfortunately none of the standard geophysical or hydrological methods can quantify vapor movement directly, therefore vapor flux is assessed in hydrology indirectly through profile temperature, moisture and matric pressure measurements and then simulated by models.

In the early phase of MRS testing and exploitation, there has been a widespread understanding, e.g. Schirov *et al.,* (1991), that MRS was not sensitive enough to detect the water in the unsaturated zone. The retained water in the unsaturated zone (capillary + bound water) was assumed as bound water, non-measurable with MRS except for carbonates rocks. As MRS field experience accumulated, it became clear that capillary water of the unsaturated zones were also contributing to the observed MRS signals e.g. the graphs summarizing the field data set inversions but not the text in Schirov *et al.,* (1991), Yaramanci *et al.* (2002), Lubczynski and Roy (2003), etc.

It is essential to keep in mind that the terminology used in NMR petrophysics may sometimes be different and misleading with respect to the terminology used in hydrogeology also adapted here. For example, in NMR petrophysics capillary-bound water term refers to the immobile water in very small pores while in hydrogeology capillary water corresponds to the fraction of water in the unsaturated zone (3 phases: solid-liquid-gas) held against gravity by capillary forces that can move by hydraulic gradient so it is mobile (see Figure 1). Capillary water in hydrogeological meaning, may correspond to water droplets up to mm in size while in NMR petrophysics capillary-bound water is in the μm or less size range and corresponds to bound water in hydrogeological meaning as adapted here and presented in Figure 1.

Except for methods exploiting permittivity contrast, e.g. GPR, which has limited depth capability in conductive environments, only a few classical geophysical techniques can provide quantitative vadose zone moisture content e.g. neutron log and NMR log. Most of the other widely used techniques have highly non-linear water content response in the vadose zone e.g. resistivity and seismic. MRS offers unique non-invasive insight into the unsaturated zone providing opportunity of unsaturated zone measurements of $\theta_{MRS}=\theta_f$. However, a full harmonization between the information provided with classical tools (θ and ψ) and with MRS (θ_{MRS} and spectrum of T_d as a function of depth) has not yet been achieved.

It is expected that MRS will bring new insight in the vadose zone particularly when multi-exponential analysis will be fully operational in its assessment and when an MRS monitoring mode will be implemented. The specific aspects for which MRS has good contribution potential include: (1) unsaturated water mode of occurrence (water films or droplets) which is linked to wettability; (2) droplet size/film thickness; (3) water content; (4) asymmetric wetting versus drying cycles; (5) unsaturated hydraulic conductivity and (6) discrete assessment of fluxes in monitoring mode. Because of the relatively small mass of water in vapor form, it is unlikely that MRS can contribute to direct vapor quantification; it may however quantify vapor through accumulated mass loss/gain over a period of time.

Multi-exponential decay analysis in its application to unsaturated zone was reported by Roy and Lubczynski (2005); an example from such procedure is summarized below. In absence of large magnetic field gradients and when signal-to-noise (S/N) ratio is large, water in unsaturated zone can be analyzed through multi-exponential MRS signal analysis that is particularly suited for unsaturated zone assessment. An example of such analysis is shown for the case of the Waalwijk-2 site where the unsaturated zone is in the upper 6 m (Figure 9), in which the ‘water size’ is displayed by 3 lines with different shades of gray. The top of the unsaturated zone is characterized only with coarse and fine water size even though the grain size locally is of medium size. In the first 2 meters, both the coarse and fine water contents are decreasing. Below 2 meters, the medium water increases rapidly until it reaches its saturated level at the water table (approximately at 6 m of depth). In fact, the sounding was done in the morning with dew on the sand surface. Part of the dew is infiltrating as fine water while the other part (coarse water) evaporate during the

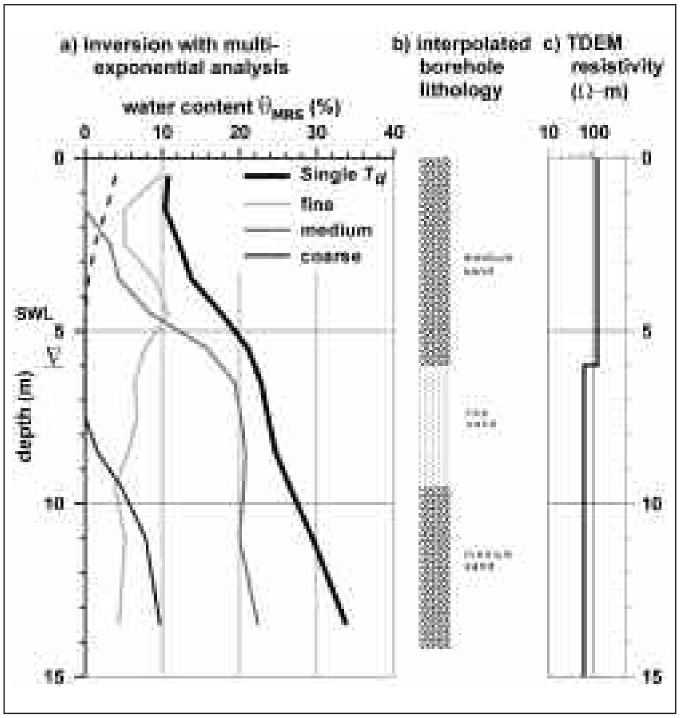

Fig. 9. Waalwijk-2 Multi-exponential decay analysis: MRS data inversion showing discrimination of 'water-size' contributing to unsaturated zone study. Roy and Lubczynski (2005). (a) MRS inversion results; (b) interpolated borehole lithology; (c) TDEM resistivity
Fig. 9. Análisis multiexponencial del tiempo de decaimiento en Waalwijk-2: inversión de datos de un SRM mostrando la discriminación del "tamaño de agua" que contribuye, en el estudio de la zona no saturada. Roy y Lubczynski (2005). (a) Resultado de la inversión del SRM; (b) Litología interpolada del sondeo; (c) Resistividad obtenida por TDEM

day. Below the water table, 'water size' is controlled by lithology.

Out of the two main characteristics of water in unsaturated zone i.e. θ and ψ, determination of θ with MRS (θ_{MRS}) is already confirmed by experiments. Concerning ψ, recently Boucher *et al.* 2006, presented hypothesis and supporting data that, the relaxation times decrease when the unsaturated medium becomes drier i.e. when soil tension pressure increases. This observation is corroborated by the Kleinberg (1996) laboratory NMR experiment that showed that the relaxation time T_2 varied depending on the tension pressure in sandstone samples. If this observation is confirmed through the MRS field experiments over a wide range of vadose environments then MRS may provide the second most important (after θ) hydrological characteristic of the unsaturated zone.

MRS provides new additional ways of characterizing the vadose zone. Classical tools are invasive, have severe constraints in terms of depth and sample representativity, and are mostly limited to a θ and ψ assessment. MRS is non-invasive, water selective, it has depth discrimination and ability to investigate vadose zone not only with regard to θ and ψ but also in terms of water film thickness or droplet size, water film continuity and eventually wettability. This leads to assessment of unsaturated hydraulic conductivity estimate involving discrimination between wetting and drying phase. There is a lot of potential for MRS in unsaturated zone assessment.

Caveats

Unsaturated zone investigations with MRS are made easy by the relative shallowness of the vadoze zone. Next to standard caveats related to the MRS performance in the "difficult" environments discussed in the storage section (see above), the unsaturated zone investigations suffer the following limitations:

(1) water content may drop below the sensitivity limit of the MRS instruments given ambient S/N;
(2) film thickness in the driest zones may be so thin that the corresponding T_d is too short with respect to the aperture window of the MRS instrument;
(3) due to soil forming processes, specific near surface layers may have magnetic susceptibility contrast making accurate measurement of T_d more complex.

Regional MRS data integration and groundwater modeling

While evaluating groundwater resources of a certain area, one of the most important issues is the assessment of spatial and depth-wise distribution of water resources. Various approaches exist in hydrogeology with respect to the integration of data from individual measurements such as: interpolation, extrapolation, stochastic modeling and numerical modeling. The objective of all those methods is to predict the unknown property distribution of the system using the available data as reference and applying certain rules. In that respect the most sophisticated is the method of numerical groundwater modeling, because using this method, data integration is done by simulating physical (hydrogeological) processes based on the commonly accepted physical laws.

In data integration very important is a common in hydrogeology problem of heterogeneity and related with that, problem of scale effect. Most of hydrogeological measurements, except of pumping tests, are restricted to very small representative volume of less than 1 m^3. In that respect MRS offers very attractive service to hydrogeological applications because the investigated by MRS volume can be adjusted by using varying sizes of loops from very low volumes up to 150x150x150 m^3 so that it can match commonly used model grid cells. Unfortunately, accurate one-to-one correspondence between the MRS loop position and the analyzed model grid cell cannot be explicitly made yet. However, the most widely used pumping test method for hydrogeological system parameterization provides even less correspondence between the model grid and the investigated volume and is more time consuming and more expensive. Therefore MRS method grows as considerable competitor to pumping tests as data provider for groundwater modeling.

The optimal strategy with respect to the use of MRS for groundwater modeling can be formulated as follows:

(1) Analyze all archive data and identify all pumping test (PT) data in the area to be modeled;
(2) If raw PT data available, reprocess it to obtain independent estimates of the hydrogeological parameters;
(3) Set MRS experiments at the sites with available PT data and derive MRS storage and flow parameters;
(4) Calibrate transmissivity by cross referencing MRS and pumping test data to obtain C_T in order to establish $T_{MRS} = C_T\ \Delta z_{MRS}\ \theta_{MRS}\ T_1^{*2}$ formula; this formula will be then specific for the area investigated, allowing then to derive T_{MRS} from MRS surveys in any other locations of that investigated area;
(5) If sufficient amount of pumping test data available spare some points for verification of T_{MRS}; if numerical model to be used requires K then derive it from T_{MRS};
(6) If pumping tests provided storage parameters compare them with MRS storage parameters to verify the latter;
(7) If discrepancies between MRS and PT data are large and/or the pumping test data are insufficient and/or not reliable, design sufficient amount of additional piezometric (consisting of well abstraction and at least one piezometer – to ensure reliable storage coefficient) pumping tests;
(8) Depending on the hydrogeological conditions in the study area modeled, particularly its size and heterogeneity, design appropriate amount of MRS survey points.
(9) Process the MRS-derived hydrogeological parameters and integrate them in the numerical model.

The advantage of numerical models in data integration, also MRS data integration, is that groundwater model solution is based on flow equations that link all spatial and temporal data types together. This means that if certain data type is not correct, then as a consequence there will be disparity in calibrated values and in water balance. For example in steady state numerical models, both aquifer transmissivity and groundwater recharge influence the position of the calibrated groundwater table. If for example certain value of T_{MRS} was largely underestimated (e.g. through the error in C_T approximation), then with given recharge, the simulated on the model groundwater table would rise beyond its realistic, expected position (sometimes even above the topographic surface). Such model performance would then confirm an error in the acquired T_{MRS} (eventually in the applied recharge). This way numerical groundwater models through the calibration process, provide additional control over the integrated in the model hydrogeological data so also over the integrated MRS data.

Experiences in groundwater modeling indicate that transient models with spatio-temporal structure are more reliable than standard steady-state models based on spatial data (hydrogeological parameters) only. Temporal hydrogeological data (hydraulic heads and groundwater fluxes such as recharge and evapotranspiration) are acquired in hydrogeology indirectly, through logger-based automated monitoring of microclimatic variables, soil moisture, matric pressure, groundwater table and eventually water uptake by trees. Determination of hydraulic heads with standard hydrogeological monitoring tools is efficient, accurate and inexpensive but none of the hydrogeological methods can provide non-invasive, direct and realistic information about flux quantity and its pattern in subsurface. This is where MRS can also contribute substantially (next to parameterization of the saturated zone) to groundwater modeling. For that purpose, several MRS experiments focusing at unsaturated zone (these in most cases would be shallow MRS instruments) would have to be installed in various locations in the monitoring mode allowing programmed interval scanning of the unsaturated zone. The temporal variability of fluxes recorded in such monitoring points could then be integrated spatially using one of the saturated-unsaturated zone models such as e.g. HYDRUS (Rassam *et al.,* 2003).

The accuracy and reliability of groundwater models depend largely upon the quantity and quality of groundwater model input. Development of such models and their calibration, require sometimes additional data to control the reliability of performance of a certain parts of the model. In standard groundwater projects, groundwater modeling follows borehole drilling so typically when models are calibrated then the additional borehole drilling and pump testing are usually not anymore permitted due to the financial constrains. With lower cost, lower time input and larger mobility of MRS as compared to borehole drilling and pump testing, MRS provides also an excellent opportunity of efficient, supplementary data acquisition during and after model calibration.

Caveats

(1) The inversion of the MRS data into hydrogeological parameters, particularly in the unknown areas, is vulnerable to error; therefore during groundwater model calibration, those parameters have to be used with prudence, definitely not as fixed independent variables.

(2) The spatial representation of the volume investigated by MRS survey is not resolved yet therefore in heterogeneous environments, it is difficult to provide one-to-one correspondence between model grid and the volume investigated by MRS.

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