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SIMULTANEOUS DETERMINATION OF THE DIELECTRIC RELAXATION BEHAVIOR AND SOIL WATER CHARACTERISTIC CURVE OF UNDISTURBED SOIL SAMPLES

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ABSTRACT

The frequency dependence of soil electromagnetic properties contain valuable information of the porous material due to strong contributions to the dielectric relaxation behavior by interactions between aqueous pore solution and mineral phases due to interface effects. Soil hydraulic properties such as matric potential are also influenced by different surface bonding forces due to interface processes. For this reason, a new analysis methodology was developed, which allows a simultaneous determination of the soil water characteristic curve and the dielectric relaxation behavior of undisturbed soil samples. This opens the possibility to systematically analyze coupled hydraulic/dielectric soil properties for the development of pedotransfer functions to estimate physico-chemical parameters with broadband HF-EM measurement techniques.

Index Terms— constitutive material parameters, dielectric spectroscopy, soil water characteristic curve

1. INTRODUCTION

Frequency dependent material properties of porous media such as soil are not only disturbance quantities in applications with high frequency electromagnetic (HF-EM) techniques (remote sensing, time domain reflectometry, ground penetrating radar) but also contain valuable information of the porous material due to strong contributions to the dielectric relaxation behavior by interactions between aqueous pore solution and mineral phases [1, 2, 3]. This circumstance opens the possibility to estimate physico-chemical parameters such as water content, texture, mineralogy and matric potential with broadband HF-EM measurement techniques. In this context, a new analysis methodology was developed, which allows the simultaneous determination of the soil water characteristic curve and the dielectric relaxation behavior of soil. For assessment of the approach a set of 25 undisturbed samples are taken from a 80 cm soil profile of a GPR test site (Taunus/Germany) with coaxial retention cells developed in Lauer at al. (2012) [4]. The samples were capillary saturated followed by a step by step de-watering in a pressure plate apparatus as well as oven drying at 40 °C, equilibrated and the frequency dependent HF-EM material properties were determined in the frequency range from 1 MHz to 5 GHz with vector network analyzer technique. The dielectric relaxation behavior were obtained by inverse modeling with a global optimization algorithm based on a generalized fractional relaxation model according to Wagner et al. (2011) [2]. Selected relaxation parameters are compared with results determined by means of empirical equations and frequently used mixture models.

2. MATERIAL AND METHODS

Undisturbed soil samples were taken in four depths (0, 30, 50 and 75 cm) from a typically soil profile developed in the Taunus area, in the south-eastern part of the Rhenish Massif, Germany (see [4] for details). In Table 1 physical, chemical and mineralogical soil properties are summarized.

2.1. Soil water characteristic curve (SWCC)

To obtain simultaneously SWCC and frequency dependent HF-EM properties of the soil samples, a two-port coaxial transmission line cell according to Lauer et al. [4] was used. The outer diameter of the inner conductor is 16.9 mm, the inner diameter of the outer conductor is 38.8 mm with the total length of 50 mm. Both conductors are designed with a cutting edge allowing easier insertion of the cell into the soil without disturbing the natural in situ soil structure. The taken soil samples were measured as-received, water saturated and stepwise dewatered by increasing negative pressure (pF 1.4/1.8/2/2.5/4.2) in a pressure plate apparatus. After each pressure step, the samples were sealed, equilibrated, weighted and the dielectric spectra were measured. After increasing the pressure to pF 4.2, permittivity measurements were carried out for saturated and air-dried samples. The in-situ bulk densities were obtained after drying at 105 °C.

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Table 1. Physical, chemical and mineralogical properties of the investigated soil (see [4]).

horizon	sand	silt	clay	organic	vermiculite/ smectite	illite/kaolinite/ mixed layer	tecto- silicates	goethite	particle density	cation exchange capacity
	[wt. %]				[wt. %]				[g/cm^3]	[mmol/100g]
Ah	18.9	57.5	24.0	2.4	2.8 / -	40.9 / 19.1 / 8.1	28.4	0.7	2.62	9.02
Btg	20.0	46.6	33.5	-	8.7 / 1.8	35.5 / 21.8 / 12.7	18.5	1.1	2.65	12.51
2Cg	43.7	31.1	25.2	-	2.2 / -	50.7 / 30.9 / 11.3	4.9	-	2.69	11.45
3Cg	61.8	20.5	17.7	-	2.8 / -	51.2 / 27.6 / 9.2	8.8	0.4	2.71	11.09

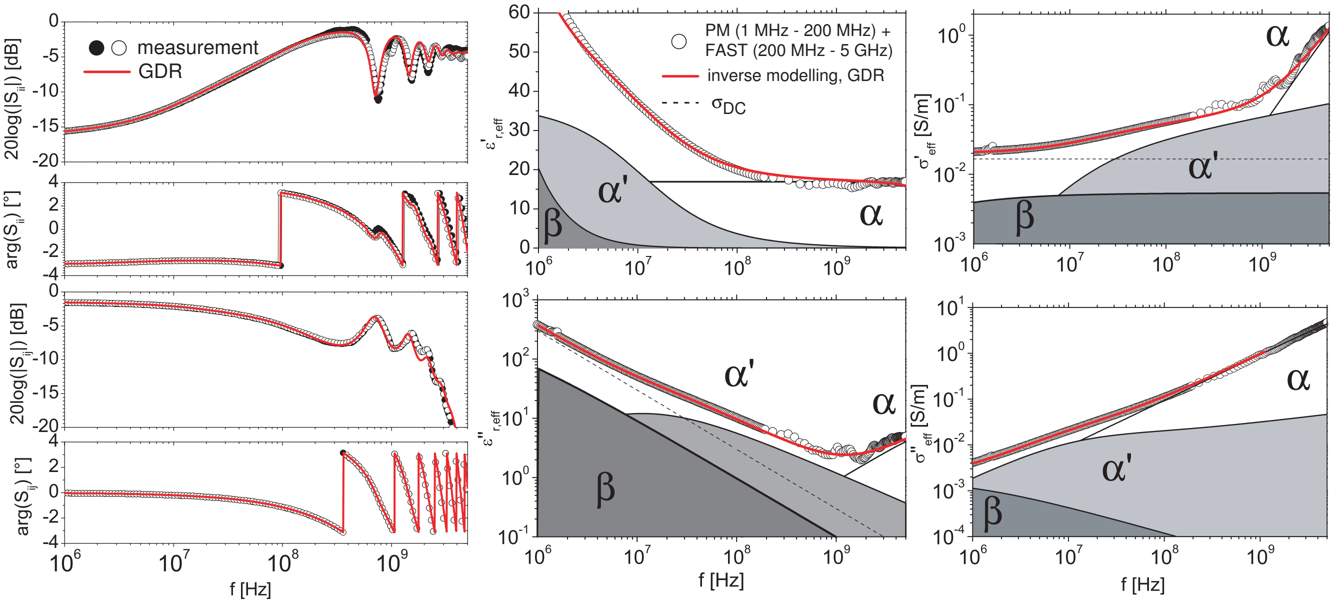

Fig. 1. (from left to right) S-Parameter S_{ij}, complex effective relative permittivity $\varepsilon^\star_{\mathrm{r,eff}}$ and complex effective electrical conductivity $\sigma^\star_{\mathrm{eff}}$ as a function of frequency of a sample from the 3Cg horizon at pF 1.8 with $\theta = 0.29\ m^3m^{-3}$ and $n = 0.41$ as well as the results of the SCEM-UA optimization (see text for the used terminology).

2.2. High frequency electromagnetic technique

HF-EM properties were determined within a frequency range from 1 MHz to 5 GHz at room temperature and atmospheric pressure with Rohde & Schwarz ZVR (1 MHz to 4 GHz) and Agilent PNA E8363B (10 MHz to 5 GHz) vector network analyzers. Full two-port calibration was done by mechanical (Rhode & Schwarz N - 50 Ω ZV-Z21) or electronically (Agilent electronic calibration kit N4691B) calibration standards (Open, Short, 50 Ω-Match, Through) at the N connector of the high-precision coaxial cable to the measurement cell. Measurement quantities are the complex scattering parameters S_{ij} of the full length coaxial line including N to 1 5/8” EIA coupling elements at both sample cell ends (Figure 1). Complex effective relative permittivity $\varepsilon_{\mathrm{r,eff}}$ was calculated by means of Agilent 85071/E materials measurement software at the frequency range from 200 MHz to 5 GHz.

In addition to Agilent 85071/E materials measurement software, complex S-parameter values S_{ij} measured with Rohde & Schwarz ZVR were used to compute $\varepsilon_{\mathrm{r,eff}}$ in the frequency range between 1 MHz to 4 GHz using the following methods implemented in matlab: classical Nicholson-Ross-Weir model (NRW), Baker-Jarvis (BJ), BJ-iterative (BJI) and propagation matrix method (PM) [4, 2]. The quasi-analytical methods were compared and validated against inverse modeling technique according to [2] based on a generalized fractional dielectric relaxation model (GDR):

$$\varepsilon^\star_{\mathrm{r,eff}} - \varepsilon_\infty = \sum_{k=1}^{N} \frac{\Delta\varepsilon_k}{(j\omega\tau_k)^{\alpha_k} + (j\omega\tau_k)^{\beta_k}} - j\frac{\sigma_{DC}}{\omega\varepsilon_0} \qquad (1)$$

with high frequency limit of permittivity ε_∞, relaxation strength $\Delta\varepsilon_k$, relaxation time τ_k as well as stretching exponents $0 \leq \alpha_k, \beta_k$ of the k-th process and apparent direct current electrical conductivity σ_{DC}.

The GDR parametrization is performed with a shuffled complex evolution metropolis algorithm (SCEM-UA) according to Vrugt et al. 2003 [5] assuming three active relaxation processes in the investigated frequency-temperature-pressure range (see [1, 2]): one primary α-process (main water relaxation) and two secondary processes caused by solid-water-ion interactions α', β (the superposing of relaxation processes due to adsorbed and hydrated water, counter ion relaxation as well as Maxwell-Wagner effects). The applicability of the HF-EM methodology was assessed by repeated measurements on a homogeneous dispersive and dielectric as well as electrical lossy nearly saturated gypsum sample and weak or non dispersive and low loss common standard materials: air, teflon measured before and after each pressure step as well as glass, zircon and baddeleyite beads with air (for details see [4]).

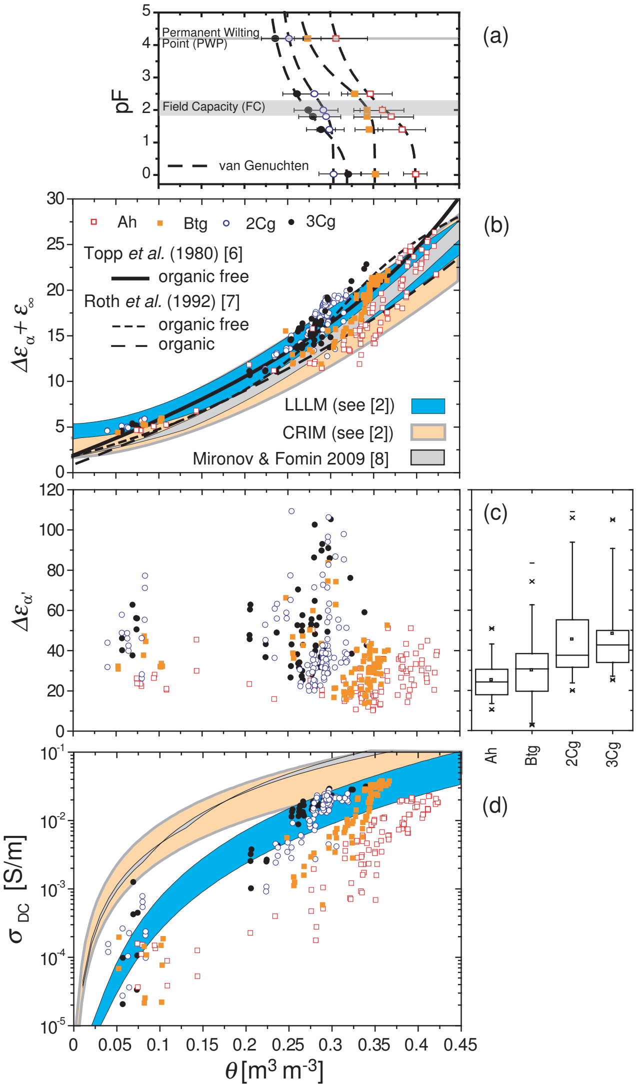

Fig. 2. (a) Soil water characteristic curve, (b) high frequency limit of permittivity ε_∞ and relaxation strength $\Delta\varepsilon_\alpha$ of free and immobile pore water, (c) relaxation strength $\Delta\varepsilon_{\alpha'}$ of the α'-process as well as box and whiskers plots of $\Delta\varepsilon_{\alpha'}$ for the appropriate soil horizon and (d) apparent direct current conductivity σ_{DC} obtained with inverse modeling as a function of volumetric water content θ (for details see [4]).

Table 2. RMSE of the obtained volumetric water content in volume % from the relaxation strength of the α-process with the empirical equations for organic free / ♣organic soils.

	Ah	Btg	2Cg	3Cg
Topp et el. (1980)	4.7 (3.5)♣	2.1	2.3	2.2
Roth et al. (1992)	4.7 (3.4)♣	2.3	2.1	2.2

3. RESULTS AND DISCUSSION

In Figure 1, the results of the direct inversion algorithms (PM+FAST) and the inverse modeling technique are represented for a soil sample from 3Cg-horizon at pF 1.8 with $\theta = 0.29\,m^3m^{-3}$ and $n = 0.41$. Clearly visible in the dielectric spectrum are the α- and α'-process with relaxation times of 9 ps or 17 ns, respectively. In the case of the β-process only the high frequency tail is visible because of a relaxation time of 0.8 μs. Hence, in the frequency range below 10 MHz, the frequency dependence of the effective complex relative permittivity was dominated by the β-process as well as the direct current conductivity contribution.

In Figure 2 the results of the parametrization for all samples are represented for the dominant α- and α'-process as well as the apparent direct current conductivity σ_{DC} in comparison to the empirical models according to Topp et al. (1980) [6] and Roth et al. (1992) [7], the semi-empirical generalized refractive mixing dielectric model (GRMDM) by Mironov et al. (2009) [8] as well as the theoretical mixture equations CRIM (Complex Refractive Index model) and LLLM (Looyenga-Landau-Lifschitz model) according to [2].

The achieved mean relative error in the relaxation strength of the α- process is below 1% in contrast to the α'- process with 24 %. Therefore, the α-process can be related to the volumetric water content, which is also confirmed by the empirical equations. In the low water content range the Topp et al. (1980) [6] equation gives better results than the Roth et al. (1992) [7] equation and in the water content range above 0.2 $\mathrm{m^3m^{-3}}$ vise versa. In Table 2 appropriate RMSEs are summarized.

GRMDM underestimate the permittivity in the low water content range below 0.2 $\mathrm{m^3m^{-3}}$ for all soils and above for the soil from the 2Cg and 3Cg horizon and overestimate the permittivity for the soil from the Ah horizon in the range below 0.4 $\mathrm{m^3m^{-3}}$. Hence, the different soil texture, structure and mineralogy are not able to predict. The relaxation strength of the α'-process shows complicated dependence on volumetric water content. Especially around 0.30 m^3m^{-3}, it rises up to 100 for all samples with exception of the Ah-horizon.

Apparent direct current conductivity σ_{DC} shows a clear textural dependence. Moreover, σ_{DC} is clearly overestimated with GRMDM due to the exponent 0.5 in the underlying CRIM equation and the difficulty to estimate the conductivity of pore water a priori [2]. The theoretical models CRIM and LLLM are more flexible to characterize the influence of the pore water conductivity as well as the different physico-chemical soil properties. However, with CRIM the same overestimation of the direct current conductivity is observed as in the case of the GRMDM regardless pore water conductivity is estimated according to the approach in [2]. This suggests to link soil water potential to the pore water conductivity.

The scattering of the relaxation strength of the α'-process can be further attributed to the influence of the non-homogeneous structure of the undisturbed samples in the cell as well as the imposition of the assumed relaxation processes and the difficulty separating them clearly with the chosen relaxation model in the investigated frequency range. Nevertheless, the strongest effects in the relaxation strength can be observed for the 2Cg- and 3Cg-horizon with smallest porosities and a permanent wilting point θ_{PWP}=25 $\pm$ 2 and 24 $\pm$ 2 respectively. In case of the soil from the Ah-horizon with θ_{PWP}=31 $\pm$ 4 relaxation strength $\Delta\varepsilon_{\alpha'}$ is nearly independent of water content corresponding with the lowest σ_{DC} and indicating the impact of organic matter. The samples from Btg-horizon with θ_{PWP}=27 $\pm$ 2 as well as the highest clay content and highest amount on swelling clay minerals show an intermediate behavior.

4. CONCLUSION

A new analysis methodology was developed, which allows a simultaneous determination of the soil water characteristic curve and the dielectric relaxation behavior of undisturbed soil samples. For assessment of the approach a set of 25 undisturbed samples from a soil profile of a GPR test site (Taunus / Germany, [4]) were analyzed in the frequency range from 1 MHz to 5 GHz with vector network analyzer technique. The dielectric relaxation behavior was determined by means of inverse modeling assuming three active relaxation processes: one primary α-process (main water relaxation) and two secondary processes α', β caused by solid-water-ion interactions . Frequently used empirical equations were related to the free water α-process which clearly confirm the great value to estimate the volumetric water content with this approaches. GRMDM according to Mironov et al. (2009) [8] used at a frequency of 1 GHz is unable to predict textural, mineralogical and structural influences on the permittivity of the α-process and clearly overestimate apparent direct current conductivity contribution. The theoretical Models CRIM and LLLM are more flexible to characterize the influence of the pore water conductivity as well as the different physico-chemical soil properties.

The relaxation strength $\Delta\varepsilon_{\alpha'}$ of the α'-process shows a complicated dependence on volumetric water content. The strongest effects can be observed for the soil from the basal periglacial slope deposit and bedrock with smallest porosities. $\Delta\varepsilon_{\alpha'}$ of the Ah-horizon is nearly independent of water content corresponding with the lowest σ_{DC} and indicating the impact of organic matter. However, the verification and validation of these observations need further systematic analysis of the obtained dataset using relaxation models in combination with mixture equations [1, 2] under consideration of the soil structure in the cell in comparison with homogeneous disturbed samples.

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