Estimation of the Soil Water Characteristics from Dielectric Relaxation Spectra - a Machine Learning Approach

Norman Wagner Institute of Material Research and Testing at the Bauhaus-University Weimar Coudraystr. 4, 99423 Weimar, Germany

Frank Daschner Microwave Group Faculty of Engineering University of Kiel, Germany Alexander Scheuermann and Moritz Schwing Geotechnical Engineering Centre The University of Queensland Brisbane, Australia

Abstract—The frequency dependence of dielectric material properties of water saturated and unsaturated porous materials such as soil is not only disturbing in applications with high frequency electromagnetic (HF-EM) techniques but also contains valuable information of the material due to strong contributions by interactions between the aqueous pore solution and mineral phases. Hence, broadband HF-EM sensor techniques enable the estimation of soil physico-chemical parameters such as water content, texture, mineralogy, cation exchange capacity and matric potential. In this context, a multivariate (MV) machine learning approach (principal component regression, partial least squares regression, artificial neural networks) was applied to estimate the Soil Water Characteristic Curve (SWCC) from experimentally determined dielectric relaxation spectra of a silty clay soil. The results of the MV-approach were compared with results obtained from empirical equations and theoretical models as well as a novel hydraulic/electromagnetic coupling approach. The applied MVapproach gives evidence, (i) of a physical relationship between soil dielectric relaxation behavior and soil water characteristics as an important hydraulic material property and (ii) the applicability of appropriate sensor techniques for the estimation of physicochemical parameters of porous media from broadband measured dielectric spectra.

I. INTRODUCTION

The success of water content estimation in porous media with high frequency (radio and microwave) non and minimal invasive electromagnetic (HF-EM) measurement techniques is caused by the dipolar character of the water molecules resulting in a high permittivity in comparison to other phases. In particular, HF-EM sensing techniques such as ground penetrating radar (GPR, [1]-[4]), conventional time or frequency domain domain reflectometry (TDR/FDR, [5]-[7]), spatial time domain reflectometry (spatial TDR, [8]-[11]), capacitance methods [12] as well as active and passive microwave remote sensing techniques ([13], [14]) offer the possibility to monitor spatial and temporal variations of soil physical state parameters, e.g. the volume fraction of free pore water, with high resolution ([2], [3], [6], [8], [10]). Hence, the objective of numerous experimental and theoretical investigations are the development of generalized electromagnetic models for a broad class of soil textures and structures ([15]–[17]). Mostly, these empirical, numerical or theoretical approaches are based on the assumption of a constant dielectric permittivity of the soil as a function of volumetric water content in a narrow frequency and temperature range ([18]–[21]). However, HF-EM techniques cover a broad frequency range between approximately 10 MHz, in the case of spatial TDR, to at least 10 GHz in X-band remote sensing applications ([6], [22]). For this reason, the knowledge of the frequency and temperature dependent HF-EM material parameters is needed for a successful application and combination of the different sensing techniques. However, interactions between the aqueous pore solution and solid phases lead to strong contributions to the electromagnetic material properties due to interphase processes ([23], [24]). Therefore, the broadband dielectric spectrum contains valuable information about porous media and it can be used for an estimation of physico-chemical parameters besides free pore water such as texture, structure, mineralogy, cation exchange capacity and matric potential as important hydraulic property with broadband HF-EM sensor techniques. In this context, a multivariate (MV) approach according to Daschner et al. (2003) [25] was applied for the simultaneously determination of soil water content, porosity and matric potential from measured frequency dependent dielectric material properties. The results of the MV-approach were compared with results obtained from empirical equations and theoretical models as well as a novel hydraulic/electromagnetic coupling approach.

II. MODELING OF SOIL DIELECTRIC RELAXATION BEHAVIOR

Organic free soil as a typical porous material mainly consists of four phases: solid particles (various mineral phases), pore air, pore fluid as well as a solid particle - pore fluid interface. In principle the fractions of the soil phases vary both in space (due to composition and density of the soil) and time (due to changes of water content, porosity, pore water chemistry and temperature). The electromagnetic properties of the solid particles are frequency independent in the considered temperature-pressure-frequency range. Real relative permittivity varies from 3 to 15 [26]. The pore fluid as well as interface fluid are mainly an aqueous solution with a temperaturepressure-frequency dependent relative complex permittivity $\varepsilon_w^*(\omega, T, p)$ according to the modified Debye model [27]:

$$\varepsilon_w^{\star}(\omega, T, p) - \varepsilon_{\infty}(T, p) = \frac{\Delta \varepsilon(T, p)}{1 + j\omega \tau_w(T, p)} - j \frac{\sigma_w(T, p)}{\varepsilon_0 \omega}, \quad (1)$$

with direct current conductivity σ_w , high frequency limit of permittivity ε_{∞} and relaxation strength $\Delta \varepsilon = \varepsilon_S + \varepsilon_{\infty}$ with static dielectric permittivity ε_S . Under atmospheric conditions the dielectric relaxation time of water $\tau_w(T)$ depends on temperature T according to the Eyring equation [23] with Gibbs energy or free enthalpy of activation $\Delta G_w^{\ddagger}(T) =$ $\Delta H^{\ddagger}_w(T) - T\Delta S^{\ddagger}_w(T)$, activation enthalpy $\Delta H^{\ddagger}_w(T)$ and activation entropy $\Delta S_w^{\ddagger}(T)$. Furthermore, Gibbs energy of the interface fluid $\Delta G_d^{\ddagger}(T)$ is assumed to be a function of the distance from the particle surface (for quantitative approaches see [23]). Soil matric potential Ψ_m is a measure of the bonding forces on water in the soil and is related to the chemical potential of soil water $\Delta \mu_W = \mu_W^\circ - \mu_W = \Psi_m V_W$ with chemical potential at a reference state μ_W° and molar volume of water V_W ([28], [29]). Thus, Hilhorst et al. ([29]–[31]) suggested an approach for the relationship between Ψ_m and ΔG_d^{\downarrow} :

$$\Psi_m(T) \cdot V_W = \Delta G_w^{\ddagger \circ}(T) - \Delta G_d^{\ddagger}(T)$$
⁽²⁾

with Gibbs energy of water at a reference state $\Delta G_w^{\ddagger\circ}(T)$ (10.4 kJ/mol at atmospheric conditions and T=293.15 K). This relationship is used to calculate Gibbs energy or free enthalpy of dielectric activation of interfacial water $\Delta G_d^{\ddagger}(T)$. The complex relative dielectric permittivity of free and interface water of a porous material, e.g. soil, in dependence of the volumetric water content θ under atmospheric conditions then can be calculated [32]:

$$\varepsilon_{a(\theta,n)}^{\star}(\theta,T) = \int_{\Psi_m(0)}^{\Psi_m(\theta)} \varepsilon_w^{\star a(\theta,n)}(\Psi_m(\theta),T) \frac{d\theta(\Psi_m)}{d\Psi_m} d\Psi_m.$$
(3)

The parameter $0 \le a \le 1$ is defined by the used mixture approach to obtain the effective complex relative permittivity of the soil $\varepsilon_{r,\text{eff}}^{\star}(\theta,T)$. The parameter *a* contains in principle structural information of free and interface water in the soil and is strictly speaking a function of volumetric water content θ and porosity *n*. However, Hilhorst 1998 (HIL, [31]) suggests the following equation

$$\varepsilon_{r,\text{eff}}^{\star}(\theta,T) = \frac{\varepsilon_1^{\star}(\theta,T)}{3(2n-\theta)} + (1-n)\varepsilon_G(T) + (n-\theta) \quad (4)$$

with porosity n and real relative permittivity of solid grain ε_G . As an alternative approach Wagner et al. 2011 [24] suggests the so called advanced Lichtenecker and Rother Model (ALRM):

$$\varepsilon_{r,\text{eff}}^{\star a(\theta,n)}(\theta,T) = \varepsilon_{a(\theta,n)}^{\star}(\theta,T) + (1-n)\varepsilon_G(T)^{a(\theta,n)} + (n-\theta)$$
(5)

with the following empirical relationships for the structure parameter a and pore water conductivity σ_w° at a reference state (T=298.15 K, [33]) with constants A_i , B_i , C_i :

$$a(\theta, n) = A_1 + B_1 n^2 + C_1 \left(\frac{\theta}{n}\right)^2$$
 (6)

$$\log\left(\sigma_{w}^{\circ}(\theta, n)\right) = \log A_{2} + B_{2}n + C_{2}\left(\frac{\theta}{n}\right).$$
(7)

In the proposed electromagnetic/hydraulic coupling approach the ALRM is used in complex refractive index model (CRIM) form with a constant structure parameter a = 0.5 [23].

III. MATERIAL AND METHODS

A slightly plastic clay soil was investigated (for soil details see [34]). The mineralogical composition is dominated by tectosilicates (36 wt.%), carbonates (36 wt%) and mica (16 wt%) with a certain amount of clay minerals (smectite 9 wt.%, kaolinite 3 wt%). The permittivity of the solid particles with 5.57 was estimated from mineralogical composition (see [32] for details).

A. Hydraulic and mechanical soil properties

Soil water characteristic curve (SWCC- relationship between volumetric water content θ and matric potential Ψ) as well as shrinkage behavior (changes in porosity *n* as a function of volumetric water content θ) were determined in separate experimental investigation (for details see [35], Fig. 1). SWCC was parameterized with a tri-modal van Genuchten equation according to Priesack and Durner (2011) [36] using a shuffled complex evolution metropolis algorithm (SCEM-UA, [37]) and shrinkage behavior was parameterized with an empirical equation to determine appropriate matric potential and porosity at defined volumetric water contents (c.f. [32]).

B. Soil dielectric relaxation spectra

The frequency dependent complex permittivity was determined in the frequency range from 1 MHz to 10 GHz with network analyzer technique according to Wagner et al. (2011) [34] by means of quasi-analytical methods as well as numerical inversion of measured four complex S-parameters based on a transverse electrical and magnetical (TEM) forward model in combination with a broadband electromagnetic transfer function (Generalized Dielectric Response - GDR, Fig. 2):

$$\varepsilon_{\mathrm{r,eff}}^{*}(\omega) - \varepsilon_{\infty} = \sum_{i=1}^{N} \frac{\Delta \varepsilon_{i}}{\left(j\omega\tau_{i}\right)^{a_{i}} + \left(j\omega\tau_{i}\right)^{b_{i}}} - j\frac{\sigma'_{\mathrm{DC}}}{\omega\varepsilon_{0}}, \quad (8)$$

with ε_{∞} the high-frequency limit of relative permittivity, $\Delta \varepsilon_i$ the relaxation strength, τ_i the relaxation time, $0 \le a_i, b_i \le 1$ stretching exponents of the *i*-th process, and σ'_{DC} apparent direct current electrical conductivity.

For the determination of the spectra, the soil sample was in a first step saturated with deionized water and prepared at liquid limit with gravimetric water content w = 0.267 g/g (volumetric water content $\theta = 0.45$ m³/m³). The obtained soil suspension was placed in a rod based transmission line cell (R-TML, see [34]). In a next step the sample was stepwise dried



Fig. 1. (top) Matric potential Ψ expressed in terms of pF=log($|\Psi|[hPa]$) and (bottom) porosity *n* as a function of volumetric water content θ .

isothermal at 23 °C under atmospheric conditions at defined humidities and equilibrated. Appropriate mass loss and sample volume change were estimated during the drying process to obtain appropriate volumetric water content. At each step a broadband electromagnetic measurement was performed.

C. Preprocessing of the relaxation spectra

Prior to the application of the MV-methods the measured dielectric relaxation spectra were reduced to 81 frequency points in the frequency range from 1 MHz to 5 GHz. The spectra were compiled in a $m \times 2n$ relative permittivity matrix

$$\underline{\varepsilon} = \begin{bmatrix} \varepsilon_{1,1}'(f_1) & \cdots & \varepsilon_{1,n}'(f_n) & \varepsilon_{1,1}''(f_1) & \cdots & \varepsilon_{1,n}''(f_n) \\ \vdots & \vdots & \vdots & \vdots \\ \varepsilon_{m,1}'(f_1) & \cdots & \varepsilon_{m,n}'(f_n) & \varepsilon_{m,1}''(f_1) & \cdots & \varepsilon_{m,n}''(f_n) \end{bmatrix}$$
(9)

for *m* measurements at *n* frequencies f_l with real $\varepsilon'_{k,l}$ and imaginary part $\varepsilon''_{k,l}$. The data-set then was transformed in its principal components **P** (PCs)

$$\mathbf{P} = \mathbf{X}\mathbf{E} \tag{10}$$

based on a singular value decomposition with loadings (matrix of eigenvectors) \mathbf{E} and mean-centered and standardized original data matrix \mathbf{X}

$$\mathbf{X} = \begin{bmatrix} \underline{\varepsilon} & -\begin{bmatrix} 1\\ \vdots\\ 1 \end{bmatrix} \begin{bmatrix} \overline{\varepsilon_1'} \cdots \overline{\varepsilon_n'} & \overline{\varepsilon_1''} \cdots \overline{\varepsilon_n''} \end{bmatrix} \begin{bmatrix} \sigma_{\varepsilon_1'}^{-1} & \cdots & 0\\ \vdots & \ddots & \vdots\\ 0 & \cdots & \sigma_{\varepsilon_n''}^{-1} \end{bmatrix}$$
(11)



Fig. 2. Real part $\varepsilon'_{r,\text{eff}}$ and imaginary part $\varepsilon''_{r,\text{eff}}$ of the experimental determined complex relative effective permittivity $\varepsilon^*_{r,\text{eff}}$ as a function of frequency for different volumetric water contents θ .

herein $\overline{\varepsilon_l'}$ or $\overline{\varepsilon_l''}$ denotes the mean and $\sigma_{\varepsilon_l'}$ or $\sigma_{\varepsilon_l'}$ the standard deviation of the data-set at each frequency. Based on principal component analysis (PCA) an appropriate lower limit of the PCs variance with $\sigma_C = 10^{-5}$ was estimated as a robust cut off criterium in the multivariate calibration step.

D. Multivariate calibration

The following multivariate methods were applied to quantitatively relate the spectra to soil physical properties such as water saturation S_W and porosity n or volumetric water content $\theta = S_W \cdot n$ as well as matric potential Ψ : principal component analysis with principal component regression (PCR), partial least squares regression (PLSR). In addition artificial neural networks (ANN) was applied to the mean-centered and standardized original data matrix \mathbf{X} using one hidden layer, which contains 10 neurons. The activation functions of the neurons in the hidden layer are nonlinear (tansig-function) while those of the output layer are linear (for details see [25], [38]).

IV. RESULTS

The complete data-set of 266 measured spectra were randomly divided into two sets with each 133 groups. One set is used for calibration and one set for validation. In Table I and Figure 3 the results of the different methods are summarized. The PLSR-technique gives the best results with



Fig. 3. Experimental determined parameters (volumetric water content θ , porosity *n*, matric potential Ψ expressed in terms of pF=log($|\Psi|[hPa]$)) versus predicted results from the dielectric relaxation spectra.

TABLE I Results of the used multivariate methods (R^2 =0.99 for all properties and methods) and root mean square error estimate for calibration RMSE_C or validation RMSE_V, respectively.

	PCR	PLSR	ANN
θ [%]	0.4 / 0.5	0.2 / 0.5	0.3 / 0.3
$n \ [\%]$	0.4 / 0.6	0.1 / 0.4	0.3 / 0.4
Ψ [pF]	0.12 / 0.12	0.09 / 0.09	0.12 / 0.12

lowest RMSEs (see Figure 1 and Tab. I). The results of the PLSR-approach were compared with the well known empirical calibration function according to Topp et al. 1980 [15] and the advanced Lichtenecker and Rother model (ALRM) according to equation (5) to (7). Furthermore the theoretical mixture rule according to equation (4) as well as (5) in four phase CRIM form were used considering soil water characteristic curve (SWCC) as well as shrinkage behavior (Fig. 1) based on the improvements suggested in section II (WS-HIL, WS-CRIM) to calculate complex relative permittivity of free and interface water according to (3).

In Fig. 4 theoretically calculated, statistically estimated and experimentally determined ε_{reff}^{*} at 1 GHz is represented for

WS-CRIM, WS-HIL, ALRM, PLSR and Topp. The models (WS-HIL, WS-CRIM, ALRM) predict the permittivity at very low water content whereas the Topp-equation clearly underestimate $\varepsilon'_{r,\text{eff}}$. The frequency and water content dependent complex effective relative permittivity is poorly predicted with WS-HIL while the qualitative characteristics is similar. Substantially better results gives WS-CRIM. The deviation between WS-CRIM and experimentally obtained imaginary part of effective complex permittivity $\varepsilon_{r,\text{eff}}^{\star}$ especially below the shrinkage limit θ_S indicates the dependence of the so called structure exponent as well as pore water conductivity on volumetric water content or porosity and saturation pointed out by Wagner et al. 2011 [24] and considered with ALRM. The overestimated real and imaginary part due to WS-HIL for volumetric water contents above approximately $0.05 \text{ m}^3/\text{m}^3$ is a result of the influence of the porosity in the mixture approach pointed out by Wagner and Scheuermann 2009 [23]. With the MV-approach the relationship between complex effective relative permittivity $\varepsilon_{r,\text{eff}}^{\star}$ and volumetric water content θ is predicted in the complete measured water content range.



Fig. 4. (left, top) Real part $\varepsilon'_{r,\text{eff}}$ and (right, top) imaginary part $\varepsilon''_{r,\text{eff}}$ of complex effective permittivity $\varepsilon^{\star}_{r,\text{eff}}$ at a measurement frequency of 1 GHz as a function of volumetric water content θ in comparison to the empirical calibration function according to Topp et al. 1980 [15], WS-HIL, WS-CRIM, ALRM and PLSR (see text for details). Volumetric water content at the shrinkage limit θ_S , plastic limit θ_P and at the liquid limit θ_L are indicated. (left, bottom) Structure parameter a and (right, bottom) effective pore water conductivity σ_W as a function of θ .

V. CONCLUSION

The applied MV-approach gives evidence, (i) of a phys-

(c.f. [7], [24], [44], [45]).

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ical relationship between soil dielectric relaxation behavior and soil water characteristics as important hydraulic material property and (ii) the applicability of multivariate methods for estimation of physico-chemical parameters of porous media from broadband measured dielectric spectra. Against this background, a better theoretical understanding is required of the HF-EM material properties of porous geo-materials in general. However, this can be only achieved if the full frequency and temperature dependence is investigated under defined hydraulic and mechanical boundary condition [39], [40]. Moreover, a knowledge of the frequency dependent material properties bridge the gap between the HF-EM methods and low frequency methods (mHz - kHz: Induced Polarization - IP / SIP, Electrical Resistivity Tomography - ERT and kHz - MHz: Electromagnetic Methods - EM [6], [41]–[43]). Therefore, from the perspective of practical applications of broadband sensor techniques (e.g. TDR) an essential information profit can be achieved. This, however, is inevitably linked to an increase in the complexity of the interpretation of measurement results under both laboratory and field conditions. Hence, the redesign of appropriate sensor systems and probes in combination with the development of robust broadband modeling and inversion schemes is required

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