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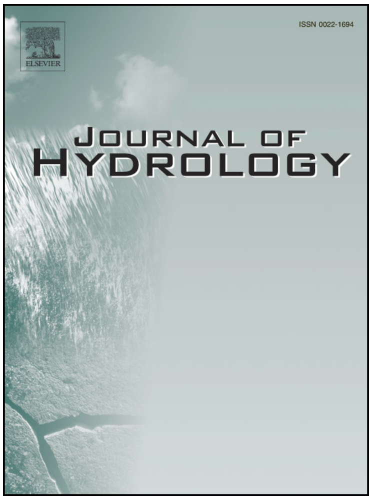

Research papers

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Hydrogeophysical characterization and determination of petrophysical parameters by integrating geophysical and hydrogeological data at the limestone vadose zone of the Beauce aquifer

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Abstract

The hydrological characterization of the vadose zone remains a major challenge considering the spatiotemporal variability of its properties and the limitations associated with hydrological measurements techniques. Geophysical methods, in particular the DC-resistivity and ground penetrating radar, can provide large scale images of hydrogeological structures and a non-invasive assessment of the subsurface dynamic processes. However, these approaches rely on the accuracy of the petrophysical relationships connecting the geophysical parameters to hydrogeological ones, where the site-specific determination of the associated petrophysical parameters is considered crucial. The first objective of this study was to investigate the relationship between the water content, geological properties, and geophysical attributes at the vadose zone of a vulnerable limestone aquifer. The second objective aimed to obtain the Archie's and Complex Refractive Index Model (CRIM) petrophysical parameters by using borehole electrical resistivity and cross-hole ground penetrating radar data. For this purpose, we adopted a grid search inversion algorithm where the field geophysical data were integrated with water content profiles simulated by using HYDRUS-1D. The vadose zone profile was divided into three layers, and the inversion was carried out for the petrophysical parameters in each of the model layers. The electrical resistivity and relative dielectric permittivity data showed a very good correspondence with the simulated and experimental water content distributions along the vadose zone profile. The petrophysical parameters estimated by the inversion showed values that fall in the ranges reported in the literature. Similar values have been observed in the different model layers, with slight differences that were attributed to the vertical heterogeneities associated with the alteration and fracturation features of the limestone vadose zone. This study showed a very good correlation between geophysical, hydrogeological and geological data, and highlighted the presence of heterogeneities that can have profound effects on the vadose zone water dynamics.

Key Words: Electrical Resistivity, Ground Penetrating Radar, Archie, Complex Refractive Index Model, Water Content.

1. Introduction

Improved understanding of water flow and transport processes in the vadose zone (VZ) is crucial, considering the critical role this compartment of the subsurface plays within the biosphere and in the transmission of water and contaminants from the surface to the groundwater. Contamination sources mainly originate in the VZ where the transfer of contaminants is impacted by the medium heterogeneities (e.g., fractures, induced preferential flow and rapid infiltration), and by interactions involving a complex interplay between coupled physical, geochemical, and microbial processes (Arora et al., 2019; Stephens, 2019; Nimmo, 2005). Therefore, a better knowledge of the hydrogeological processes and water content distribution within the VZ is essential to protect groundwater resources.

Conventionally, water content measurements were carried out by single-point techniques, such as time domain reflectometry (TDR) or neutron probes (He et al., 2021; Isch et al., 2019; Skierucha et al., 2012; Evett, 2008; Verhoef et al., 2006; Evett, 2003). Advancements in these techniques (e.g., multi-TDR systems) provided the possibility of time-lapse water content monitoring and eventual preferential flow paths detection (Herkelrath et al., 1991). However, such measurements are intrusive, limited to very shallow depths, and provide restricted information at only a series of point locations. These measurements are often not representative of the field scale spatial water content distribution (Robinson et al., 2003). The difficulties involved in obtaining 2-D or 3-D hydrologic images by exploiting such sparse local data introduced geophysical methods as alternative ways of monitoring water content distribution and water fluxes within the VZ (Binley et al., 2015; Vereecken et al., 2006; Rubin and Hubbard, 2005).

Geophysical methods have shown a great potential in providing large-scale and high spatial resolution images of the subsurface hydrogeological processes (Binley et al., 2015; 2010). Several surface and cross-borehole geophysical methods have been recently used for different hydrological applications. These methods include the ground penetrating radar (GPR) (Dafflon et al., 2011; Lunt et al., 2005; Binley et al., 2001), seismic techniques (Blazevic et al., 2020), electrical resistivity (ER) (Mallet et al., 2021; Johnson et al., 2015; Robinson et al., 2008), self-potential (Abbas et al, 2017; Ahmed et al., 2014; Jardani et al., 2012), induced polarization (Johnson et al., 2010) and nuclear magnetic resonance (Vilhelmsen et al., 2014). Additionally, geophysical methods have been recently used to characterize and quantify processes and interactions in the soil–rhizosphere–atmosphere agricultural ecosystem continuum (Garré et al., 2021).

In particular, the GPR and ER methods have been frequently used to investigate water flow dynamics and identify hydrodynamic parameters (Klotzsche et al., 2019, 2018; Paz et al., 2017; Binley et al., 2015). Thanks to well-established petrophysical relationships between water content and both electrical resistivity (e.g., Archie, 1942) and dielectric permittivity (e.g., Topp et al., 1980) of porous media, these methods can provide valuable information on water flow that can be used to parameterize and constrain hydrogeological models. Relative variations of water content distribution in VZ profiles have been successfully estimated by GPR and ER data. These observations were used to monitor infiltration experiments and visualize flow patterns, quantify petrophysical parameters, characterize preferential flow pathways in fractured media (De Jong et al., 2020; Gance et al., 2016; Wehrer and Slater, 2015; Klotzsche et al., 2013; Steelman and Endres, 2011; Brunet et al., 2010; Cassiani et al., 2009b ; Looms et al., 2008; Linde et al., 2006; Kowalsky et al., 2005; Huisman et al., 2003; Binley et al., 2002a; Hubbard et al., 2001a), and even assess the variations of the soil water content associated with root water uptake (Mary et al., 2018; Hagrey, 2007).

Generally, the water content estimates derived from GPR and ER data showed high accuracy and a good reproducibility. However, geophysical methods cannot directly provide water content values. This approach is dependent on the empirical relationships between the sensed physical parameters and the subsurface parameters of interest (e.g., porosity and water saturation), especially in complex heterogeneous mediums such as carbonate environments, which are often characterized by a complex multiple-porosity system consisting of matrix porosity and fissures, vugs, fractures and karst networks (Mallet et al., 2022; Aldana et al., 2021; Ammar and Kamal, 2017; Mount and Comas, 2014 ; Lucia, 2007). Difficulties arise in the need of time-consuming and expensive laboratory calibration of the petrophysical relationships that are basically suitable only for homogeneous formations, and influenced by properties such as the porosity and tortuosity patterns of the medium under study (Mohamed and Hamada, 2017; Glover, 2016). Estimating parameters such as the water content and porosity from geophysical data by using documented literature values of petrophysical parameters can induce a lot of uncertainties in the absence of site-specific calibration. Achieving an efficient determination of site-specific petrophysical parameters is expected to reduce such uncertainties, and can provide a large-scale and time-saving estimation of water content by avoiding destructive and time-consuming hydrogeological measurements and laboratory calibrations.

The presented study is carried out within the framework of the “Observatory of Transfers in the Vadose Zone” (O-ZNS) platform. The general objective of the O-ZNS platform is to investigate the water-rock-biosphere interactions and their associated mass and heat transfer processes in the VZ. This can provide a better understanding of the VZ dynamics and coupled processes by providing physical, biogeochemical and spatially resolved hydrodynamic parameters capable of characterizing water flow patterns and parameterizing transport models. This study first investigates the relationship between geophysical attributes, water content and geological heterogeneities at the vadose zone of a vulnerable limestone aquifer. An inversion algorithm is then used to obtain the Archie's and CRIM's petrophysical parameters by integrating borehole electrical resistivity and cross-hole ground penetrating radar data with water content profiles simulated by HYDRUS-1D.

2. Study site

2.1. Description

This study was carried out at the O-ZNS observatory, located in the vicinity of the Beauce limestone aquifer at an agricultural site in Villamblain, France (Fig. 1) (DMS coordinates: X = 48°1′5.131″; Y = 1°34′55.333″). The observatory offers a unique experimental setup, composed of an exceptional well having a depth of 20 m and a diameter of 4 m, along with a number of instrumented boreholes and piezometers. Additionally, the observatory will be equipped with innovative complementary environmental sensors such as fiber-optic sensors (e.g., distributed acoustic sensing, distributed temperature sensing), water content monitoring probes (e.g., TDR), and samplers. These sensors can provide quantitative measurements relative to fluid and heat transfer processes within the VZ. During its exploitation, which is planned for several decades, the observatory will allow acquiring original and unique data on the mass (water, solutes, organic and inorganic contaminants, gases, etc.) and heat (induced by temperature gradients, microbiological reactions, etc.) transfer processes across the continuum "Soil-VZ-Capillary Fringe -Aquifer" for environmental issues and water management. A detailed description of the observatory instrumentation setup can be found in Abbar et al. (2021).

2.2. Geology

Direct observations of undisturbed cores complemented with optical log imagery revealed significant vertical and lateral lithological heterogeneities within the VZ units. Three main lithological units have been identified by the direct core observations (Fig. 1): (1) A first top soil unit having a thickness ranging between 0.9 and 1.8 m, and a silt loam texture referred to as a Hypereutric Cambisol (IUSS Working Group WRB, 2015); (2) a second unit characterized by highly heterogeneous and altered (i.e., fractures, weathering, oxidation) incoherent limestone facies reaching a depth of around 7 m; and (3) a third unit of hard limestone rock (Pithiviers limestone) extending from a depth of around 7 m down to 20 m with a clear evolution of alteration, fracturation and karstification with depth. The water table had an average depth ranging between 16.5 m and 20.5 m over the last decade, with observed historical variations ranging between 14.5 m and 22.5 m since 1966 (Isch et al., 2022).

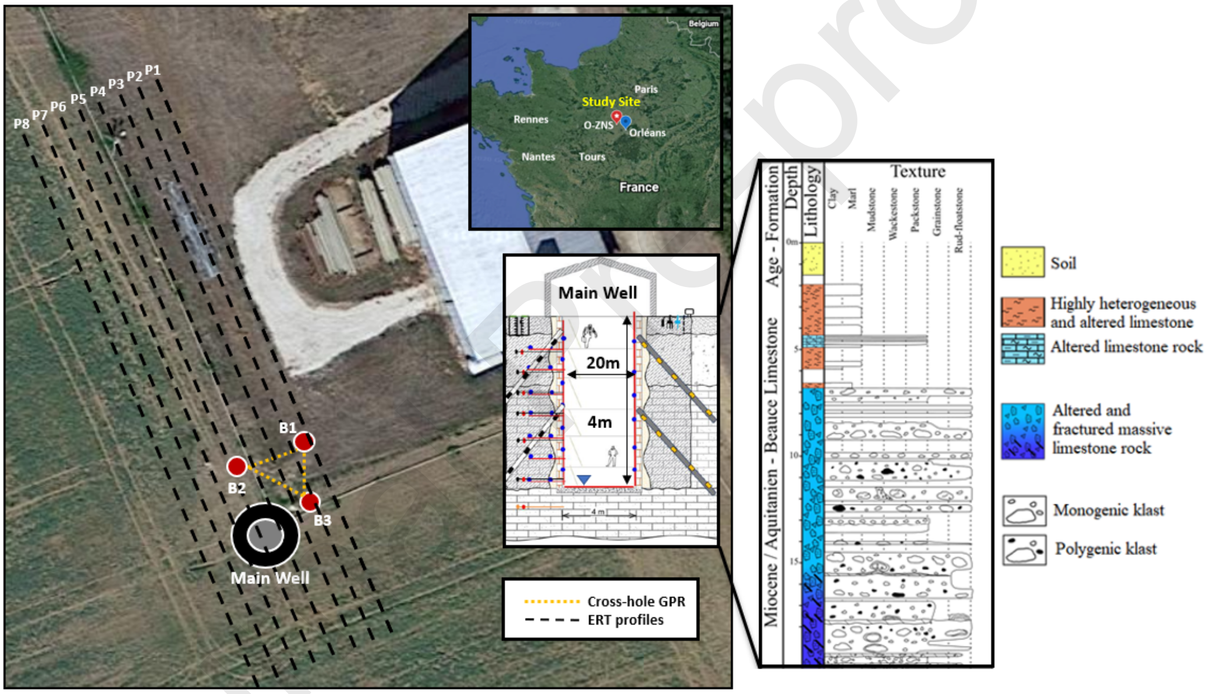

Fig. 1. Study site location, instrumentation, geology and geophysical measurements setup. The figure only shows the boreholes used for this study, several other boreholes surrounding the main well are present at the study site.

3. Methods

3.1. Geophysical data acquisition

The O-ZNS infrastructure allows the combination of different geophysical methods and focuses on integrating borehole, cross-hole and surface geophysical techniques that are sensitive to transfer and flow processes. In this section, we present the acquisition protocols of the electrical resistivity tomography (ERT), borehole ER and cross-hole GPR data used in this study.

3.1.1. Electrical Resistivity

A total of 8 ERT profiles were acquired on the 18th of April, 2019 by using a Syscal-Pro 96 resistivity meter (Iris Instruments, France) connected to a Syscal Switch Pro 96. The profiles had 48 electrodes each, with an inter-profile spacing of 5 m (Fig. 1). A 2.5 m electrodes spacing was chosen in order to ensure both, an acceptable resolution, and a maximum investigation depth of about 23 m. The measurements were acquired in Dipole-Dipole and Wenner-Schlumberger configurations. Basic filtering steps have been conducted on the acquired ERT profiles (e.g., exterminating bad data points). The profiles were then inverted by Res2Dinv (Loke and Barker,1996) that uses a smoothness-constrained Gauss-Newton least-squares inversion technique to obtain a 2D electrical resistivity model of the subsurface from the field apparent resistivity data (Griffiths and Barker, 1993). The result is a 2D smoothness-constrained distribution of electrical resistivity in the VZ. The effect of temperature variations was considered negligible on the electrical resistivity data along the first 20 meters of the subsurface. This was assumed due to the observed low variations of temperature as a function of depth in the VZ at this time of the year.

On the other hand, the ER borehole data were obtained from three different boreholes logs (B1, B2 and B3, cf. Fig. 1) on the 23rd of March, 2017 by means of the dual induction-laterolog (DIL) method. This method consists of focused electrical measurements that rely on transmitter and receiver coils. The measurements are based on an alternating current that generate eddy currents which in turn produce a secondary electromagnetic field. The latter induces an alternating voltage proportional to the formation electrical conductivity in the receiver coil. The transmitter-receiver pair which uses a low frequency is designed to minimize the effects of the borehole and optimize the depth of investigation and the measurement vertical resolution. A measurement point spacing of 2 cm was used, with a maximum penetration depth varying between 18 m and 19 m depending on each of the borehole's maximum accessible depth.

3.1.2. Ground Penetrating Radar

The cross-hole GPR measurements were acquired by using a ProEx GPR system (Malå Geosciences) on the 24th of January, 2019. The measurements were done by using 100 MHz borehole antennae with a sampling frequency of 1000 MHz and a measurement period of 240 ns. Zero offset profiles (ZOP) were acquired between the three boreholes B1, B2 and B3 (TXB2_RXB1, TXB1_RXB3 and TXB2_RXB3) (Fig. 1). The ZOP method is a commonly used approach for borehole GPR acquisition surveys (Klotzsche et al., 2019). Throughout the ZOP measurements, the transmitting (Tx) and receiving (Rx) antennas are moved simultaneously in two different boreholes with a fixed step size. To conduct the ZOP measurements, the antenna were first pushed to the bottom of each of the boreholes where the maximum accessible depth was 18.98 m (water table). The antennae were then pulled simultaneously towards the surface by using a 0.5 m fixed step size.

One-dimensional velocity profiles were then determined by a standard ray-based analysis approach. For simplicity, the medium was assumed to have no horizontal variation of velocity while obtaining the one-dimensional velocity profiles. After picking the first arrivals (in ReflexW©), the arrival time (t) and the distance between the boreholes were used to determine the GPR electromagnetic wave velocity (v) through the following equation:

$$\mathrm{v} = \left(\frac{\mathrm{d}}{\mathrm{t} - \mathrm{T}_0}\right), \tag{1}$$

where T_0 is the time-zero offset, which was obtained by conducting multi-offset measurements with the antenna in free-space. In low-loss and non-magnetic material such as carbonate formations (e.g., limestone), the relative dielectric permittivity (ε_r) can be then determined at different depths by using the following equation:

$$\varepsilon_r = (c/v)^2, \quad (2)$$

where c is the velocity of an electromagnetic wave in vacuum (~0.3 m/ns). Relative dielectric permittivity profiles were then determined from the obtained velocity profiles by using Eq. 2.

3.2. Hydraulic properties measurements and simulation of water flow within the VZ

3.2.1. Hydraulic properties of the vadose zone samples

Fifteen undisturbed samples representative of the VZ (0-20 m deep) were chosen according to the lithological observations made from the three cored boreholes B1, B2 and B3 (Isch et al., 2022). The samples included three soil samples (S_A, S_B and S_C), four soft sediments and powdery limestone samples (P_A, P_B, P_C and P_D), two calcareous sand samples (I_A and I_B), and six limestone rock samples (R_A, R_B, R_C, R_D, R_E and R_F). These samples were used to estimate the water retention θ(h) and hydraulic conductivity K(h) curves by applying the multistep outflow method (Aldana et al., 2021). The multistep outflow experiments were conducted by using a triaxial system based on the experimental procedure described by Eching et al. (1994). The hydraulic conductivity was calculated from the outflow data based on the method described by Gardner (1956).

3.2.2. Simulation of water flow in the vadose zone

Simulation of water flow within the VZ was then performed over a 55 years period (1966-2020) on a 23 m deep VZ profile (borehole B2) composed of fifteen layers and reconstituted with the HYDRUS-1D software (Šimůnek et al., 2016). The simulation of water flow was based on the one-dimensional vertical water flow in the VZ described by Richards equation (Richards, 1931):

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[K\left(\frac{\partial h}{\partial z} + 1\right)\right] - S, \tag{3}$$

where θ is the volumetric water content (cm^3/cm^3), z is the coordinate along the vertical axis (cm), t is the time, h is the matric head (cm), K is the hydraulic conductivity (cm/d) and S is a sink-source term. The Mualem-Van Genuchten analytical model (MVG) was used for the description of the VZ hydraulic properties. The van Genuchten's expression (van Genuchten, 1980) was used to describe the water retention curve:

$$\theta(h) = \begin{cases} \theta_r + \dfrac{\theta_s - \theta_r}{[1 + |\alpha h|^n]^m} & h < 0 \\ \theta_s & h \geq 0 \end{cases} \tag{4}$$

$$\text{with} \qquad m = 1 - \frac{1}{n} \qquad n > 1,$$

where θ_r and θ_s are the residual and saturated volumetric water content (cm^3/cm^3) respectively. α is an empirical parameter related to the matric head (cm^{-1}), and n is a pore size distribution parameter (-). The statistical pore connection model of Mualem (1976) was then used to predict the hydraulic conductivity from the water retention curve:

$$K(h) = K_s S_e^l \left[1 - (1 - S_e^{\frac{1}{m}})^m\right]^2 \tag{5}$$

$$\text{with} \qquad S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r},$$

where K_s is the saturated hydraulic conductivity (cm/d), S_e is the effective saturation (-) and l is a pore connectivity parameter (-) fixed at the value of 0.5 (Mualem, 1976). The measured water retention and hydraulic conductivity data were fitted to the θ(h) and K(h) curves with the MVG model (Eq. 4 and Eq. 5) by using the RETC software (van Genuchten et al., 1991) to infer the VZ hydraulic properties used in our simulations. The representation of the VZ profile for B2, the values of experimental and fitted (with RETC) saturated volumetric water content (θ_s) and fitted hydraulic conductivity (K_s, in cm/d) are given in Table 1. Water table level and meteorological data were collected from monitoring stations located at the villages of Poiseaux (4 km from the study site) and Bricy (20 km from the study site) respectively. While the weather conditions at the study site may differ slightly during intense and localized rainy events relative to those observed at the Bricy station, these are however considered to be representative over a period of more than 50 years.

Table 1. (a) Description of the samples considered for the representation of the VZ profile and the simulation of water flow with HYDRUS-1D: depth, description, saturated water content (θ_s), experimental saturated water content ($\theta_{s\text{Exp.}}$), hydraulic conductivity (K_s), α, and n.

Geological Unit	**Depth (m)**	**Sample**	**Description**	**θ_s (cm3/cm3)**	**$\theta_{s\text{ Exp.}}$ (cm^3/cm^3)**	**K_s (cm/d)**	**α cm^{-1}**	**n (/)**
1	0.00-0.30	S_A	Soil	0.4735	0.4864	30.24	0.0242	1.15
	0.31-0.60	S_B	Soil	0.4661	0.4612	53.57	0.0242	1.16
	0.61-0.90	S_C	Soil	0.5002	0.4162	47.52	0.0366	1.16
2	0.91-1.30	P_A	Powdery limestone	0.4511	0.4230	7.31	0.0247	1.17
	1.30-3.50	P_B	Powdery limestone	0.3659	0.3525	0.455	0.0073	1.25
	3.51-4.10	I_A	Calcareous sand	0.3918	0.3775	35.22	0.0715	1.20
	4.11-4.60	P_C	Powdery limestone	0.2969	0.3080	0.143	0.0031	1.22
	4.61-4.90	I_B	Calcareous sand	0.3698	0.4336	285.49	0.1600	1.23
	4.91-5.20	R_A	Altered rock	0.2984	0.3400	5000	0.5156	1.36
	5.21-5.50	I_B	Calcareous sand	0.3698	0.4336	285.49	0.1600	1.23
	5.51-6.60	P_D	Powdery limestone	0.3527	0.3491	0.185	0.0040	1.22
3	6.61-9.00	R_B	Massive rock	0.1547	0.1499	1.32	0.0150	1.16
	9.01-11.20	R_D	Massive rock	0.0949	0.1180	0.402	0.0096	1.17
	11.21-11.40	R_C	Massive rock	0.0504	0.0491	0.0097	0.0014	1.23
	11.41-14.00	R_D	Massive rock	0.0949	0.1180	0.402	0.0096	1.17

14.01-16.00	R_E	Massive rock	0.1172	0.1333	500	0.1266	1.15
16.01-19.00	R_F	Massive rock	0.1452	0.1639	500	0.1371	1.19

4. Petrophysical Modeling

4.1. Relative Permittivity

The CRIM is a three-phase dielectric mixing model commonly used to describe the relationship between relative dielectric permittivity and subsurface properties such as water content and porosity (Huisman et., 2003; West et al., 2001; Roth et al., 1990):

$$\varepsilon_r^\alpha = \phi S_w \varepsilon_w^\alpha + (1-\phi)\varepsilon_s^\alpha + \phi(1-S_w)\varepsilon_a^\alpha, \tag{6}$$

where ϕ and S_w are the porosity and water saturation respectively, ε_a is the relative dielectric permittivity of air (given a value of 1), ε_w is the relative dielectric permittivity of water, ε_s is the relative dielectric permittivity of the solid phase, considered as a source of uncertainty to be accounted for when using the CRIM.

Besides the ε_s, the second source of uncertainty to be accounted for is the factor α which describes the orientation of the electrical field with respect to the geological formations' geometry (West et al., 2003; Chan and Knight, 1999; Knoll, 1996; Roth et al., 1990; Birchak et al., 1974).

4.2. Electrical Resistivity

In geological formations characterized by medium to coarse grained sediments, the grain surface conductivity effect can be neglected and the bulk electrical resistivity (ρ_0) can be related to subsurface properties such as porosity and fluid saturation by the following modified form of Archie's equation (Winsauer et al., 1952 ; Archie, 1942):

$$\rho_0 = a\rho_f\phi^{-m}S_w^{-n}, \quad (7)$$

where ρ_f is the fluid or pore water electrical resistivity, a is an empirical constant originally referred to as the tortuosity or lithology constant (Winsauer et al., 1952), m is the cementation exponent which is considered to be influenced by the degree of cementation of the rock fabric (Glover, 2010; 2009), and n is the saturation exponent which is independent of the rock matrix and describes how the pore water is connected (Glover, 2017; Looms et al., 2008a; Hendrickx et al., 2002).

Even though Archie's law does not take the surface conduction into account, it is considered to be applicable if the pore fluid conductivity is largely greater than the surface conduction, especially in the case of low clay content formations such as the limestone rock described within the VZ of our study site (Fig. 1). The need of including the surface conductivity arises when other conducting phases such as clay minerals are present in the rock formation. Therefore, during this study, we applied our approach to the limestone rock facies located at a depth between 6.61 m and 19 m, where geological and mineralogical studies (Aldana et al., 2021) suggested that the surface conduction can be practically neglected.

4.3. Inversion

This study aims to estimate the Archie's and CRIM's parameters that can vary according to the study site conditions, and that are considered as sources of uncertainties in the application of these models for the estimation of water content variations. The numerical approach used in this study is based on a grid search inversion algorithm (Fig. 2). The inversion workflow is based on testing the possible combinations of the petrophysical parameters that can provide the best fit between the measured and simulated data. The estimated data are the electrical resistivity and relative dielectric permittivity values calculated by using the Archie's and CRIM's equations respectively. The ER measured data are the 1D electrical resistivity data acquired by the borehole's ER measurements, while the dielectric permittivity measured data are those generated from the 1D velocity profiles obtained from the GPR cross-hole measurements. The fit between the measured and calculated data is evaluated through calculating the corresponding root mean square error (RMSE) while the algorithm varies the Archie's (a and m) and CRIM's (α and ε_s) petrophysical parameters to be estimated:

$$\mathrm{RMSE} = \sqrt{\frac{\sum_{i=1}^{N}(x_i - \hat{x}_i)^2}{N}}, \tag{8}$$

where x_i represents the observed data, $\hat{x}_i$ represents the data estimated by the model and N is the total number of data points. The procedure is done separately for the Archie's and CRIM's models. The water content profiles data used to calculate the dielectric permittivity and electrical resistivity in the CRIM's and Archie's equation are those simulated by HYDRUS-1D software. The geophysical data, water content and porosity data used for both models are obtained from the geophysical measurements and hydrogeological model of borehole B2. The fluid resistivity in the Archie's equation is given a value of 510 µS/cm obtained from probes and calibrated by laboratory measurements, while the relative dielectric permittivity of water is assumed to be 79.5 at a temperature of 22.0 °C (Buchner et al., 1999). The model was divided into three layers, and the inversion was carried out for each of the layers separately. This step was done to investigate the effect of geological vertical heterogeneities on the obtained petrophysical parameters. The model discretization and layering were designed according to the geological characteristics and hydrogeological simulations results (see section 5.3.1).

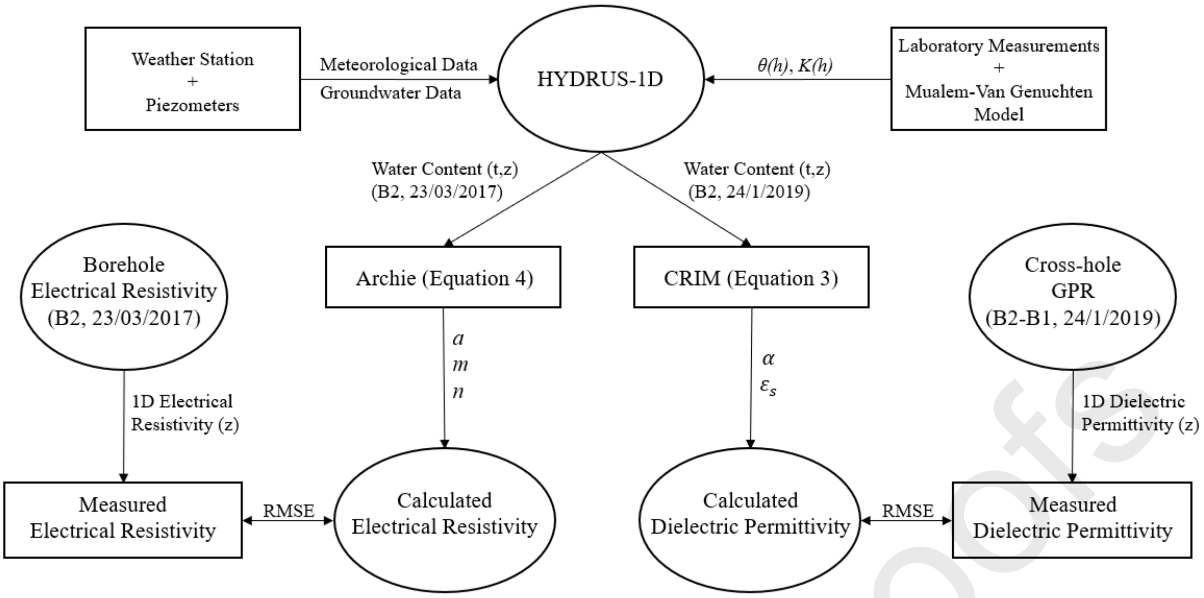

Fig. 2. The inversion algorithm workflow which was done for the Archie and CRIM models separately. The inversion procedure is based on finding the combinations of petrophysical parameters that can provide the best fit between the measured geophysical data and the geophysical profiles calculated by using the water content profiles simulated by HYDRUS-1D.

The results analysis is based on obtaining the combined values of the varied Archie (a and m) and CRIM parameters (α and ε_s) that have the minimal observed RMSE while the algorithm fits the calculated and the measured data. The ranges of variability set for each of the parameters during the inversion were based on common ranges provided in literature for limestone formations. However, the parameters were set to also have values outside these ranges to avoid directing the inversion towards literature values, and to compare our results with those reported in previous studies. Table 1 shows the ranges of the Archie and CRIM parameters used for this inversion and those most commonly reported in the literature for limestone formations. To improve the inversion performance and reduce the different parameters dependencies, the saturation exponent n was fixed to a value of 2 and the calculation was done only for the a and m parameters in the Archie equation. Even though values ranging between 1.4 and 2.5 have been previously given to n in the literature for rocks (e.g., Schön, 2004; Sweeney and Jennings, 1960; Rust, 1952), in practice, the saturation exponent is commonly set to 2 for most types of rocks in the absence of laboratory measurements (e.g. Yaramanci et al., 2000; Looms et al., 2008a, 2008b). On the other hand, α was given a range based on its extreme values which are 1 and -1. The lower boundary (-1) represents the harmonic arrangement of dielectric components in series, while its upper boundary (1) represents the arithmetic arrangement of dielectric components in parallel (Chan and Knight, 2001;1999).

Table 2 : The ranges of the Archie (a, m and n) and CRIM (α and ε_s) parameters used for the inversion and those commonly reported in the literature for limestone formations.

Model	Parameter	Literature (limestone)	Inversion
Archie	a	$0.2 \leq a \leq 2.3$	$0.1 \leq a \leq 10$
	m	$1.6 \leq m \leq 3$	$1.0 \leq m \leq 10$
	n	$1.5 \leq n \leq 2.5$	$n = 2$
CRIM	α	$-1 \leq \alpha \leq 1$	$-1 \leq \alpha \leq 1$
	ε_s	$4 \leq \varepsilon_s \leq 11$	$1 \leq \varepsilon_s \leq 20$

5. Results and discussion

5.1. Geology

Knowing that a strong coherence was observed between the ERT and borehole ER profiles, throughout this work, the ERT profiles are only used for the lithological description and 2-D representation, while the borehole ER data will be used for the water content analysis and as an input in the inversion for its higher resolution (2 cm) and larger number of data points.

In correspondence with the geological description, the ERT (profile P2 in Fig. 1) showed three main layers corresponding to the three main geological units shown in Fig. 1 (Fig. 3). The data showed a first low ER unit representing the top soil layer. The latter is followed by a moderate

ER layer down to a depth of around 7 m. This layer corresponds to the incoherent and altered limestone formation. Lateral ER variations (Fig. 3) and dispersed dielectric permittivity values (Fig. 4b) were observed in this layer, which reflects the heterogeneity of this formation. A clear transition zone between the incoherent limestone layer and the underlaying hard limestone rock layer is evident in the relative permittivity and ER data at depths between 6.5 m and 9 m. This is followed by a third relatively higher ER layer corresponding to the massive limestone rock layer. This layer shows lower dielectric permittivity values which started to increase again as the measurements got closer to the water table level (Fig. 4b).

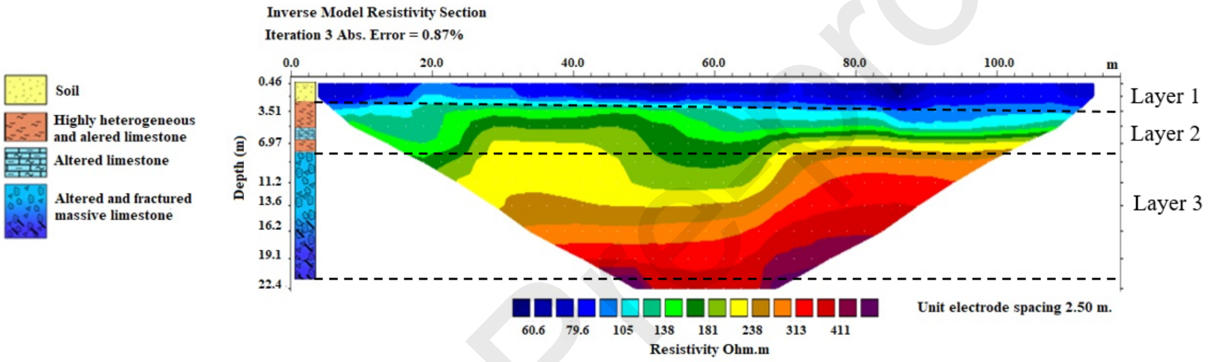

Fig. 3. The 2D smoothness-constrained distribution of electrical resistivity of profile P2. showing 3 main units in accordance with the geology data presented in Fig. 1. All the ERT profiles showed similar results in terms of the lithological structure, therefore, only profile P2 is presented in this work.

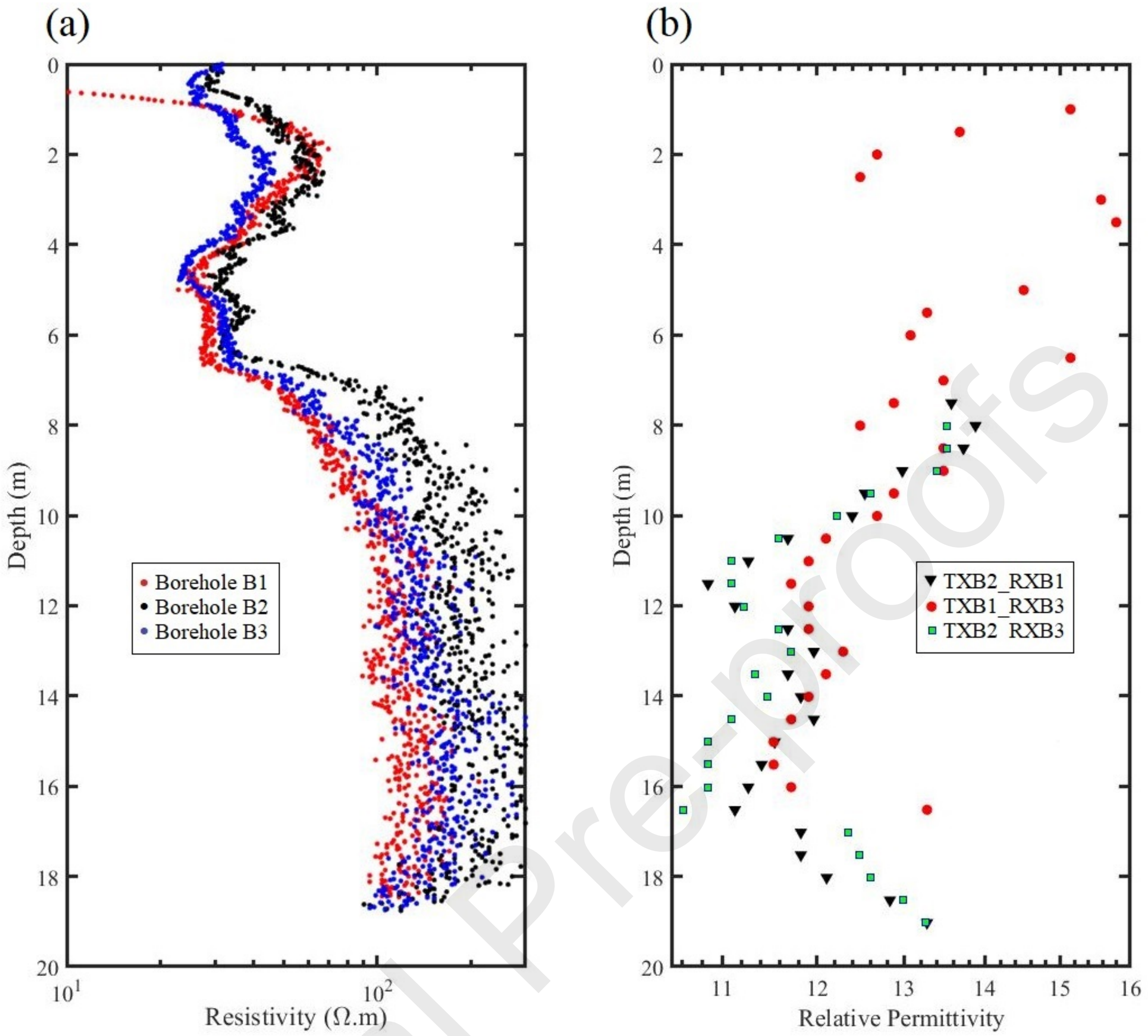

Fig. 4. (a) Electrical resistivity borehole data showing the ER variations in boreholes B1, B2 and B3 (23/03/2017). (b) Relative permittivity results obtained from the cross-hole GPR profiles acquired between boreholes B1, B2 and B3 (24/01/2019).

5.2. Hydrogeology

As shown in Fig. 5, the simulated water content profile obtained by the model for borehole B2 (23/03/2017) showed a good agreement with experimental water content ($R^2 > 0.885$) measured at the same date. This model, which focused on the simulation of the water movement within the matrix components of the VZ, seemed to constitute a first simplified but suitable approach for the unidimensional simulation of water flow within the VZ of the Beauce limestone aquifer.

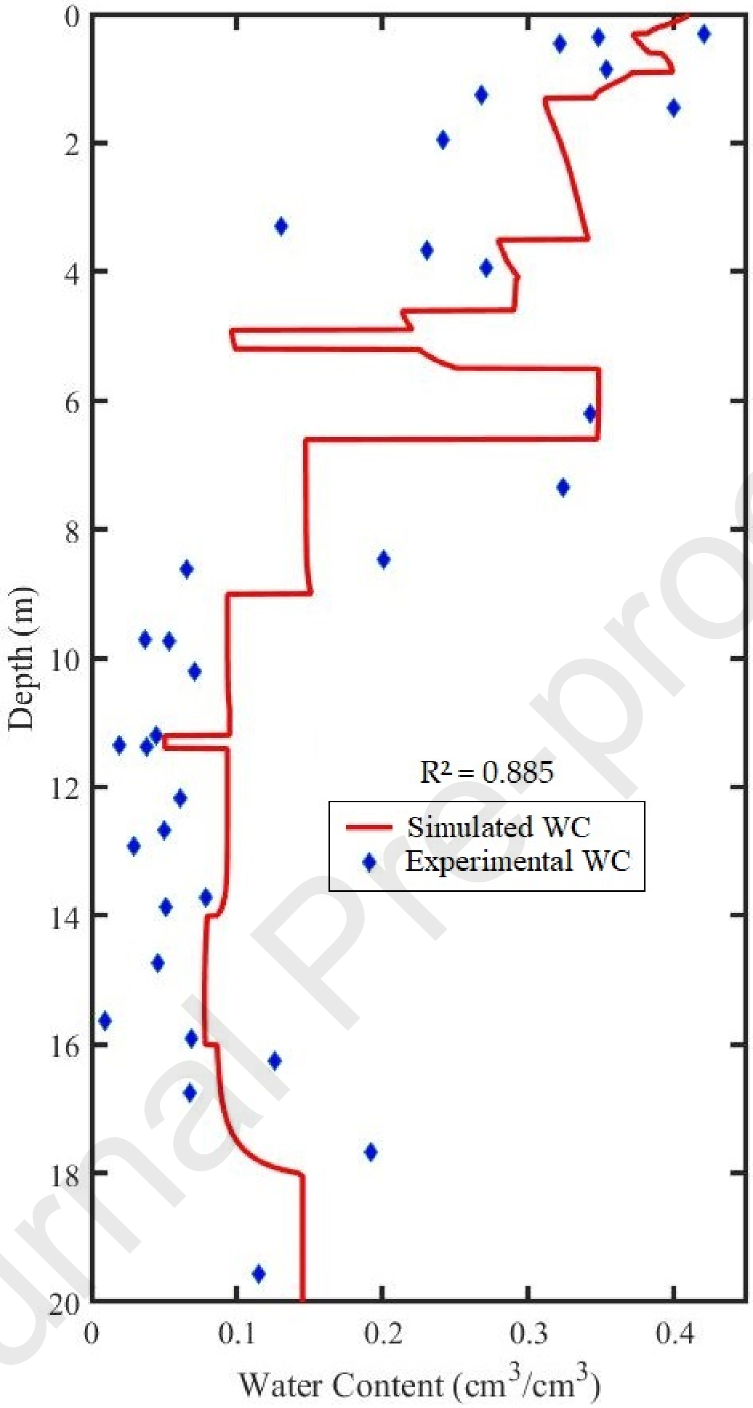

Fig. 5 : Experimental water content (WC) plotted against the simulated water content obtained in borehole B2 with the HYDRUS-1D software (23/03/2017).

The borehole ER data (23/03/2017) showed a good global correspondence with the simulated water content distribution at the same date (Fig. 6a). This correspondence is characterized with a global increase in the ER values along with the global decrease in the water content. This was followed by a decrease in the ER values with the increase in the water content close to the water table level. Similarly, the relative permittivity data showed a good correspondence with the water content variations (Fig. 6b). A significant coherent decrease in the relative permittivity and water content was observed at a depth between 6.5 m and 9 m located at the transition zone between the incoherent limestone and the hard limestone formations. This was followed by a significant increase in the relative dielectric permittivity values along with the increase in water content close to the water table level. The water content profiles simulated for the dates of the ER (Fig. 6a) and GPR (Fig. 6b) data showed similar values with slight but noticeable differences in the top 6 meters and at a depth between 17 m and 19 m. This was expected knowing that these profiles were simulated for two close periods of the year (23rd of March and 24th of January).

A similar pattern was observed in the three boreholes ER data and in the three dielectric permittivity profiles, which shows a good repeatability of the field geophysical data. This observation also indicates that the zones around and between the boreholes are globally and relatively homogeneous, despite the presence of local lateral heterogeneities that were observed in each of the geophysical profiles.

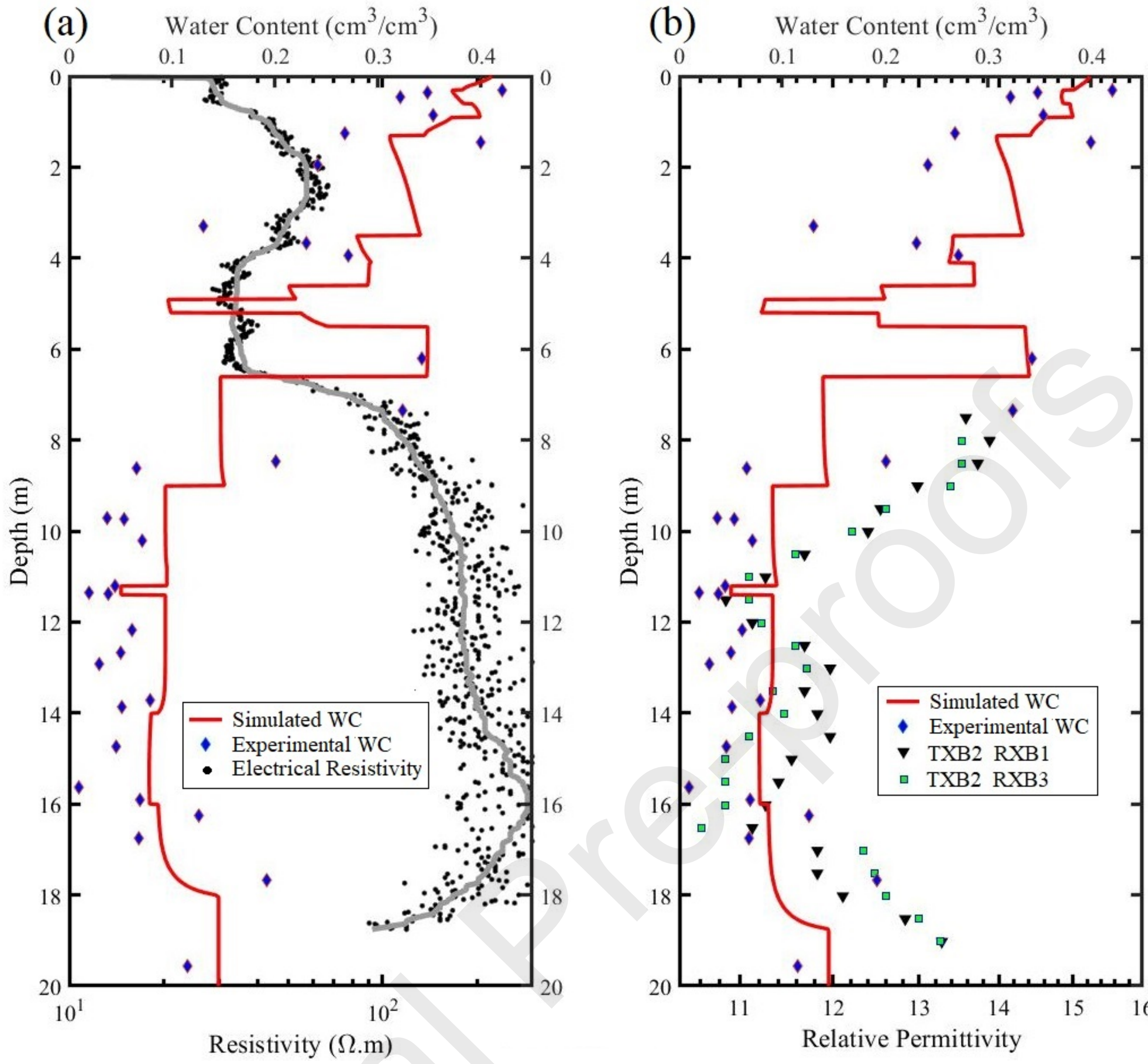

Fig. 6. (a) Borehole ER variations with respect to water content variations simulated by HYDRUS-1D (B2, 23/03/2017), (b) Relative dielectric permittivity distribution obtained from the GPR measurements with respect to water content variations simulated by HYDRUS-1D (B2, 24/01/2019). The water table in borehole B2 had a depth of 18.71 m during the ER measurements and a depth of 18.98 m during the GPR measurements.

5.3. Determination of Petrophysical Parameters

To determine the Archie (a and m) and CRIM (α and ε_s) petrophysical parameters, the measured ER and relative permittivity data and the simulated water content distributions were used in the inversion algorithm described in section 4.3.

5.3.1. Model Structure

As explained previously in section 4.2, the calculation was done for the part of the VZ located at a depth between 6.61 m and 19 m, where the well-cemented microcrystalline texture of the hard limestone rock along with its very low amount of fine-grained material (Aldana et al., 2021) permits the neglection of the grains surface conductivity. Therefore, the inversion model was applied on the geological unit number 3 (Table 1), which was divided into three sub-layers according to lithological description, the hydrogeological model discretization and the water content variations. Layer 1 is located at the top of the unit at a depth between 6.61 m and 9.00 m. This layer, which is considered as the transition zone between the incoherent limestone (P_D) and the massive rock (R_B) materials (Table 1), showed simulated water content variations ranging between 0.147 and 0.151 cm^3/cm^3 (Fig. 5). Layer 2 is located at a depth ranging between 9.01 m and 14.00 m, and is characterized by a limestone rock showing few fissures and slight alterations (R_D) with intercalations of massive limestone rock banks (R_C) (Mallet et al., 2022) which presented a very low porosity (Table 1). Layer 2 showed a simulated water content variation ranging between 0.050 and 0.095 cm^3/cm^3. Layer 3 corresponds to the altered limestone rock that showed a highly heterogeneous structure characterized by an increased evolution towards fracturation and karstification with depth. Layer 3 is located at a depth ranging between 14.01 m and 19 m, and showed the highest water content variation with values ranging between 0.078 and 0.145 cm^3/cm^3. The simulated water content values described here are those obtained for the ER measurements date (23/03/2017), while similar value ranges were also obtained for those of the GPR measurements date (24/01/2019). The inversion was carried out for each of the model's layers separately in order to investigate the effects of vertical heterogeneities on the obtained parameters. This gives us a total of 6 inversions (3 for the CRIM and 3 for the Archie's model).

5.3.2. Inversion Results

The inversion results of the Archie's parameters showed a value of 1.60 for the cementation exponent m in Layers 1 and 2 and a value of 1.47 in Layer 3. One can look at the cementation exponent as a measure of connectedness of the pore network which decreases as the m exponent increases (Glover, 2017). Most sediments or sedimentary rock consisting partially or completely of sand-sized fragments have cementation exponents ranging between 1.5 and 2.5 (Glover et al., 1997), while lower connectedness and vuggy limestone formations are expected to be represented by higher m values. A wide range of values have been reported in the literature for limestone formations (Worthington, 1993). Values ranging between 1.6 and 2.4 have been reported for carbonates (Schön, 2004; Carothers, 1968; Hill and Milburn, 1956), while it was also suggested that they can also have higher values ranging between 2.5 and 5 due to their poorly connected pore space (Tiab and Donaldson, 2011, 2004). However, knowing that connectedness is a term which also describes the extent to which transport pathways are available, low porosity rocks characterized by relatively direct flow paths due to a well-developed fracture network could have lower values or values close to unity reflecting a fairly good connectedness provided by the fractures network. Therefore, the relatively low values obtained in our study could be related to a well-developed fracture network which is thought to be present in the study site but not fully characterized yet. Even though we used a simple porosity model that doesn't take fractures network into account in the porosity parameter, the relative effect of the fracturation could be reflected in the field resistivity data that have a major influence on the obtained m value during the inversion. Layer 3, which showed a lower m value (1.47) relative to Layers 1 and 2, has a highly heterogeneous structure characterized by increased alteration, fracturation and karstification features relative to the other layers, which might explain the relative decrease of m in this layer. Indeed, complex structural formations have been observed in the limestone VZ at the O-ZNS site (Fig. 7), where fissures, fractures and karst networks were observed at the field scale (Aldana et al., 2021). For example, millimetric vugs induced by dissolution processes have been observed in the weathered rock formations located at the water table fluctuation zone and corresponding to Layer 3. Further dissolution episodes could have increased the vugs diameters and enhanced the permeability at this layer. As it is evident in the Archie's equation (Eq. 7), the higher is the cementation exponent the higher is the sensitivity of the electrical resistivity values to changes in porosity (Ellis and Singer, 2007). The relatively similar m values that were obtained in the three layers indicate a similar sensitivity of the electrical resistivity values to the slight differences in porosity observed in the different layers.

Fig. 7. Images of the altered and fissured limestone formation taken while drilling the main well at the O-ZNS observatory.

Table 3. The Archie's petrophysical parameters obtained in the three layers of the model.

Layer	Depth (m)	a	m	n
1	6.61-9.00	0.80	1.60	2.00
2	9.01-14.00	0.70	1.60	2.00
3	14.01-19.00	0.60	1.47	2.00

The inversion results showed a value of 0.8 for the parameter a in layer 1, while it showed a value of 0.7 and 0.6 in layers 2 and 3 respectively. Even though no real correlation was found between this parameter and tortuosity or lithology, a is an empirical constant which is believed to have a role in the compensation for systematic errors in the porosity, electrical resistivity or pore fluid resistivity measurements (Glover, 2016, 2015). This empirical factor which appeared in the Winsauer et al. (1952) modification of the Archie's first law usually provided improved fits with experimental data, especially when dealing with low-quality and sparse types of datasets. It is commonly assumed that the size of a is a measure of the extent to which an overall systematic error is present in the measurements. Recent research suggested that these errors produce non-unity values of a, while the closer this parameter is to unity, the better is the data quality. Additionally, a has an important role in the calculation of a more accurate m value, since it compensates for the experimental errors present in the parameters used to calculate m during the fitting procedure (Glover, 2016). Throughout the inversion, a takes the appropriate fitted value to compensate for the presence of systematic errors and reduce their effects on the obtained m value. Therefore, the value of a obtained from the fit can be considered as an empirical parameter that describes the accuracy of the measured data in the Archie equation. The observed decreasing behavior value of a, from 0.8 in layer 1 to 0.6 in layer 3 could be attributed to the increase in the measurements errors associated with the evolution of alteration, fracturation and karstification with depth. This phenomenon can increase the medium heterogeneities and produce errors in the field measurements which the fitted value of a compensated for during the inversion. Even though a was not shown to have an underlying physical meaning, few studies suggested a values ranging between 0.4 and 2.3 in the case of limestone formations (Timur et al., 1972; Porter and Carothers, 1970; Carothers, 1968). In accordance with our inversion results, the most recent studies reported values of a ranging between 0.2 and 1.8 for limestone formations (Glover, 2016, 2015).

The inversion of the CRIM showed a ε_s value of 7.99 in Layer 1, 7.97 in Layer 2 and 8.00 in Layer 3. ε_s is mainly influenced by the mineralogy and rock formation characteristics. Therefore, similar values were expected to be observed in the three layers, knowing that they are all considered as part of the limestone rock main geological unit (Table 1). However, the slight differences in the ε_s values observed in the three layers can be attributed to the differences in the geological characteristics of the layers in terms of materials heterogeneity and degree of alteration which evolved with depth. Nevertheless, these slight differences, as small as they are, could also be simply induced by the mathematical procedure of the inversion. In accordance with our results, values ranging between 4 and 13 have been reported in the literature for the solid phase dielectric permittivity of limestone formations, which is considered as one of the main sources of uncertainties in the electromagnetic waves application of the CRIM model (Mount and Comas, 2014; Reynolds, 2011; Cassidy, 2009).

The inversion of the CRIM showed an α value of 0.50 in Layer 1, 0.58 in Layer 2 and 0.61 in Layer 3. Values ranging between -1 and 1 were reported for α over the last few decades, which is a geometrical factor connecting the effective layering direction of the components to the applied electric field direction (West et al., 2003; Knoll, 1996; Roth et al., 1990). Several GPR studies indicated that most geological facies can take an α value of 0.5 (West et al., 2003; Knoll, 1996). Values ranging between 0.46 and 0.65 have been previously obtained during laboratory measurements (Mount and Comas, 2014; Moysey and knight, 2004).

Table 4. The CRIM's petrophysical parameters obtained in the model layers.

Layer	**Depth (m)**	**α**	**ε_s**
1	6.61-9.00	0.50	7.99
2	9.01-14.00	0.58	7.97
3	14.01-19.00	0.61	8.00

This approach was shown to produce acceptable results reflected in a very good fit between the measured and calculated data in the three layers, and with values that generally fall in the ranges reported in previous studies. The degree of accuracy of this approach is defined by the resolution of the hydrogeological model and its capability in capturing the VZ water content variations. The water content distribution is strongly influenced by the extent of heterogeneities incorporated in the hydrogeological model and in the porosity parameter of the empirical relationships, especially in limestone formations with complex porosity patterns. Characterizing the impact of the observed fissures and fractures networks on the water flow at the field scale of the O-ZNS VZ is indeed crucial. Therefore, our future work is focused on the development of a precise description of the water flow through the whole porosity of this highly heterogeneous VZ by combining 3D experimental observations and numerical simulations with dual-porosity or dual-permeability approaches. This will form the basis to incorporate the complex multiple porosity patterns in the petrophysical relationships in order to provide an improved estimation of petrophysical parameters. The geological heterogeneities encountered at different study sites might explain the wide range of values reported in the literature for the Archie's and CRIM's parameters, especially in carbonate geology environments, which are complex mediums that can develop different porosity patterns, fractures networks and flow paths.

6. Conclusion

This study attempted to investigate the relationship between geophysical properties and water content distribution, and determine the Archie's and CRIM's petrophysical parameters by integrating ER and dielectric permittivity data with simulated water content data at the scale of a highly heterogeneous limestone VZ. The simulated and experimental hydrogeological data displayed a very good correspondence with the geophysical data reflected in coherent variations in water content, ER and relativity permittivity. These observations showed a significant sensibility of geophysical methods to water content variations, and demonstrated the potential of these methods in investigating hydrogeological processes at our study site.

The inversion results of the Archie model showed values ranging between 0.6 and 0.8 for a and between 1.47 and 1.60 for m. On the other hand, the inversion results of the CRIM showed values ranging between 0.50 and 0.61 for α and between 7.97 and 8.00 for ε_s. Similar results were obtained in the three model layers, with slight differences that were attributed to the vertical heterogeneities of the limestone rock formation (e.g., degree of alteration, fracturation, karstification). This observation demonstrates the sensitivity of petrophysical parameters to vertical geological heterogeneities that should be taken into account when calculating these parameters. Given the ranges of variability used in the inversion, the obtained values are within the bounds of values found in the literature, where a wide range have been reported for carbonate formations due to their complex geological features that might vary greatly among different study sites.

Throughout this study, the petrophysical parameters were successfully obtained with a very good fit between the measured and simulated data. However, the demonstrated approach showed an important sensitivity to the resolution of water content variations captured by the used hydrogeological model, and to the geological heterogeneities of the medium. Therefore, the perspectives include further improvements to this approach by conducting extensive studies at larger scales, and combining 3D experimental observations and numerical simulations using dual-porosity and dual-permeability modeling approaches that can capture the water content and geological heterogeneities at a higher resolution in complex and fractured limestone formations. In this context, our future work is focused on the development of a geological model constrained by laboratory calibrations that can give a better estimation of the limestone complex porosity patterns to be incorporated in the hydrogeological model and empirical relationships.

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Table 5. (a) Description of the samples considered for the representation of the VZ profile and the simulation of water flow with HYDRUS-1D: depth, description, saturated water content (θ_s), experimental saturated water content ($\theta_{s\text{Exp.}}$), hydraulic conductivity (K_s), α, and n.

Geological Unit	**Depth (m)**	**Sample**	**Description**	θ_s **(cm3/cm3)**	θ_s **Exp. (cm³/cm³)**	K_s **(cm/d)**	α cm^{-1}	n **(/)**
1	0.00-0.30	S_A	Soil	0.4735	0.4864	30.24	0.0242	1.15
	0.31-0.60	S_B	Soil	0.4661	0.4612	53.57	0.0242	1.16
	0.61-0.90	S_C	Soil	0.5002	0.4162	47.52	0.0366	1.16
2	0.91-1.30	P_A	Powdery limestone	0.4511	0.4230	7.31	0.0247	1.17
	1.30-3.50	P_B	Powdery limestone	0.3659	0.3525	0.455	0.0073	1.25
	3.51-4.10	I_A	Calcareous sand	0.3918	0.3775	35.22	0.0715	1.20
	4.11-4.60	P_C	Powdery limestone	0.2969	0.3080	0.143	0.0031	1.22
	4.61-4.90	I_B	Calcareous sand	0.3698	0.4336	285.49	0.1600	1.23
	4.91-5.20	R_A	Altered rock	0.2984	0.3400	5000	0.5156	1.36
	5.21-5.50	I_B	Calcareous sand	0.3698	0.4336	285.49	0.1600	1.23
	5.51-6.60	P_D	Powdery limestone	0.3527	0.3491	0.185	0.0040	1.22
3	6.61-9.00	R_B	Massive rock	0.1547	0.1499	1.32	0.0150	1.16
	9.01-11.20	R_D	Massive rock	0.0949	0.1180	0.402	0.0096	1.17
	11.21-11.40	R_C	Massive rock	0.0504	0.0491	0.0097	0.0014	1.23
	11.41-14.00	R_D	Massive rock	0.0949	0.1180	0.402	0.0096	1.17
	14.01-16.00	R_E	Massive rock	0.1172	0.1333	500	0.1266	1.15

	16.01-19.00	R_F	Massive rock	0.1452	0.1639	500	0.1371	1.19

Table 6 : The ranges of the Archie (a, m and n) and CRIM (α and ε_s) parameters used for the inversion and those commonly reported in the literature for limestone formations.

Model	**Parameter**	**Literature (limestone)**	**Inversion**
Archie	a	$0.2 \leq a \leq 2.3$	$0.1 \leq a \leq 10$
	m	$1.6 \leq m \leq 3$	$1.0 \leq m \leq 10$
	n	$1.5 \leq n \leq 2.5$	$n = 2$
CRIM	α	$-1 \leq \alpha \leq 1$	$-1 \leq \alpha \leq 1$
	ε_s	$4 \leq \varepsilon_s \leq 11$	$1 \leq \varepsilon_s \leq 20$

Table 7. The Archie's petrophysical parameters obtained in the three layers of the model.

Layer	**Depth (m)**	**a**	**m**	**n**
1	6.61-9.00	0.80	1.60	2.00
2	9.01-14.00	0.70	1.60	2.00
3	14.01-19.00	0.60	1.47	2.00

Table 8. The CRIM's petrophysical parameters obtained in the model layers.

Layer	**Depth (m)**	**α**	**ε_s**
1	6.61-9.00	0.50	7.99
2	9.01-14.00	0.58	7.97
3	14.01-19.00	0.61	8.00