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Pore-Scale Petrophysical Models for the Simulation and Combined
Interpretation of Nuclear Magnetic Resonance and Wide-Band
Electromagnetic Measurements of Saturated Rocks

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Pore-Scale Petrophysical Models for the Simulation and Combined Interpretation of Nuclear Magnetic Resonance and Wide-Band Electromagnetic Measurements of Saturated Rocks

by

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Dedication

To my love, Margarita,

and my parents, Claudine and Bernard,

who patiently waited and supported my decisions all these years
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The interpretation of well logs in terms of hydraulic permeability, irreducible and free fluid saturations, hydrocarbon grades, and wettability is currently approached with oversimplified models of electrical resistivity and nuclear magnetic resonance (NMR). Inconsistent interpretations arise in the presence of clay, complex rock morphologies, and mixed wettabilities. Wide-band electromagnetic (WBEM) measurements in the kHz-GHz range are sensitive to all these petrophysical attributes but cannot be interpreted in an independent fashion. New interpretation methods are necessary that can effectively combine the resolving capabilities of NMR and WBEM measurements performed under complex petrophysical conditions.

This dissertation develops numerical models to simulate NMR and WBEM measurements in saturated rocks using explicit pore-scale spatial distributions of grains and saturating fluids. The purpose of such models is three-fold: (1) to describe the
fundamental properties of NMR and electromagnetic measurements using pore-scale physics; (2) to benchmark the accuracy and reliability of standard macroscopic models used for the interpretation of NMR and WBEM measurements; and (3) to show the complementary nature of NMR and WBEM measurements for the petrophysical evaluation of complex petrophysical conditions.

Two geometrical models are developed to simulate electrical conductivity, NMR, and WBEM measurements in saturated rocks. The first model consists of continuous 3-dimensional dense packs of grains. Immiscible fluids are distributed in the ensuing pore-space with adherence to capillary and saturation history. Random walkers diffusing throughout these pore geometries accurately reproduce DC conductivity and NMR magnetization decay as functions of porosity, rock morphology, saturation history, fluid types, wettability, rock surface relaxation, and NMR pulse sequences. The second model is constructed with 2-dimensional digital pore maps, where pixels are assigned contrasting electrical properties for grain, clay and fluids. KHz-GHz dispersions of effective conductivity and dielectric permittivity are computed for each pore map. These wide-band dispersions exhibit measurable sensitivity to brine salinity, grain/pore eccentricity, fluid saturation, and wettability.

The 3D model accurately reproduces resistivity index hystereses in mixed-oil-wet rocks and incorporates the combined effects of saturation history, microporosity and clay-exchange cations on rock conductivity. In the case of NMR measurements, unaccounted saturation history leads to erroneous petrophysical interpretations in addition to known adverse effects due to grain morphology and paramagnetic clays. Rock morphologies and fluid configurations where NMR measurements do not lend
themselves to accurate petrophysical interpretation are shown to exhibit characteristic
dielectric dispersions. This result suggests a practical procedure to quantitatively
integrate both NMR and WBEM techniques to improve the assessment of
permeability, wettability, and fluid content.
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$$(1 - \exp(-TW/T)) \times \exp(-t/T)$$

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Chapter 1: Introduction

This chapter defines the scope, methodology, and organization of the dissertation. Current limits of standard interpretation methods of conductivity and nuclear magnetic resonance (NMR) measurements emphasize the lack of accurate and reliable interpretation models for general formation evaluation. We introduce wide-band electromagnetic (WBEM) measurements to improve the reliability of those models. Previous work has shown that pore-scale phenomena embody the information required to refine macroscopic petrophysical models. However, existing pore-scale models lack a multiphysics approach that integrates rock morphology, fluid distribution and type, and fluid wettability. New pore-level petrophysical numerical models are introduced for diffusion processes (Direct-current (DC) conductivity and NMR) and wave propagation (WBEMs) that incorporate these different elements.

1.1 Problem Statement

1.1.1 Limits of Conventional Log Interpretation Models

Macroscopic petrophysical models and mixing laws are commonly used to interpret suites of borehole measurements and to assess hydrocarbon reserves and producibility. Usual examples include the calculation of water saturation from low-frequency resistivity measurements using Archie’s equations (Archie, 1942), or the assessment of irreducible fluid saturations and hydraulic permeability from NMR relaxation time spectra. These models were developed several decades ago for simple petrophysical cases. Archie’s equations assume water-wettability, homogeneous pore sizes, absence of near-wellbore invasion, etc. NMR interpretation assumes that pore
water relaxes independently from surrounding pore water, neglects the restricted
diffusion of light hydrocarbons, and assumes that pores are filled with only one fluid.
From a practical viewpoint, however, the validity of most of these assumptions has
been increasingly questioned. It is now established that oil- and mixed-oil wettabilities
occur in reservoirs much more frequently than believed 20 years ago, where both oil
and water are simultaneously present in the same pores. The alteration of rock
wettability by drilling mud filtrate in the near-wellbore invaded formation, where most
in-situ borehole geophysical measurements are conducted, is a new area of research.
As conventional siliciclastic reservoirs deplete, the relative proportion of hydrocarbon
reserves contained in carbonate rocks with complex pore structures and wettabilities is
constantly increasing. Moreover, the high cost of deepwater exploration, in which most
new major exploration projects occur, places ever-increasing pressure on the quality of
petrophysical wellbore measurements and on the accuracy of their interpretation.

For the most part, the response of the industry to the increasing demand for
refined petrophysical interpretation consists of ad hoc adjustment of parameters,
cutoffs, and empirical correlations with little predictive power. The challenge remains
to determine correct values of permeability, fluid saturations, and wettability in
complex reservoirs. For the case of electrical conductivity, Archie’s power laws are
still widely used despite a number of reasons (including variations in rock morphology,
wettability, imbibition cycle, porosity, even water saturation) why its exponents, $m$ and
$n$, depart from what are sometimes still believed to be universal constants equal to 2.
Besides, sparse core measurements are required to determine the values of Archie’s
parameters $a$, $m$, $n$, and sample cation exchange capacity (CEC). High homogeneity of
rock morphology and wettability has to be assumed to consider these values as
formation characteristics. The variation of brine resistivity between different reservoir compartments is also often neglected. As a result, the application of Archie’s laws is very inaccurate. Likewise, NMR measurements strongly depend on pore size, rock fabric and mineralogy, and the pore-level distribution of fluids. The quantification of fluid volumes and rock permeability stems from the application of relaxation time cutoffs which are defined a priori or just based on data from a few core samples. These cutoffs are usually enforced regardless of local rock heterogeneity, pore geometry, and fluid distributions. Diffusion coupling occurring in micritized carbonate rocks is one phenomenon among many others that are disregarded by the “standard” 90-ms relaxation cutoff value in carbonate rocks (Toumelin et al., 2003a). Finally, mapping NMR measurements into hydraulic permeability assumes a universal relationship between pore size and permeability. In fact, NMR measurements usually probe diffusion lengths of 5 to 10 pores, which ought to be insufficient to characterize the flowing capacity of a rock. As a result, permeability estimation from NMR measurements remains controversial.

1.1.2 Using Wide-Band Electromagnetic Measurements

Current interpretation models lack reliability for application to complex rock geometries and fluid distributions, which causes the limitations discussed previously. Multifrequency electromagnetic phenomena in the kHz-to-GHz range have the potential to investigate pore structure and surface effects, with sensitivities that complement those of NMR measurements. A large array of electromagnetic tools already exists to provide some of these measurements, such as the array induction log or the laterolog in the 10-kHz range, the logging-while-drilling (LWD) induction log in the 2-MHz range, or the electromagnetic propagation log in the GHz range.
Petrophysical interpretation of WBEM measurements was a subject of intense research in the 1980s. Numerous geometrical mixing laws were developed to explain the frequency dependence of dielectric measurements (Sihvola, 2002), which mostly used concepts of polarization averaging over distributions of grain (or pore) shapes in the MHz range, or fluid partial porosities in the GHz range (Complex Refractive Index Method CRIM). Parametric models fit measurements very accurately as the sum of a geometric, Maxwell-Wagner-type contribution and an electrochemical, power-law contribution (Bona et al., 1998, 2001; Myers, 1991, 1996); however, the values of the fitting parameters have not been quantitatively related to rock properties. Practical considerations and the absence of convenient interpretation models prevented further use of multifrequency measurements for general formation evaluation. Now, NMR measurements provide new measurements of pore space, such as pore size or fluid saturations, independently of porosity, which was a critical gap in WBEM measurements. Therefore, it is timely to reconsider WBEM measurements for petrophysical use and to develop methods that effectively combine the resolving capabilities of WBEM and NMR measurements performed under complex petrophysical conditions.

1.1.3 Existing Pore-Scale Approaches

Since Fatt’s first pore network (Fatt, 1956), pore-scale models have matured to successfully model multiphase fluid flow in porous media, even in the presence of complex rock wettability, based on generic rock topologies (three-phase flow for Mani and Mohanty, 1998, and Dijke et al., 2004) or advanced three-dimensional (3D) digital rock reproductions (two-phase flow for Jackson et al., 2003, and Øren and Bakke, 2003). High accuracy has also been obtained for the prediction of interface curvatures
between fluids in simple realistic grain packs (Gladkikh and Bryant, 2003). Use of these pore-network models has yielded good accuracy to simulate DC conductivity measurements in saturated rocks for drainage saturation cycles; however, the simulation of rock electrical properties during imbibition cycles has not given consistent results in the presence of complex wettability (Sallier and Hamon, 2005). Standard pore-network models also neglect the presence of thin wetting films and pendular rings. For instance, Bryant and Pallatt (1996) assume that neglecting wetting films is the reason for the inaccuracy of pore network calculations in water-wet rock models. Furthermore, the node-bond structure of pore-network models is unable to incorporate intragranular porosity and it prevents from reproducing surface contacts between conductive clay zones and pore brine. As a result, the range of rock morphologies that can be studied is limited. One of the few attempts to integrate saturation history into NMR models was made by Chang and Iasonidis (2001), who used pore-network models to distribute fluid phases in the pore space and performed magnetization balance at the pore nodes; however, they assumed that pores were totally filled by one fluid simultaneously, thereby excluding mixed-oil-wet fluid descriptions.

Diffusive random walks and transport analogy between diffusion and DC electrical conduction have so far been the most successful and versatile simulation methods to account for a variety of rock morphologies formed by anisotropic, disordered grain packs (Schwartz et al., 1989) and cubic-centered clay coatings (Johnson et al., 1986). Ramakrishnan et al. (1999) also used random-walk diffusion within cubic-centered packs of bimodal, self-similar, microporous grains to approximate the NMR response of micritized carbonate rocks. Olayinka and Iasonidis
(2002) also used diffusion random walks to simulate the single-phase NMR response of voxel-based stochastic rock replicas. However, none of these random-walk models incorporated the NMR effects of diffusion within background magnetic field gradients at the same time as surface relaxation effects (Toumelin et al., 2003b). Despite the versatility of random-walk techniques to incorporate complex pore geometries, little progress has been reported to adapt them to multiphase problems for either DC conductivity or NMR modeling.

Wide-band electromagnetic analysis also suffers from a lack of efficient numerical simulation. Given the numerical complexity of Maxwell’s equations (Balanis, 1989) in a disordered medium and for a wide frequency range, WBEM modeling has been limited to analytical solutions and to mixing laws riddled with limitations (Sihvola, 2002). For instance, mixing laws neglect electromagnetic coupling between brine bodies within the rock and incorporate limited information, such as distribution of pore shapes or grain shapes, but not both simultaneously; they also fail to incorporate pore connectivity as a critical factor of rock electrical response. Those analytical studies provided invaluable physical insight into wide-band dielectric and conductive phenomena in rocks but were not appropriate for quantitative petrophysical interpretation. For instance, the effect of charged grain surfaces on the frequency-dependent dielectric response of clays has been approached as the combined solution of electrical and diffusion potentials at the molecular scale (Fixman, 1980; Lacey and White, 1981; Chew and Sen, 1982). However, these double-layer responses were considered as phenomena isolated from any influence of fluid saturations and rock pore structure. The geometrical arrangement of clays, which should affect the spatial distribution of the surface charges, has also been systematically neglected by
double-layer models. Lima and Sharma (1992) reported one of the few efforts to calculate the dielectric response of a mixture made of spherical clays, rock, brine and hydrocarbons using mixing laws to upscale the influence of clay double-layers at the rock level. However, their simulations were constrained by the usual limitations of dielectric mixing laws. To our knowledge, no standard pore-scale numerical model exists to synthesize WBEM rock responses from pore-scale arguments.

Therefore, it is timely to develop new pore-scale approaches that simultaneously integrate rock structure information, fluid distribution, fluid types, and wettability to numerically simulate the NMR- and electromagnetic response of saturated rocks.

1.2 RESEARCH OBJECTIVES

This dissertation develops petrophysical numerical models to simulate and integrate NMR and WBEM measurements in saturated rocks on the basis of explicit pore-scale description of grains and saturating fluids. The purpose of such models is three-fold: (1) to describe the fundamental properties of NMR and electromagnetic measurements using pore-scale physics; (2) to benchmark the accuracy and reliability of standard macroscopic models used for the interpretation of NMR and WBEM measurements; and (3) to emphasize the complementary nature of NMR and WBEM measurements for the petrophysical evaluation of complex petrophysical conditions.

1.3 METHODOLOGY

We construct new pore-scale numerical models using recent advances in computational power, numerical algorithms, and an understanding of pore-scale
physics. In particular, the sudden increase of computational speed during the last
decade allows fast resolution of diffusion random-walk methods, which, until now,
were constrained by processor speed. A similar increase in available computer memory
and the development of efficient mathematical tools also make it possible to solve
Maxwell’s equation in the frequency domain for large grids.

We define a 3D framework on the basis of grain packs, overlapping fluid blobs
centered on pore units, and wetting films. This approach reproduces the pore-scale
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Random-walk trajectories are then drawn within the conductive zones of the pore
space to compute the rock DC electrical conductivity. We also compute the NMR
response of the fluids saturating the rock model by solving Bloch’s equations along
similar trajectories within the volume formed by each saturating fluid phase
independently. The WBEM frequency dispersions are also computed from pore-scale
simulations in which explicit pixel-based distributions of grain, clay, and fluids define
the 2D geometry of saturated rocks.

Both the 3D-diffusion and 2D-electromagnetic models make assumptions of the
fluid distribution within the pore space and of the rock topology. In particular, the 3D
model assumes a spherical shape for all the grains and fluid blobs that populate the
pore space. The model defined by Kovscek et al. (1993) is also used to determine the
geometrical prototype of different pore types with respect to their saturation history.
Pore-to-pore and film-growth mechanisms are assumed as exclusive alternate
mechanisms of drainage and imbibition; wettability alteration is also assumed
homogeneous throughout the pore model. Variation from these assumptions may
therefore yield results different from those presented in this work, in particular
concerning wettability effects. However, the numerical approaches introduced in the dissertation remain valid and general enough to be applied to specific rock geometries and wettability conditions.

The 2D pixel-based model also makes assumptions of fluid distribution but is mainly limited by model resolution and the absence of a third dimension. The results obtained with this 2D model, therefore, exhibit differences with respect to core measurement values; however, the model captures the appropriate behavior of WBEM measurements. We remain confident that future developments in computational power will allow our model to be used as a quantitative predictive tool as well.

1.4 ORGANIZATION OF THE DISSERTATION

The dissertation consists of six additional chapters following this introductory chapter. Chapter 2 first defines the 3D geometrical framework that implements random walks to simulate diffusion-based pore-scale transport phenomena in realistic porous structures and the fluid distribution. The DC conductivity simulations validate the approach and show that this method is an efficient and accurate approach to simulate (a) the resistivity index curves of mixed-oil-wet rocks, as well as (b) the electrical response of complex distributions of clay exchange cations and microporosity.

Chapter 3 introduces a general formulation to simulate NMR measurements in porous media using diffusing random walks. The random walkers define trajectories along which one solves the complete set of Bloch’s equations, or just the phase shift measured for Carr-Pucell-Meiboom-Gill (CPMG) acquisition. This numerical method places equal emphasis on both surface relaxation and enhanced relaxation due to diffusion within inhomogeneous magnetic fields. It, therefore, provides a viable
method to describe multiphase fluid relaxation in explicit descriptions of porous rocks and a novel way to synthesize parametric, multidimensional NMR maps.

In Chapter 4, we study the impact of saturation history on diffusion/relaxation NMR maps by using the NMR simulation algorithm defined in Chapter 3, in combination with the rock/fluid framework defined in Chapter 2. With this objective, 2D NMR maps are inverted from the magnetization decay data that was successively simulated during saturation cycles in water-wet and mixed-oil-wet homogeneous rock models. This analysis quantifies the relative importance of saturation cycle, wettability, and fluid type on the petrophysical interpretation of 2D NMR maps.

Chapter 5 focuses toward WBEM modeling. We introduce a new algorithm to numerically simulate the frequency dispersions of electrical conductivity and of the dielectric constant of saturated rocks. The geometrical distribution of rock and fluids is described with discretized pixels forming a 2D digital pore/fluid map. Maxwell’s equations are solved using an integral equation formulation using the Method of Moments in which pulse functions coincide with pixels locations. The computed internal electric fields and currents in the pore map are then matched to those of a homogeneous scatterer to estimate the effective conductivity and dielectric constant of the rock model.

Chapter 6 extends the WBEM model described in Chapter 5 to specific cases where stand-alone NMR measurements lend themselves to ambiguous interpretation. Emphasis is placed on the assessment of the WBEM response characteristic (a) of complex rock morphologies, namely micritized carbonate rocks, and (b) of wettability type and fluid saturation in clayey sandstones. In both cases, the WBEM model
provides characteristic dielectric dispersions which testify to the sensitivity necessary to complement NMR measurements.

Chapter 7 summarizes the general conclusions of the dissertation and provides recommendations for future research work.
This chapter introduces a new 3D methodology to simulate DC electrical conductivity phenomena for a wide variety of petrophysical systems of saturated rock formations. The methodology is based on the use of random walks that simulate the late-time behavior of diffusion phenomena in the pore space. Such a procedure accurately reproduces the formation factor and resistivity index of a large class of pore systems, including the cases of hysteresis-dominated oil-wet rocks. We construct pore-scale rock models with dense packs of grains that exhibit explicit intragranular porosity as well as coating clays whose effective conductivity depends on the salinity of connate water. Fluids are distributed in the ensuing pore space in the form of oil blobs, wetting films, and pendular rings using the Kovscek model for mixed-oil-wet saturation systems. Moreover, we describe the spatial distribution of fluids in the pore space with adherence to capillary principles of drainage and imbibition.

Our simulations successfully reproduce measured values of Archie’s saturation exponent, $n$, as a function of porosity, wettability, saturation cycle, and grain structure. For water-wet rocks, we find that the case of $n = 2$ arises in homogeneous rocks with low surface roughness, whereas the case of $n < 2$ arises in cases of substantial surface roughness or microporosity. For mixed-oil-wet rocks undergoing drainage and imbibition above the critical water saturation, $n$ remains between 3 and 4 for homogeneous rocks and around 2 for microporous rocks. Finally, $n$ increases to or above 10 for cases of mixed-oil-wet imbibition below critical water saturation.


2.1 INTRODUCTION AND BACKGROUND

2.1.1 Limits of Archie’s Power Laws

Two of the most widely used electrical petrophysical properties of rocks are the resistivity formation factor, \( F_R = \rho_{Sw=100%}/\rho_{bulk} \) (ratio of resistivity measured on a fully brine-saturated rock and the bulk resistivity of the brine), and the resistivity index, \( I_R = \rho_{Sw<100%}/\rho_{Sw=100%} \) (ratio of the electrical resistivity measured on a partially-saturated rock and the electrical resistivity measured on a fully-water-saturated rock). Using a collection of water-wet rock samples acquired from unrelated wells, Archie (1942) was the first to observe that logarithmic values of resistivity index linearly correlated with logarithmic values of rock porosity, \( \phi \) (for \( F_R \)) and brine saturation \( S_w \) (for \( I_R \)). Since then, it has been customary to relate these quantities via the empirical power-laws \( F_R = a\phi^{-m} \) and \( I_R = S_w^{-n} \). The so-called cementation (or lithology) exponent, \( m = 2 \), and tortuosity factor, \( a = 1 \), are intended to describe the effect of rock tortuosity on electrical conduction through the pore space. The saturation exponent, \( n = 2 \), incorporates the effect of additional electrical resistance due to presence of electrically insulating hydrocarbons. Similar power laws have been derived for shaly sandstones based on empirical observations, with exponents corrected for the presence of clay double-layer electrical conduction (Argaud et al., 1989).

A plethora of experimental data has shown that Archie’s power-laws could be inaccurate when petrophysical conditions depart from the generic case of clean water-wet rocks with regular grain morphology. Many attempts have been made to explain the physical origin of the variations of \( m \) with rock facies. By contrast, only a handful of studies have been published to explain the behavior of \( n \) with respect to rock morphology and saturation. In many cases, \( n \) depends on rock type, mineralogy,
porosity, wettability, and even $S_w$ itself, which makes the power-law a non-general rule. For instance, Wei and Lile (1991) reported variations of $n$ within the same sandstone samples in both water-wet and oil-wet states, as a function of drainage/imbibition saturation history. Measured values of $n$ in the water-wet state did not vary with variations of saturation history and water saturation, whereas those measured in the oil-wet state exhibited marked sensitivity to saturation history and water saturation (Fig. 2.1a). These measurements emphasized the presence of two resistivity-index hystereses cycles for oil-wet rocks: one between primary drainage and imbibition (Cycles A-B and B-C) and one between imbibition and secondary drainage (Cycles B-C and C-B). Earlier measurements performed by Sweeney and Jennings (1960) on a collection of carbonate rock samples reported relatively constant values of $n$ for preferentially water-wet saturation; conversely, it was found that $n$ could vary widely with water saturation and rock morphology for the preferentially oil-wet samples (Fig. 2.1b). All the resistivity index curves in Fig. 2.1b exhibit water saturations (in increasing order: 32%, 55% and 80%) below which $n$ abruptly increases from 2 or 3, to 10 or more.

2.1.2 Outstanding Technical Issues in Rock Conductivity Modeling

Despite significant experimental evidence of the unconventional electrical behavior of many saturated rocks, only in the last two decades have quantitative pore-scale models been available to explain the non-Archie behavior of electrical conduction via percolation principles. Pore network models have been widely used to assess the impact of pore connectivity and fluid distribution on capillary pressure hysteresis and relative permeability during cycles of drainage and imbibition (e.g., Jackson et al., 2003; Gladkikh and Bryant, 2003). However, the pore-scale simulation
of resistivity hysteresis cycles remains inaccurate for drainage and imbibition, especially in the case of oil-wet rocks. This is due to the fact that electrical conduction occurs not only through pore throat openings, such as in the case of hydraulic conduction, but also through other pathways that are usually neglected in pore-scale modeling. For instance, electrical conduction may occur through (a) wetting films of brine in water-wet rocks, (b) pendular rings in oil-wet rocks, (c) sub-micron intragranular microporosity in a general sense, and (d) exchange cations at clay mineral surfaces in low-salinity sandstones.

For the case of wettability modeling, Sharma et al. (1991) successfully reproduced the hysteresis cycles only at high values of water saturation by incorporating wetting films; their formulation included non-realistic rock/throat geometries. Man and Jing (2001), on the other hand, considered more accurate throat geometries but they reached unrealistically low values of resistivity index in their oil-wet simulations and failed to obtain positive curvatures (i.e., bending upward of the saturation-resistivity index logarithmic cross-plot toward low values of water saturation) of resistivity index during imbibition. Zhou et al. (1997) reported improved simulations of hysteresis between primary drainage and imbibition of oil-wet rocks using a three-dimensional (3D) cubic network based on concepts borrowed from the theory of effective percolation; however, their approach did not include the effects of rock morphology on electrical conduction. To our knowledge, the upper hysteresis cycle due to imbibition and secondary drainage has never been reproduced numerically with pore-scale simulations of electrical conduction.

As emphasized by Stalheim et al. (1999), rock morphology can have a strong impact on resistivity index/water saturation cross-plots. Intragranular porosity, in the
form of microporosity or fractures, clay conduction pathways, certain vug types, or surface roughness, decrease the resistivity index of the saturated rock and create a negative curvature. Other types of vugs and oil-wettability increase the rock’s resistivity and create a positive curvature. Comparison of the oil-wet imbibition critical saturations described in Fig. 2.1b indicates that the effects of rock morphology on DC electrical conduction are not negligible. Fleury (2002) reports completely non-linear resistivity index curves measured on a variety of carbonate samples. Schwartz and Banavar (1989) emphasized that the geometrical approximations invoked in modeling the electrical conduction of disordered porous media remain valid only for the case of distributions of relatively homogeneous pore and grain sizes, and are therefore inappropriate to simulate the effects of complex rock morphologies. It is customary to rely on high-resolution digital cores (either scanned by computer tomography (CT) or statistically reconstructed) to reproduce the geometrical complexity of complex rock facies. Voxel discretization of the medium, however, in general impairs the accurate modeling of fine rock microstructure (Liang et al., 2000). In addition, wettability effects can be readily included in such models. Digital rocks are often used as skeletons to construct network models (Øren and Bakke, 2003) but remain constrained by the same practical limitations of voxel discretization approaches.

Therefore, the technical challenge remains to quantify the value of $n$ when there are competing electrical conduction effects between wettability and morphology. This conflict arises, for instance, in fractured, microporous, or clayey rocks (wherein the resistivity index-saturation plot exhibits a negative curvature) that are also oil wet (positive curvature).
2.1.3 Objective and Methodology

This chapter describes a new approach to simulate electrical conduction phenomena at the pore scale of rocks. The objective is to accurately reproduce electrical conduction effects due to rock morphology, clay distributions, and wettability. We reproduce realistic spatial distributions of pore and grain objects in the pore space. Diffusive random walks are used to numerically simulate electrical conduction in the pore space to calculate the corresponding values of electrical formation factor and resistivity index.

The use of diffusive random walks to model steady-state petrophysical transport properties governed by Laplace’s equation, such as DC electrical conduction, heat transfer, or molecular diffusion is not new (e.g., Johnson et al., 1986; Schwartz and Banavar, 1989). Random walks reproduce the thermal agitation of particles within a fluid of bulk (free) diffusion coefficient $D_{bulk}$. In so doing, random walks consist of a succession of microscopic 3D displacements of length $\delta r$ and duration $\delta t$ constrained by Einstein’s relation (Einstein, 1956):

$$\delta r^2 = 6D_{bulk} \delta t .$$

(2.1)

If $\mathbf{r}$ is the position vector of a walker in the pore space, and $t$ is the walk time, the effective diffusivity of the fluid is related to the mean-square displacement during the walk time $t$ over all diffusing walkers:

$$D(t) = \frac{\langle \|\mathbf{r}(t) - \mathbf{r}(0)\|^2 \rangle}{6t} .$$

(2.2)

The diffusion tortuosity associated with the fluid in the pore space is given by $\tau = L'/L$, i.e., by the ratio of the distance $L'$ measured along the diffusion path between two points, and the straight-line distance $L$ between the same two points. This
tortuosity is the inverse of the asymptotic value of the normalized diffusivity at long times:

\[
\tau^2 = \left( \frac{D(t \to \infty)}{D_{\text{bulk}}} \right)^{-1} = D_{\text{bulk}} \left[ \frac{\lim_{t \to \infty} \left( \frac{\|\mathbf{r}(t) - \mathbf{r}(0)\|}{6t} \right)}{1} \right] > 1. \quad (2.3)
\]

For the case of DC electrical conduction phenomena, resistivity indices are directly related to ratios of electrical conductivity \(\sigma\), as opposed to ratios of diffusivity, \(D\). However, both resistivity indices are also related to \(\tau\) and are obtained by considering the diffusion of bulk ionic brine and ionic brine saturating a rock sample (Clennell, 1997; Rasmus, 1986):

\[
\begin{align*}
F_R &= \frac{\sigma_{\text{brine}}}{\sigma_{\text{sample}}} = \frac{1}{\phi} \frac{\tau_{S_w=100\%}}{\tau_{S_w=100\%}} = \frac{1}{\phi} \frac{D_{\text{brine}}}{D_{\text{bulk}}(t \to \infty)}, \quad (2.4) \\
I_R &= \frac{\sigma_{\text{sample}}}{\sigma_{\text{sample}}} = \frac{1}{S_w} \left( \frac{\tau_{S_w<100\%}}{\tau_{S_w=100\%}} \right)^2 = \frac{1}{S_w} \frac{D_{\text{brine}}^{\text{S_w=100\%}}(t \to \infty)}{D_{\text{brine}}^{\text{S_w<100\%}}(t \to \infty)}. \quad (2.5)
\end{align*}
\]

These conceptual definitions, usually regarded as of negligible practical interest because tortuosity cannot be measured directly in rocks, become central components to our simulation algorithm. Figure 2.2 shows the variation of water diffusivity computed from Eq. (2.2) in a 20% porosity (or 20 p.u.) tortuous pore space, as a function of random walk travel time \(t\) for different values of water saturation.

In the past, random-walk methods were successfully used to simulate single-phase petrophysical measurements for rock geometries as varied as disordered grain packs or fractal rocks (Schwartz and Banavar, 1989; Kostek et al., 1992) and, more recently, microporous carbonate rocks (Ramakrishnan et al., 1999; Toumelin et al., 2003). No attempt, however, has been reported to use the same principles to study electrical conduction effects due to multiphase fluid saturations, saturation history, and variable wettability.
Given the scale contrasts between the fluid and the relevant geometrical features of the rock (nm-thick film, sub-μm micropores, μm-scale pores, sub-mm grains, mm-scale vugs), we perform random-walk trajectories in the pore space using step sizes that are dynamically adjusted to be several times smaller than the smallest surrounding boundaries (e.g. the throat size of an occupied pore or the film thickness within a wetting water film). To optimize the number of random walkers (and therefore the total simulation time) necessary to determine $D_{\text{brine}}^{\text{brine}}(t \to \infty)$ for a given pore configuration, we perform the simulations sequentially with series of 10 to 50 walkers. The resulting long-time effective diffusivities are averaged across as many series of walkers as needed to obtain a smooth time decay curve, and for simulation times long enough ($10^5$ to $10^7$ ms equivalent diffusion time, for $D_{\text{bulk}}^{\text{brine}} = 2 \mu m^2/\text{ms}$) to reach asymptotic convergence with ±5% error or less.

The next sections of this chapter describe examples of application of the pore-scale simulation methodology based on random walks. Section 2.2 describes the rock/fluid geometry formed by overlapping grains and fluid blobs in terms of grain and pore geometrical objects amenable to the simulation of random walks. Section 2.3 describes the modeling process and provides a theoretical basis for the enforcement of capillary pressure concepts in the simulation of drainage and imbibition cycles of water saturation. We consider both cases of complete water-wettability and mixed-oil-wettability for a generic grain pack model. Section 2.4 quantifies the effects of grain roughness, morphology, clay content, and intragranular microporosity on the electrical conductivity of rock formations.
2.2 **OBJECT-ORIENTED GEOMETRICAL MODEL**

We make use of a general geometrical framework to quantify the effects of grain morphology, clay content, fluid content, and wettability, on the calculation of formation factors and resistivity indices. To this end, we consider the rock skeleton as a dense and disordered pack of spherical grains with intergranular pores. Grains and pores are then assigned geometrical properties, and the non-wetting phase is included in the pore space as overlapping spheres which are concentric with the pores and which ensure percolation of the fluid phases throughout the pore space. Subsequently, we invoke drainage and imbibition concepts to include the pore objects within the network of connected pores following Kovscek’s model for mixed-oil wettability (Kovscek *et al.*, 1993). The geometrical description is designed to maximize the efficiency of random-walk tracking in the pore space.

2.2.1 **From Grain Pack to Pore Units**

The rock skeleton consists of dense and disordered 3D packs of spherical grains intended to represent the effects of geological events (and time) acting on both siliciclastic and carbonate rocks. Finney’s data set (Finney, 1970) provided the first measurement of locations of identical grains randomly but densely arranged to form the rock’s skeleton. Since then, several methods have been used to construct dense grain packs with arbitrary grain size distributions. One example is Visscher-Bolsterli’s algorithm (Visscher and Bolsterli, 1972), extensively used by Schwartz (e.g., Schwartz and Banavar, 1989) to simulate random walks. Another example is the discrete element modeling algorithm (Cundall and Strack, 1979), now commonly used in rock fracture analysis (e.g., Park *et al.*, 2004). It must be noted that these methods require the presence of walls between which the grain packings are generated; unrealistically
ordered grain arrangements may ensue close to such boundaries. A subset of the grain pack constructed far away from the walls must therefore be considered for subsequent analysis. Recently, methods have been developed to generate grain packs that directly extract grain positions, sizes, and shapes from 3D CT scans of rock samples (Saadatfar et al., 2005). The grain pack examples used in this chapter were either adapted from the Finney pack or generated from discrete elements in elastic equilibrium. Once a pack of given grain-size distribution is constructed, the grains are overgrown to replicate the effects of diagenesis, overburden pressure, and cementation. In this chapter, we decrease the porosity of the original grain packing by homogeneously increasing the grain radii. Dissolution vugs can be reproduced by discarding grains or clusters of grains from the pack invoking criteria for percolation or size.

Once the rock skeleton is constructed, we partition the bulk volume using a Quickhull algorithm (Barber et al., 1996), which results in the Delaunay tessellation of conforming tetrahedra whose nodes are formed by the grain centers (Fig. 2.3). In this tessellation, each tetrahedron joins a set of four-closest grains and defines a pore unit in its void space. Each face separating two tetrahedra becomes a triangle that links three neighboring grain centers. As detailed in Section A.1 of Appendix A, such a geometrical description provides a convenient way to keep track of the tetrahedron that includes the random walker at a given point in the walk. The location of the random-walker is then defined by the four grains which delimit the apices of that tetrahedron, and by the geometric pore features of that tetrahedron. Each pore throat is assigned the same center and size as the largest disc that can be positioned between the three adjoining grains on the corresponding triangular face. This throat size is used for two reasons: (1) to define the optimal step size of the random walk within the pore unit, and
(2) to determine the percolation ability of that pore. Likewise, the pore volume of a tetrahedron is formed by the complementary volume of the four grains within that tetrahedron; the largest sphere that can be positioned between the four grains determines the pore center and size. Sections A.2 and A.3 of Appendix A contain detailed descriptions of the calculation of pore and throat geometrical properties. Finally, pendular rings are included at the intersection of each pair of grains. Figure 2.4 describes the various elements of this pore geometry.

2.2.2 Grain Objects: Including Microporosity and Clays

The rock skeleton consists of spherical grains with intragranular properties. As illustrated in Fig. 2.5, six types of grains are considered in our model, where the difference among the first four is the intragranular morphology. Specifically:

(1) The solid grains are full spheres. When the distance between the walker and the center of the sphere is smaller than the grain radius, random walkers bounce back to the pore space.

(2) The microfractured grains represent mineral grains which have been fractured along the direction of maximal overburden stress and consequently provide unidirectional opening to fluids. These grains are split along their diameter by a slit of rectangular section which makes an angle $\theta_x$ with the x-axis of the geometrical framework, and an angle $\theta_y$ with the y-axis. Section A.4 of Appendix A describes the equations that govern random walk trajectories within the slit pore space. We assume that all such microfractures are connected to the intergranular pore space.

(3) The coupled microporous grains are intended to reproduce grains with intragranular microporosity connected with the intergranular pore space, e.g.
carbonate micrites (Ramakrishnan et al., 1999) or microporous cherts (Worthington and Pallat, 1992). To improve the efficiency of the random-walk algorithm, we assume that microporosity consists of a uniform and periodic cubic-centered packing of consolidated micrograins. This assumption follows from the self-similar geometry suggested by Ramakrishnan et al. (1999). The step of random walks performed through pore space formed by microporous grains is dynamically reduced to a fraction of the micropore throat size.

(4) Uncoupled microporous grains represent grains similar to those of type (3) above, except that crystal or cement has grown at the surface of the microporous grain. Such a solid barrier isolates the intragranular microporosity from the intergranular pore space. The fractional porosity within these uncoupled microporous grains becomes part of the total porosity, but not of the effective porosity of the rock model.

The next two grain types are intended to reproduce discrete distributions of clays by considering them as volumes where the electrical conductivity (i.e., its equivalent diffusivity for the random-walk problem) is different from that of the pore brine. Several publications have described this dual conductivity approach: Argaud et al. (1989) considered the macroscopic effect of the ratio of “excess conductivity associated with the clay conductor” and the bulk brine conductivity in pores. They measured the ratio between both conductivities to be within 0.02-2 for a variety of sandstones and brine salinities. De Lima and Sharma (1990) used explicit dual distributions of conductivities in a formulation based on effective-medium theory to account for the effect of dispersed and coating clays on electrical conduction. Effective clay conductivities were parameterized using published data on clay gels.
Subsequently, the same authors used an electrochemical double-layer formulation to quantify the DC electrical conductivity of clays as a function of brine conductivity, clay surface charge, and clay size (de Lima and Sharma, 1992 – see also Chapter 6, Section 6.3.2). Johnson et al. (1986) first used the coating-clay geometry in combination with diffusive random walks to model the effect of clay-coating electrical conduction in single-phase, cubic-centered grain packs. We make use of similar grain objects in the geometrical description of the pore space to define the last two grain types as clayey grains:

(5) Coating-clay grains consider clay as micron-thick spherical shells surrounding solid-isolating mineral cores. While they bounce at the boundary between the clay layer and the solid grain core, random walkers can cross the interface between pore brine space and the clay layer. Electrical boundary conditions at the brine/clay interface require that the probability of passage through that interface be proportional to the ratio of conductivities of the brine and clay zones. When the clay/brine interface is crossed, walkers change diffusivity and the relation between step size and duration is modified via Eq. (2.1).

(6) Structural clay grains represent pore-bridging amalgamates of clay flakes. In similar fashion to grain type (5), random walkers can cross the brine/clay interface if they meet the passage probability required by the conductivity contrast ratio.

2.2.3 Pore Objects: Two-Phase Fluid Configurations for Water-Wet and Mixed-Oil-Wet rocks

As shown in Fig. 2.6, within each pore that is partially saturated with oil and water, the volume occupied by hydrocarbon in water-wet cases is delimited by a sphere centered on the pore space. The radius of that sphere is equal to the pore radius $R$
multiplied by a factor $\alpha_o$. Continuity of the fluid phase from one pore to another is ensured when $\alpha_o$ is large enough (usually of the order of 2 to 3) to reach the pore throat between the two neighboring pores. If the fluid phase does not wet the rock surface, then a wetting film of thickness $T$ is included at the grain surface. Irreducible water saturation becomes the remaining component of the pore space. Water pendular rings are included in the pore corners that are not reached by non-wetting phase blobs.

This general pore geometry is intended to capture the canonical fluid configurations advanced by Kovscek’s mixed-oil-wet model (Kovscek et al., 1993; Øren and Bakke, 2003). Figure 2.7 illustrates the five pore types considered in our model, namely:

(1) Fully water-saturated pores represent pores that have never been invaded by hydrocarbons (irreducible water), or water-wet pores in which the process of imbibition has completely displaced any previously existing hydrocarbons.

(2) Hydrocarbon-saturated (with either oil or gas) water-wet pores maintain a water film thickness $T_w$ at the surface of the surrounding grain objects. Continuity of the wetting water phase from one tetrahedron to another is ensured by the wetting films, while that of the hydrocarbon is only ensured if the blob reaches the pore throats. Snap-off of hydrocarbon blobs occurs if the blob radius decreases and loses contact with all throats, or if the wetting films are thick enough to fill all the throats.

(3) Oil-saturated mixed-oil-wet pores represent pores where wettability alteration has occurred from water-wet into mixed-oil-wet conditions over geologic time, depending on factors such as capillary pressure, grain curvature, or chemical composition of the fluids, or during oil-base mud-filtrate invasion at the near-
wellbore scale. Upon wettability alteration of an oil-saturated pore, all the fluid within the oil blob of radius \( R_o = \alpha_o R \) becomes oil and the water film disappears from pore type (2). The pendular rings located outside \( R_o \) remain water-filled and water-wet. Continuity of the oil phase from one tetrahedron to another is ensured through the pore throats, while that of water is ensured through the pendular rings only.

(4) Water-saturated mixed-oil-wet pores represent cases where the water phase has re-entered the oil-wet regions of the pore space. Oil films of thickness \( T_o \) still exist at the surface of grain objects within a radius \( R_o = \alpha_o R \) of the pore center. In certain cases of oil imbibition through oil film growth (see Section 2.3.5), these oil films become thick enough to occupy all the throat apertures, whereupon snap-off of the water phase ensues (Panel 4a of Fig. 2.7).

(5) For asphaltene-rich oils, oil/water emulsion films are stable and bridge the oil films of neighboring grains across pendular rings (Kovscek et al., 1993), thereby possibly trapping the water occupying the pendular rings.

In terms of random-walk trajectories, once the walkers are determined to belong to the volume formed by one of the pore objects defined above, distances are calculated between random-walker location and pore center and grain centers. The length of a random-walk step is equal to the smallest quantity between \( 1/20^{th} \) of the pore radius and \( 1/5^{th} \) of the smallest open throat size of that pore, while that within a wetting film is equal to \( T/3 \).

2.2.4 Drainage and Imbibition Mechanisms

Pore objects defined in the previous section are distributed throughout the connected pore space based on simple heuristic arguments (Kovscek et al., 1993;
Knight, 1991). Kovscek’s mixed-oil-wet model implements a size cutoff between populations of smaller pores which become oil-wet and larger pores which remain water-wet. This criterion neglects the physical constraint that pores must be hydraulically connected to allow fluid displacement between them. We enforce the displacement of fluids from pore to pore according to the various mechanisms described in this section. First, for both water-wet and mixed-oil-wet cases, our drainage cycles assume that the non-wetting phase is displaced in the form of $\alpha_0 R$–radius blobs from pore A to pore B starting on a face of the cubic simulation domain (e.g., $x < 0$) provided that three conditions are met:

1. the blob which initiates displacement (centered on pore A) must be large enough to reach the throat leading to the pore candidate for drainage (pore B);
2. the throat between pores A and B is open to flow, i.e., the throat size is larger than the wetting film thickness, $T$;
3. the throat size exceeds a pre-specified threshold.

When the above conditions are met the non-wetting phase extends continuously from pore A to B, and the process is iterated with other neighboring pores. On the other hand, experimental results (e.g., Chen et al., 2005) suggest that imbibition can be driven by two different processes which lead to snap-offs of isolated non-wetting phase:

(a) The pore-to-pore piston-like displacement mechanism follows the principles of the drainage mechanism described above. Wetting-phase re-invades the pores connected to the inlets as long as throat sizes between pores located in the displacement path exceed a new threshold. If pores saturated with non-wetting phase become surrounded by re-invaded pores, then they become disconnected.
from the original non-wetting phase inlets. The non-wetting phase in this type of pores becomes trapped.

(b) The film thickening mechanism assumes that the wetting phase invades pores by the growth of films which wet the pore surface. Starting from the minimal thickness $T$ of the wetting film after drainage, the film-thickening process incrementally increases $T$ and the blob size decreases to $\beta T$ in order to account for curvature corrections in all the pores where the non-wetting phase is connected. If conditions (1) or (2) above are not met in a pore saturated by non-wetting phase, then snap-off occurs and the pore is automatically discarded from further film growth.

Figure 2.8 summarizes the modeling and drainage procedures described above.

### 2.2.5 Electrical Conduction through Multiple Pathways

At any saturation stage, it is important to isolate the brine volumes which do not contribute to electrical conduction, i.e., the water included in electrically isolated pores and water snap-offs in oil-wet imbibition cycles. Displacement of walkers within these isolated volumes is finite and therefore the corresponding long-time diffusivity is zero. Including these walkers in the calculation of the mean diffusivity of Eq. (2.2) could substantially bias that mean diffusivity in oil-wet configurations. Electrical conduction between pores can occur simultaneously through (a) water-filled pore throats (as long as they are larger than the wetting oil film thickness, in case of oil-wettability), (b) pendular rings, and (c) microporous and clayey grains.
2.3  SIMULATION OF WATER-WET AND OIL-WET SATURATION CYCLES IN A GENERIC ROCK MODEL

We now proceed to show how the pore-space fluid displacement model reproduces saturation cycles and the corresponding resistivity indices. First, we select a generic rock model by extracting 1000 spherical grains from the Finney pack (Finney, 1970; Gladkikh and Bryant, 2003). As depicted in Fig. 2.1a, this grain pack fits within a cube-shape simulation domain, and involves almost 6000 Delaunay tetrahedra. The porosity of the sample is then adjusted by applying uniform growth of the grain size without changing the coordinates of the grain centers. A suite of grain packs of different porosities is created to be used as benchmark in future comparisons (in Section 2.4), and the corresponding formation factors are computed with random walks via Eq. (2.4) and plotted in Fig. 2.9 as a function of porosity. These results match very well the formation factors calculated with pore networks (Bryant and Pallatt, 1996), and also agree well with published measurements of clay-free sandstones (see Section 2.4.2 on this topic). Without loss of generality, we select a 20 p.u. rock model (which corresponds to a reasonably large porosity encountered in hydrocarbon reservoirs) to study saturation cycles and the corresponding values of resistivity index. The formation factor of the 20 p.u. Finney pack is approximately equal to 12, which is lower than the 18-20 range usually measured in 20 p.u. rock formations. This does not preclude the simulation of the main effects of saturation history and wettability on resistivity index. Additional effects on resistivity index due to complex rock morphologies are described in Section 2.4.
2.3.1 Cycle 1: Water-Wet Drainage through Pore-to-Pore Blob Displacement

The originally fully water-saturated formation is first invaded with non-wetting hydrocarbons. The non-wetting phase is put in contact with one face of the cube-shaped grain pack. All the pores opening to that face become possible inlets. Starting from each inlet, the general drainage algorithm is applied to allow pore-to-pore displacement of non-wetting oleic or gaseous phase, into successions of blobs of radii equal to \( \alpha_o R \), where we assume that \( \alpha_o \) is identical throughout the pack. Given that real rock grains exhibit surface roughness and that the spheres of our model are smooth, we set the thickness of the wetting water layer equal to \( T_w = 30 \text{ nm} \). (see Section 2.4.1 on this topic). The pore-to-pore drainage algorithm described in Section 2.4 is applied to the 20 p.u. Finney pack to yield the spatial distribution of oil shown in Fig. 2.10. In this figure, oil inlets are located to the left \((x<0)\) and percolation across the initially fully water-saturated pores ensues at four of the five other sides of the cubic simulation domain. No pressure gradient is imposed across the sample; the direction of drainage is solely driven by the directional distribution of throat sizes. Therefore, the imposed drainage is isotropic if the throat size distribution is also isotropic.

The homogeneous blob radius factor \( \alpha_o \) is adjusted for each grain pack to match the target irreducible water saturation when most pores are invaded with non-wetting phase (i.e. by selecting a very small throat threshold). Irreducible water saturation \( S_{wir} \) exists in both the pendular rings and the pores which are the least connected. Because the throat size threshold controls the percolation process, it is natural to relate capillary pressure \( P_C \) (assumed inversely proportional to the significant geometrical dimension under consideration, i.e. radius of capillary tube, local curvature of pore walls, etc.) with the inverse of throat threshold. Figure 2.11 shows that pseudo-
capillary-pressure curve for the 20-p.u. Finney pack with three values of $\alpha_o$. These curves exhibit the conventional features of capillary-pressure curves for primary drainage in well-sorted grain packs: (a) high curvature of $P_C$ at high values of water saturation, (b) quasi-horizontal plateau and increasingly steeper $P_C$ slope at decreasing values of water saturation, and (c) steep increase of $P_C$ close to irreducible water saturation. The agreement is remarkable, thereby corroborating the physical basis of the heuristic nature of the drainage algorithm.

Figure 2.12 shows the resistivity indices, $I_R$, calculated from Eq. (2.5) along the drainage cycle with respect to water saturation. We make use of a bilogarithmic plotting convention so that $n$ appears as the negative slope of the curve. Points simulated along the drainage curve match measurements made on a 20 p.u. clay-free sandstone sample (core T1 from Argaud et al., 1989) reasonably well, with a simulated value of $n = 2.1$. Random-walk results also compare well to pore network simulations obtained with the same Finney pack (Bryant and Pallatt, 1996), including a remarkable increase around 50% water saturation. At this saturation, the pore network simulations exhibit an increase in resistivity index due to unaccounted electrical conduction through thin water films. Our simulations, which explicitly incorporate presence of water films, also yield a slight increase of resistivity index at this value of water saturation but instead exhibit a smooth transition.

2.3.2 Cycle 2: Water-Wet Imbibition through Pore-to-Pore Displacement and Snap-Off

Starting from the drainage end point of saturation ($S_w = 14\%$) for $\alpha_o = 2.25$, pore-to-pore, we now consider the case of piston-like imbibition by putting the inlet face of the simulation domain $x < 0$ in contact with brine. The throat threshold that controls pore-to-pore brine displacement is reset to a large value and progressively
decreased to yield a new pseudo-capillary-pressure curve. Because the threshold controls imbibition and no longer drainage, the pseudo capillary pressure is taken equal to that of the imbibition onset minus the inverse of the varying imbibition threshold. Figure 2.13 shows the hysteresis curve of pseudo-capillary-pressure resulting from subsequent drainage (Cycle 1) and imbibition (Cycle 2) for $\alpha_o = 2.25$. These curves are in very good agreement with the capillary-pressure hysteresis expected for a homogeneous Finney pack. Presence of 12% irreducible non-wetting hydrocarbon saturation is due to the progressive isolation of hydrocarbon-filled pores from the inlet. Figure 2.14 shows the record of isolated pores and pore throat threshold as a function of $S_w$.

### 2.3.3 Cycle 3: Water-Wet Imbibition through Film Growth and Oil Snap-Off

We apply the film-thickening imbibition process starting from the end of cycle 1 at $S_w = 14\%$. This time, we make use of no throat threshold but we iteratively increase the thickness $T_w$ of the water film at the same time we reduce the non-wetting blob size by $\beta_w T_w$. The parameter that controls the maximal water saturation of the cycle (i.e., the saturation of snapped-off oil or gas) becomes $\beta_w$. For the 20 p.u. Finney pack, values of $\beta_w$ equal to 0.5 and 1 yield irreducible hydrocarbon saturations of 27% and 13%, respectively. For the case under consideration we selected $\beta_w = 0.5$. Figure 2.15 shows the evolution of water film thickness and number of created snap-offs for increasing values of $S_w$. Both curves overlap remarkably well. We monotonically increase the value of $T_w$ in pores where oil is continuously connected and stop the process in pores where oil has snapped-off.

Resistivity indices $I_R$ are computed with random walks performed at discrete stages of each imbibition process. Figure 2.16 compares the evolution of $I_R$ for both
imbibition mechanisms (Cycles 2 and 3) along with the drainage results (Cycle 1) obtained previously. Curves representing Cycles 1 and 2 are very close to each other, with $n$ close to 2, and exhibit slight hysteresis due to presence of some snap-offs during imbibition. However, the difference of resistivity index between the two branches of that hysteresis cycle remains within the 10% numerical error bar associated with random walks. No definitive conclusions can therefore be drawn. Figure 2.16 shows another hysteresis cycle of resistivity index between drainage and film-growth imbibition (Cycles 1 and 3). The slope of $I_R$ sharply decreases from the onset of Cycle 3 ($n > 10$) until it reaches the line $n = 1$ around $S_w = 30\%$. At this value of saturation, only 7\% of the pores have snapped-off, whereupon the incremental film thickness of 3 $\mu$m (or 3\% of grain radius) is present in most pores. This thickness hardly restricts brine diffusion, and therefore $1/R_w I_S$; low values of $n$ ensue. In real rocks exhibiting no conductive clays, the combination of both pore-to-pore and film-growth imbibition mechanisms can explain measurements of $n$ lower than 2.

2.3.4 Cycle 4: Oil-Wet Primary Drainage through Pore-to-Pore Blob Displacement

When wettability alteration occurs, 3\% of the fluids consist of isolated water zones that remain water-wet for all oil-wet cycles. At this point, thin water films separating oil blobs from grain surface break apart. Because oil becomes the predominant wetting phase, drainage now refers to the displacement of oil by water, whereas imbibition refers to the displacement of water by oil. In analogy to the water-wet case, drainage occurs via pore-to-pore displacement of brine starting from the same inlet, $x < 0$. These pores become Type-4 pores (see Fig. 2.7) and re-establish both hydraulic and electrical connection with water-wet pendular rings and isolated water-
filled pores. We set the thickness of oil film thickness \( (T_o) \) equal 30 nm for all the simulations of drainage.

Starting from the completion of Cycle 1 at \( S_w = 14\% \), the evolution of \( S_w \) as a function of throat threshold is regarded as a new pseudo-capillary-pressure curve. In similar fashion to Cycle 2, the pseudo capillary pressure is transformed to the inverse throat threshold \( \text{subtracted} \) from the value at the onset of Cycle 4. The resulting pseudo-capillary-pressure curve is shown in Fig. 2.17a, which can be compared to the theoretical mixed-oil-wet capillary-pressure curves calculated by Kovscek et al. (1993) and sketched in Fig. 2.17b. Our model excludes oil snap-offs during oil-wet drainage and therefore, unlike Kovscek et al. (1993)’s results, we obtain no irreducible oil saturation. Despite this difference, a very good agreement is obtained with Kovscek’s results in view of our simplifying assumptions.

2.3.5 Cycle 5: Oil-Wet Imbibition through Film Growth and Water Snap-Offs

After enforcing a 90%-drainage, oil imbibition proceeds via film-thickening. In similar fashion to Cycle 3, a blob-shrinkage coefficient \( \beta_0 \) is defined equal to 0.5. Figure 2.18 shows the evolution with wetting oil saturation of the incremental oil film thickness and of the amount of water trapped into snap-offs during imbibition. It is remarkable that the incremental oil film thickness grows with wetting oil saturation in the same fashion as the incremental water film thickness grows with wetting water saturation in Cycle 3 (Fig. 2.15). The build-up of water snap-offs and isolated water saturation, however, is very different from the water-wet case: instead of exhibiting the progressive influence of film thickness (as in Fig. 2.15), water snap-offs occur as a step function above a threshold of 67% oil saturation (Fig. 2.18).
2.3.6 Cycle 6: Secondary Drainage through Blob Displacement

A final drainage cycle is sustained that progressively reconnects water snap-offs as the drainage throat threshold decreases. Figure 2.17a shows the evolution of pseudo-capillary pressure with saturation during Cycle 6. This curve compares well to Kovscek’s theoretical curve (shown in Fig. 2.17b).

Figure 2.19a describes the resistivity indices calculated from random-walk simulations performed on the 20 p.u. Finney pack during mixed-oil-wet Cycles 4 to 6. For comparison, plots of Wei and Lile (1991)’s measurements (Fig. 2.1a) for the same saturation cycles are shown in Fig 19b. The agreement between the two figures is remarkable. There are only two important differences between the two plots: the irreducible saturations, and the value of critical water saturation below which the saturation exponent increases abruptly during imbibition (about 40% water saturation for our model, 50% for the measurements). This critical saturation also corresponds to the saturation at which water snap-offs form abruptly, which in turn explains the resistivity enhancement across the sample. It is also remarkable that the lower hysteresis cycle exhibits the same 40% critical water saturation as that reported by Zhou et al. (1997) for their 3D effective percolation method which neglected specific details of rock morphology. Such evidence supports our intuitive understanding that the incorporation of more realistic rock morphologies reduces the difference between simulated and measured critical saturations.

2.4 Effect of Grain Morphology on Electrical Rock Conductivity

As discussed in Section 2.1.2, it is well known that rock morphology can have a strong impact on the electrical conductivity of saturated rocks. We consider several
rock models to illustrate the effects of rock roughness, grain clustering, intragranular microporosity, and clays on formation factor and resistivity index.

2.4.1 Effect of Grain Roughness on Resistivity Index

Diederix (1982) reported measurements of clay-corrected resistivity indices of shaly sandstones that exhibited an abnormal decrease of $n$ from 2.1-2.2 to 1.3-1.5 below a critical water saturation, $S_{wcr}$, close to 60%. Because the rock formation under consideration was salt-saturated, it followed that the contribution of clay exchange cations to electrical conduction was negligible compared to pore-water conduction, and therefore the rock electrically behaved as a clay-free saturated rock. No other petrophysical data are available from wells considered in Diederix’s (1982) study; however, reported $n$ values in the range of 2.1-2.2 suggest the validity of a Finney pack-type rock model to study the reported behavior of electrical conduction. The conductivity enhancement occurring below $S_{wcr}$ was explained by Diederix (1982) as a consequence of the roughness created by the coating clay texture at the grain surface. Diederix (1982) reached this conclusion by comparing the resistivity index measured for smooth and rough water-wet glass-bead samples. We now attempt to reproduce such non-Archie behavior with our pore-scale random-walk method.

As illustrated in Fig. 2.20, substantial roughness created by clay flakes at the grain surface causes an effective increase of the thickness of the brine film between water-wet rock and oil. The same argument justifies the choice of a thickness of 30 nm brine at the surface of our smooth spherical grains to represent some grain roughness, instead of the 5 to 10 nm thickness expected for a flat rock/water/oil interface (Hirasaki, 1991). Because clay conductivity is negligible, we keep the same rock model as in Section 2.3 (20-p.u. overgrown Finney pack of 100-μm grains) and
increase the thickness of the brine wetting film from 30 to 300 nm during drainage (Cycle 1). Figure 2.21 shows the corresponding simulation results for $I_R$, along with simulation results obtained previously for 30-nm brine films, and the experimental trends measured by Diederix (1982). Both measured and simulated critical water saturations $S_{w \text{crit}}$ (around 55%) and abnormal resistivity index slopes (around 1.3) agree extremely well. This result is rather surprising given that no morphological effects, including porosity or formation factor, were adjusted in the generic-rock simulations. Moreover, results suggest that the negative curvature of $I_R$ versus $S_w$ below $S_{w \text{crit}}=55\%$ could solely be due to wetting effects, and that wetting films as thick as 0.3% of the grain radius are enough to reproduce the measured trend regardless of rock geometry at 20% porosity.

### 2.4.2 Effect of Grain Clustering on Formation Factor

As emphasized earlier, for porosities above 15% uniform overgrowth of the Finney pack underestimates the intrinsic tortuosity of real rocks, and therefore the formation factor. To understand this behavior, let us consider the fused-glass-bead pack and sandstone micrographs shown in Fig. 2.22. Marked differences exist between relatively high-porosity samples of glass beads and rocks. Specifically, Fig. 2.22c shows that grains constituting the rock sample form small clusters, while Fig. 2.22a suggests that beads from the fused pack are homogeneously distributed in space. At low values of porosity, however, the clusters of squashed rock grains are no longer apparent in Fig. 2.22b, and the sample acquires the same morphology as a tight packing of fused beads. If we regard the Finney pack as a good approximation of a fused glass bead pack, this observation explains why the corresponding formation
factor agrees well with sandstone measurements at low values of porosity but not at high values of porosity.

We construct packs with a more realistic normal grain size distribution in the range of 30 to 160 μm, and subsequently modify them to exhibit variable degrees of clustering. Local grain clustering is achieved by including grain attractors in the packs and by displacing the remaining grains toward the attractors by a distance \( a/r^2 \), where \( a \) is a constant and \( r \) is the distance between the grains and the attractors. Packs 1 to 3 are characterized by increasing values of \( a \). Figure 2.23 shows formation factor curves simulated for these grain packs, indicating that grain clustering can result in values of formation factor closer to those measured in the 20 p.u. range. Similar results could be obtained by growing the grains on a cluster basis, instead of homogeneously during the porosity reduction process.

### 2.4.3 Effect of Microporosity and Clay Distributions on Formation Factor

We proceed to construct a suite of rock models where grains exhibit intragranular microporosity. The connectivity of the intragranular micropore space with the intergranular pore space depends on whether cement is present on the pore walls. Therefore, as described in Table 1.1, we vary the distribution of coupled microporous grains (Type 3 in Fig. 2.5) and uncoupled ones (Type 4 in Fig. 2.5) with total porosity. In this table, \( \phi_{total} \) is the total porosity of each model, \( \phi_{inter} \) is the intergranular porosity, and \( \phi_{intra} \) is the intragranular porosity that develops within the grain objects; \( \phi_{eff} \) is the effective, or connected, porosity comprising intergranular pore space and coupled intragranular microporosity within grains of Type 3; \( \phi_{eff} \) is the porosity value that is used to calculate the formation factor (Eq. 2.4). At high values of porosity (above 20 p.u.), the rock model is constructed with a Finney pack where 1/3
of the grains are solid and 2/3 are coupled microporous. The objective is to reproduce the structure of a micritized carbonate sample described by Toumelin et al. (2003, 2004) to relate pore structure and the corresponding nuclear magnetic resonance (NMR) response. Below $\phi_{\text{total}} = 17\%$ (or $\phi_{\text{inter}} = 8\%$), the proportion of coupled microporous grains decreases gradually in favor of uncoupled grains (isolation by cements and crystallization) and solid grains (incomplete micritization). The formation factor in these microporous rock models is then calculated from random-walk simulations and plotted in Fig. 2.24. We observe a minor difference between the curve associated with the microporous model and that of the Finney pack with solid grains. While the effective diffusivities computed in the microporous model are much larger than those computed in the solid Finney pack for similar intergranular porosities, the division by $\phi_{\text{eff}}$ in Eq. (2.4) normalizes the results and yields very similar curves.

Finally, we consider distributions of grain-coating clay randomly distributed in the Finney pack. Thirty percent of the grains are assigned a 3-$\mu$m clay coat (as described in the type-4 grains of Fig. 2.5), so that the corresponding clay volume amounts to 2% of the solids. The porosity is reduced by homogeneously growing all the grains and by maintaining the 3-$\mu$m clay coat with grain growth regardless of porosity. We consider contrasts between effective clay conductivity and pore brine conductivity, $\sigma_{\text{clay}} / \sigma_{\text{brine}}$, equal to 1:1000, 1:10 and 1:1, which correspond to decreasing brine salinities. Figure 2.24 shows the resulting plot of formation factor vs. porosity. The slope of the line now becomes the clay-corrected Archie-type exponent $m^*$ (Clavier et al., 1984). As expected, the 1:1000 conductivity contrast yields the same results as the solid-grain Finney pack (Fig. 2.21). However, we remark that formation factors can substantially decrease for lower values of conductivity contrast.
When clays become as conductive as the pore brine (a situation that is common in low-salinity shaly sands), $m^*$ decreases to 1.5 for the Finney rock model.

### 2.4.4 Effect of Porosity and Microporosity on Resistivity Index

We now consider the case of a consolidated Finney pack with 7% porosity. A procedure similar to that previously used for the 20-p.u. rock model yields a blob factor $\alpha_o = 3.6$. Cycle 1 (water-wet drainage) is then performed down to $S_{wir} = 20\%$. Next, wettability is altered and Cycle 4 (oil-wet drainage) is simulated up to $S_w = 80\%$. Finally, oil-film growth is implemented for Cycle 5 (oil-wet imbibition) down to $S_w = 54\%$. Figure 2.25b shows the corresponding resistivity indices calculated with our random-walk algorithm. Comparison with resistivity index cycles previously obtained for the 20-p.u. Finney pack (Fig. 2.25a) emphasizes several differences due to the decrease of porosity. First, the value of $n$ for water-wet drainage (Cycle 1) remains equal to 2 for both porosity models. However, for oil-wet drainage (saturation Cycle 4), $n$ remains between 3.5 and 4, up from the value $n = 3$ found with the 20 p.u. model. This behavior is due to the fact that $\alpha_o$ increases when porosity decreases, which in turn decreases the accessibility to pendular rings. When water films break at the rock surface, conductive paths through the pendular rings become more tortuous and the resistivity index increases. Second, the critical water saturation below which the resistivity index increases abruptly during oil-wet imbibition now increases from about 40\% (at 20 p.u.) to 60\% (at 7 p.u.).

Finally, we consider the case of a partially microporous grain pack and calculate the associated resistivity index during the same saturation cycles. We select the 22.5 p.u. grain pack described in Table 1, which is roughly based on a 14-p.u. consolidated Finney pack where 2/3 of the grains are considered microporous and
diffusively coupled with the intergranular pore space. Due to the amount of intragranular microporosity (amounting to 38% saturation of the fluids in the rock model), irreducible water saturation is set to 45%, with a blob factor $\alpha_o = 3$. Figure 2.25c shows the resistivity index values calculated for Cycles 1, 4 and 5 for this microporous rock model. Major differences appear with respect to results previously obtained for solid-grain packs. Both water-wet and oil-wet drainage curves exhibit negative curvature (thereby decreasing $n$) when $S_w$ decreases below 60%. At these values of water saturation, most of the electrical conduction occurs through intragranular microporosity. Furthermore, two characteristics of the resistivity-index curve during oil-wet imbibition resemble those reported by Sweeney and Jennings (1960), shown in Fig. 2.25d: the value of $n$ (decreased to 2) and the critical water saturation below which non-Archie behavior occurs (increased to 75%). This suggests that Sweeney and Jennings’ carbonate rocks could include an unaccounted amount of intragranular porosity.

The above results conclusively suggest the strong morphological origin of the non-Archie behavior of oil-wet rocks.

## 2.5 SUMMARY AND CONCLUSIONS

We introduced a new pore-scale approach to simulate the electrical conductivity of two-phase saturated rocks as a function of saturation history, preferential wettability, and intragranular grain morphology. The simulation approach reproduced measurements of conductivity hysteresis in both water-wet and oil-wet rocks, including several types of drainage and imbibition cycles. Our simulation procedure was successfully used to compute the electrical resistivity of a variety of
grain and rock morphologies, including microporous rocks and clayey sands. To date, no pore-scale modeling results have been published that undertake the same complexity of petrophysical problems.

Simulation results obtained in this chapter shed significant light on the behavior of Archie’s saturation exponent $n$ across the complete range of water saturation. Specifically, the simulation work presented in this chapter corroborates the following known experimental behavior of $n$:

1. Standard $n$ values in the neighborhood of 2 are deemed characteristic of water-wet rocks where the dominant fluid displacement process is pore-to-pore connectivity.
2. Values of $n$ tend to decrease when brine saturation decreases in water-wet rocks that exhibit conductive pathways other than pore throats and thin films, such as in the presence of thick films resulting from substantial surface roughness, clay exchange cations, or intragranular porosity.
3. Values of $n$ between 3 and 4 are associated with oil-wet and clay-free rocks during their primary drainage for all values of water saturation, and during imbibition at high values of water saturation.
4. Oil-wet saturation cycles could be associated with values of $n$ as low as 2 for the case of microporous rocks.
5. Values of $n$ equal or larger than 10 arise during oil-wet imbibition cycles below a given value of critical water saturation. The corresponding value of critical water saturation increases with a decrease of porosity and in the presence of intragranular porosity.
Water-wet hysteresis of resistivity indices is theoretically possible if the imbibition is controlled by a film-growth mechanism. Oil-wet hystereses of resistivity index can be explained by the effect of oil-wettability and water snap-off independently of rock morphology. Rock morphology influences the critical water saturation below which the brine forms isolated patches and electrical resistivity abruptly increases.

Several additional conclusions stem from the observed behavior of $m$ with grain morphology:

1. Values of $m$ increase when porosity decreases.
2. Asymptotic values of $m$ at low and high values of porosity do not vary significantly with rock morphology as long as intragranular porosity and clays are absent from the rock matrix. Between 10 and 25 p.u., however, $m$ is strongly affected by grain clustering. Such grain clustering yields values of formation factor that are closer to those measured in real sandstones than those simulated with the Finney pack.
3. Coupled intragranular porosity significantly enhances effective water diffusivity throughout the rock model, compared to rocks with similar intergranular porosity but with no intragranular porosity. However, because the formation factor is normalized by effective porosity, no significant change in formation factor is obtained in the presence of intragranular porosity.
4. Values of $m$ strongly depend on intragranular conductive shortcuts when these shortcuts are associated with low values of porosity. For instance, the presence of clay exchange cations can significantly decrease the apparent lithology exponent $m^*$ for low values of salinity.
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Table 1.1: Distribution of grain types, intergranular, and intragranular porosities in the microporous rock model as a function of total porosity.
Figure 2.1: Resistivity index cycles measured (a) by Wei and Lile (1991) during drainage and imbibition cycles of an oil-wet sample of Berea sandstone and (b) by Sweeney and Jennings (1960) during imbibition of a variety of preferentially oil-wet carbonate samples (plain lines). The dashed line in panel (b) describes the trend of Wei and Lile’s imbibition curve shown in panel (a), and is used for comparison purposes.
Figure 2.2: Examples of diffusivity time decays simulated for water molecules ($D_{\text{bulk}} = 2 \, \mu m^2/\text{ms}$) at different values of water saturation, $S_w$, in a 20 p.u. tortuous pore space.

(a) (b)

Figure 2.3: From grain pack to Delaunay tessellation: (a) example of a 1000-grain subset from the Finney pack constructed with the basic length of 100 $\mu m$ per grain, and (b) corresponding Delaunay tessellation. All the dimensions are given in $\mu m$. 

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Figure 2.4: From Delaunay tetrahedra to pore space: graphical description of one cell which defines one pore, four throats, and six pendular rings (PR).

Figure 2.5: Description of the six grain types used in the geometrical framework considered in this chapter. Color is used to code the diffusivity values enforced during random walks by zones (blue: \(D_w\); yellow: \(D_w\) – disconnected from the blue connected brine; green: \(D_{clay}\) – connected to blue brine via probability of passage).
Figure 2.6: Description of the geometry of two-phase fluid saturation in a Delaunay tetrahedron. A non-wetting blob occupies the intersection between the pore space and a sphere of radius $R_o$ concentric with the pore shown in Fig. 2.4. Thin wetting films of thickness $T$ are included between the blob and the grains.

Figure 2.7: Description of the five pore types used in the geometrical framework considered in this chapter (gray: rock, blue: water; red: oil).
Figure 2.8: Two-dimensional description of the procedure used in this chapter to model pore-space fluid drainage. (a) Real rock topology from a thin section (white is quartz and blue is pore space). (b) Model representation that includes the grains (yellow circles) and the Delaunay cells (dashed triangles). (c) Fluid drainage configuration for oil inlet at the bottom-right. The oil (red) region in each pore is delimited by a sphere (blue circles) of radius $R_o = \alpha_o R$, where $R$ is the pore size. Drainage stops at the arrowed pore throat, where the throat size threshold is not met. (d) Same as (c), but with a lower throat size threshold fluid flow is allowed through the arrowed throat.
Figure 2.9: Cross-plot of formation factor and total porosity measurements of clay-free sandstones (Doyen, 1988) together with the corresponding simulations obtained with pore networks (PN: Bryant and Pallatt, 1996) and random walks (RW: this work) for the case of a 20-p.u. Finney pack.
Figure 2.10: Visualization of the Delaunay tetrahedra invaded by oil during Cycle 1 to reach 22% oil saturation in the 20 p.u. Finney pack (17 μm throat threshold). The oil inlets are located at face $x=0$ (circled 1’s). Breakthrough is reached at faces $x=1600$ μm (circled 2), $y=0$ (circled 3), $z=0$ (circled 4) and $z=1600$ μm (circled 5). The color scale describes the $z$-coordinate of the pore centers drained with oil.
Figure 2.11: Pseudo-capillary-pressure curves for primary drainage in the 20-p.u. uniformly consolidated Finney pack. The curves describe pseudo-capillary pressure values as a function of water saturation for different non-wetting blob-size factors $\alpha_o$ involving different values of irreducible water saturation, $S_{wir}$. 
Figure 2.12: Evolution of resistivity index during primary drainage in a 20 p.u. clean water-wet rock: comparison between measurements performed on clay-free sandstones (core T1 from Argaud et al., 1989), pore-network simulation results performed on a cemented Finney pack neglecting thin-film conduction (Bryant and Pallatt, 1996), and random-walk simulation results carried out for the same Finney pack but allowing thin-film electrical conduction.
Figure 2.13: Pseudo-capillary-pressure curves for primary drainage (Cycle 1) and imbibition (Cycle 2).

Figure 2.14: Evolution with (wetting) water saturation of pore throat threshold (left scale, plain curve), and fraction of pores where oil snap-off occurs (right scale, dashed curve with open markers).
Figure 2.15: Evolution with (wetting) water saturation of: incremental water film thickness (left scale, plain curve), and fraction of pores where oil snap-off occurs (right scale, dashed curve with circle markers).
Figure 2.16: Resistivity index hysteresis due to drainage and imbibition cycles for the water-wet 20-p.u. overgrown Finney pack with 13% irreducible water saturation.
Figure 2.17: (a) Pseudo-capillary-pressure curves simulated for primary and secondary oil-wet drainage cycles involving different values of irreducible water saturation, $S_{wir}$. (b) Theoretical capillary-pressure curves for oil-wet cycles that exhibit similar values of irreducible water saturation (adapted from Kovscek et al., 1993).
Figure 2.18: Evolution with (wetting) oil saturation of: incremental wetting oil film thickness (left scale, plain curve with dot markers), proportion of pores with water snap-offs (right scale, dashed curve with circle markers), and water saturation isolated from the water network (right scale, plain curve with diamond markers) during Cycle 5 (oil-wet imbibition).
Figure 2.19: Resistivity-index hysteresis (a) simulated with a 20-p.u. Finney pack assuming mixed-oil-wettability for saturation Cycles 4 to 6, and (b) measured in 19-p.u. Berea plugs previously chemically treated to remain oil-wet (see Fig. 2.1a).
Figure 2.20: Effect of surface roughness on the effective thickness of the brine wetting film for an equivalent smooth surface: (a) relatively smooth grain surface; (b) rough grain surface. Single-headed arrows represent conduction currents through the brine film.

Figure 2.21: Influence of water film thickness on the resistivity index drainage curve: comparison between the random-walk simulation results performed for the generic rock model with different wetting films thicknesses (30 nm and 300 nm), and in-situ measurements of salt-saturated shaly sandstones containing smooth grains (as in Fig. 2.20a: Well 4 data from Diederix, 1982) and rough grains (as in Fig. 2.20b: Well 1 data from Diederix, 1982).
Figure 2.22: Micrographs of fused packs of glass beads and rocks exhibiting different values of porosity.
Figure 2.23: Cross-plot of formation factor and total porosity values measured in clay-free sandstones (Doyen, 1988) and formation factors simulated with random-walks (RW) for packs of normally distributed grain sizes and different degrees of grain clustering (pack 1 is the least clustered and pack 3 is the most).

Figure 2.24: Cross-plot of formation factors and total porosity values for the case of microporous rock models (dashed with circles) and clayey rock models exhibiting different contrasts of clay-to-brine electrical conductivity (plain lines).
Figure 2.25: Comparison of resistivity index curves simulated for saturation Cycles 1, 4 and 5 for three different rock models: (a) 20-p.u. generic Finney pack; (b) 7-p.u. homogeneously overgrown Finney pack; (c) 22.5-p.u. microporous grain pack based on a 14-p.u. Finney pack. Black vertical arrows designate the wettability alteration between Cycles 1 and 4. Sweeney and Jennings’ (1960) imbibed measurements of oil-wet carbonates are plotted in panel (d) for comparison purposes.
Chapter 3: Random-Walk Approach for the Simulation of NMR Measurements and 2D NMR Maps in Porous Media with Relaxing and Permeable Boundaries

This chapter revisits random-walk methods to simulate the NMR response of fluids in porous media using Bloch equations and relaxing or permeable boundaries. We generalize existing NMR numerical methods used in biology and engineering into a single formulation that combines the effects of surface relaxivity, membrane permeability, inhomogeneous magnetic fields, and arbitrary pulse sequences of the NMR signal. When fluids exhibit low $T_1/T_2$ contrasts and when CPMG pulse sequences are used to acquire NMR measurements, we verify that classic NMR numerical models neglecting $T_1$ effects accurately reproduce surface magnetization decays of saturated granular porous media. However, when fluids exhibit substantial $T_1/T_2$ contrasts, when they include several components, or when magnetic fields are strongly inhomogeneous, we show that the solution of the complete set of Bloch’s equations is necessary to obtain accurate simulation results. This random-walk formulation accurately reproduces the magnetization echoes stemming from fundamental spin dynamics calculations, in arbitrary background magnetic field maps. By simulating longitudinal and transversal magnetizations for specific bulk fluid properties and fluid/solid boundary geometries, this random-walk algorithm is used to generate parametric multidimensional $T_1/T_2$ and $D/T_2$ NMR maps for the characterization of pore structures and saturating fluids.
3.1 INTRODUCTION

The non-invasive and non-destructive nature of NMR measurements and their sensitivity to both in-situ fluid composition and pore structure make them extremely valuable to a wide class of engineering and biological applications. Specific areas of application include oil exploration, soil hydrology and remediation, synthetic microporous materials characterization, tissue engineering, osteology, and biomedical imaging. Specific problems of interest include fluid displacement imaging, pore-size characterization, in-situ fluids characterization, and ions characterization, among others.

3.1.1 Pore Structure and Fluid Characterization

The application of NMR measurements for pore-size characterization is motivated by two relationships between measurable quantities and the pore surface-to-volume ratio \( (S/V) \) of porous media saturated with a single fluid phase. Firstly, longitudinal and transversal relaxation times of a fluid \( (T_1 \) and \( T_2 \), respectively) are related to the product \( \rho (S/V) \), where \( \rho \) is the relaxivity of the pore surface. This relationship remains valid in the fast-diffusion limit (Brownstein and Tarr, 1979) when paramagnetic centers are present at the pore wall surface. Secondly, the short-time asymptotic behavior of the effective fluid diffusivity \( D \) is directly related to \( (S/V) \) (Latour et al., 1993; Song, 2000). Practical limitations exist when applying these two relationships to the interpretation of NMR measurements. Namely, it is normally assumed that (1) pores are well defined and isolated, and (2) inversion techniques can reliably and accurately estimate the distribution of surface-to-volume ratios. Experimental evidence shows that pores spanning different length scales can be connected and, therefore, that the estimated values of \( (S/V) \) should be interpreted in
an average sense. The recently identified phenomenon of diffusion coupling in heterogeneous and low-surface-relaxivity carbonate rocks is representative of such a limitation of NMR measurements (Ramakrishnan et al., 1999). In addition, effective pore values of \((S/V)\) sensed by protons in a fluid phase depends on the relative saturation of that phase within the pore: when several fluid phases are present in the same pore space the actual and effective values of \((S/V)\) for that pore may differ substantially. The case of pore geometrical anisotropy, whether in rocks or in biological tissue, is of prime interest and is generally approached using simplified models that neglect the complex pore geometries and the permeability of boundary membranes (Meerwall and Ferguson, 1981; Pfeuffer et al., 1998; Stanisz et al., 1997; Zientara and Freed, 1980).

Special acquisition techniques have been developed to improve fluid characterization (Hürlimann and Venkataramanan, 2002; Sun and Dunn, 2002; Callaghan et al., 2003; Sun and Dunn, 2005), including: (1) suites of magnetic pulse sequences of different magnitudes, orientations, and characteristic times, e.g. CPMG-like sequences with different echo-times and wait-times, and (2) multidimensional inversion of the measured magnetization decays in the form of cross-plot distributions of \(T_1\), \(T_2\) and \(D\). This inversion procedure is sensitive to fluid diffusivity contrasts, restricted diffusion, surface relaxation, and wettability. To date, however, no NMR method exists that can reliably and accurately differentiate ambiguous porous medium morphologies (e.g., rock facies and irregular texture) and fluid distributions within the same saturated rock.
3.1.2 **Objective and Scope**

Modern NMR applications require integrated simulation and interpretation methods that can incorporate the complexity of real porous media and multiphase fluid saturation at the pore scale. Accurate simulation methods have been proposed based on a quantum mechanical framework for the case of bulk fluids (Hürlimann and Griffin, 2000), or based on analytical diffusion propagators for the case of periodic porous microstructures (Dunn, 2002). The disordered nature of most biological and mineral porous media, however, demands sophisticated approaches for numerical simulation.

The main thrust of this chapter is to formulate an accurate algorithm for the simulation of NMR measurements of saturated microporous media in a general context. Namely, the algorithm is designed to remain valid for known distributions of (a) pore boundaries and surface characteristics (i.e. geometry and surface relaxation $\rho$ and/or diffusion permeability $P$), (b) static and susceptibility-induced magnetic fields, (c) fluid phases and their bulk properties, and (d) corresponding velocity fields which superimpose to the diffusive Brownian motion in the case of ionic displacement (Johnson and He, 1989) or hydraulic motion (Caprihan and Fukushima, 1990). For this, the fluid NMR magnetization is computed as the solution of Bloch’s equations along the continuous non-interacting random walk of diffusing spins. This approach remains valid when the magnetization coupling between spins in a fluid is governed by constant longitudinal and transversal bulk relaxations, and when Bloch’s equations remain valid to describe magnetization, i.e., both in the low-field NMR measurement of spins $\frac{1}{2}$, and in the high-field $^1$H measurements of water.
3.2 NMR Theory

Let us first define the geometrical orthonormal basis, $\Gamma = (0, \hat{x}, \hat{y}, \hat{z})$, and the rotating frame, $\Sigma = (\hat{x}', \hat{y}', \hat{z})$, which rotates with the magnetic dipoles around the direction of the permanent magnetic field $B_0$ exerted by the NMR tool. The frame $\Gamma$ is centered with the geometrical center of the volume of investigation, 0, while the direction of the unitary vector $\hat{z}$ is imposed by the static magnetic field exerted by the permanent magnet of the NMR tool, $B_0 = B_0 \hat{z}$. As explained later in this chapter, the permanent field $B_0$ can vary as a function of position and time within the NMR sensitive volume; it is therefore quantified by its difference $\Delta B_0$ with respect to a reference ‘sweet spot.’ The frame $\Sigma$ rotates with respect to $\Gamma$ along $\hat{z}$ at the same frequency as the spin Larmor frequency at the sweet spot, $\omega = \gamma B_{0\text{sweet spot}}$, where $\gamma$ is the gyromagnetic ratio for the spin of interest. Since $\Sigma$ rotates with the spin, the effective contribution of the permanent magnetic field which affects the spin is $\Delta B_0$.

3.2.1 Bloch-Torrey Equations

Bloch’s equations describe the dynamics of spins $\frac{1}{2}$ as equivalent magnetic dipoles. The magnetization of the collective magnetic moments of spins can be expressed with the vector $M = (M_x, M_y, M_z)^T$ in the rotating frame $\Sigma$ (the subscript $^T$ denotes vector transposition). At equilibrium, the spin is aligned with $B_0$ and the corresponding equilibrium magnetization vector is $M_0 = M_0 \hat{z}$. If $B = (B_x, B_y, B_z)^T$ is the effective magnetic field that affects the walker in the rotating frame and $T_1$ ($T_2$) is the total longitudinal (transversal) relaxation time, Bloch’s equations modified by Torrey (Torrey, 1956) can be written in vector form as

$$\frac{dM}{dt} = \gamma B \times M - \frac{M_x}{T_2} \hat{x}' - \frac{M_y}{T_2} \hat{y}' - \frac{M_z}{T_1} \hat{z} + \frac{M_0}{T_1}.$$

(3.1)
To illustrate the “mechanics” of Eq. (3.1), consider the CPMG (Carr-Purcell-Meiboom-Gill) pulse sequence that is widely used in low-field NMR applications. The $B_1$ field that forces spin refocusing and the creation of NMR echoes is applied in the form of RF pulses along the rotating axes $\hat{x}'$ and $\hat{y}'$. Punctually, these pulses add to $\Delta B_0$ so that the effective magnetic field applied to the spins during pulse enforcement is $B = \Delta B_0 + B_1$. These $B_1$ pulses are applied with finite duration $t_\theta$ and are quantified by the amount of magnetization tilting, $\theta = \gamma \| B_1 \| t_\theta$, they create through the curl term in Eq. (3.1) – usually $\pi / 2$ or $\pi$. For instance, regular CPMG pulse sequences take the form of a $\pi / 2$-pulse along the $\hat{x}'$ axis followed by a series of $\pi$-pulses along the $\hat{y}'$ axis separated by the inter-echo time $TE = 2\tau$. This pulse sequence is denoted as $(\pi / 2)_x - \tau - (\pi)_y - 2\tau - (\pi)_y - 2\tau - ...$

Spin echoes are stimulated between two successive $\pi$ pulses. Figure 3.1 illustrates the successive positions of the magnetization vector $M$ in the rotating frame $\Sigma$ during and between the first two RF pulses, assuming that the amplitude $\| M \|$ remains constant (i.e., $T_{1,2} \rightarrow \infty$) in the process. The durations of the $\pi / 2$ and $\pi$ pulses are termed $t_{90}$ and $t_{180}$, respectively.

### 3.2.2 Time- and Space-Dependent Magnetic Fields

The effective field $B = \Delta B_0 + B_1$ applied to the spin varies as a function of time and space. First, as described in Appendix B, the geometrical configuration of the magnet itself may yield inhomogeneous field maps (Hürlimann and Griffin, 2000). Next, the presence of susceptibility contrasts between the fluid and the solid grain within the porous medium can distort this background field map and induce internal fields (Dunn, 2002; Weiskoff et al., 1994). Finally, additional background field gradients $\nabla B_0$ are imposed to enhance the NMR decay due to diffusivity contrasts...
between fluids in low-field applications, or to encode the spin position in high-field magnetic resonance imaging (MRI) applications. In this last case, $\Delta B_0$ will be not only a function of walker location $\Delta r$ with respect to the sweet spot, since $\Delta B_0(\Delta r) = (\nabla B_0 \cdot \Delta r) \hat{z}$, but also a function of time when these gradients are enforced.

Figure 3.2 shows an example of 3-dimensional (3D) MRI encoding sequence that includes both RF pulses and background gradient pulses.

### 3.2.3 Relaxation Processes

Macroscopically, it is normally considered that three independent processes affect the time decay of the measured NMR signal: (1) bulk fluid relaxation, with characteristic longitudinal and transversal times $T_{1B}$ and $T_{2B}$, mainly due to spin dipole-dipole interactions or spin rotation within the fluid; (2) surface relaxation, characterized by effective relaxation times $T_{1S}$ and $T_{2S}$, which occurs because of the proximity with paramagnetic centers at interfaces between pore fluids and grain solids; and (3) relaxation due to the presence of background magnetic field heterogeneities, $T_{2D}$. Mathematically, the measured NMR time decay of a fluid-saturated sample exhibits a total relaxation time given by

$$\frac{1}{T_2} = \frac{1}{T_{2B}} + \frac{1}{T_{2S}} + \frac{1}{T_{2D}}. \quad (3.2)$$

$T_{2B}$ and $T_{2S}$ relaxations are intrinsic properties of the system and are governed by fluid, rock and thermodynamic states (pressure, temperature). They are responsible for the magnetization decay, in the sense of energy loss. By contrast, $T_{2D}$ is an experimentally controllable quantity affected not only by the fluid diffusivity and the internal fields due to clays, but also to experimental parameters (tool gradient, echo time values). $T_{2D}$ appears solely because the NMR signal is acquired in the $(\hat{x}', \hat{y}')$ rotating frame, and more specifically along the $\hat{y}'$ axis. As illustrated in Fig. 3.3, even
if the magnetization vector keeps a constant magnitude, its projection along $\hat{y}'$ is weighted by the cosine of the phase shift $\phi$; the sum of all these cosines over all the walker population collectively creates an apparent decay in $\exp(-t/T_{2B})$, $t$ being time. This concept is capital to understanding the microscopic treatment of our numerical method.

3.3 **RANDOM-WALK RESOLUTION**

Numerous NMR models have been used in different disciplines to reproduce the NMR response of fluids in porous rocks, bones, semi-permeable biological tissue, etc. Random walks reproducing the diffusive motion of the spins proved to be the only technique amenable to the simulation of NMR responses due to a variety of porous medium geometries, including fractal or 3D disordered porous media (Schwartz and Banavar, 1989; Wilkinson *et al.*, 1991). All these algorithms simulate the projection of spin packets in the transversal plane of the rotating frame, i.e., in the plane of measurement of an NMR tool antenna, and describe either surface relaxation effects (Ramakrishnan *et al.*, 1999; Bergman *et al.*, 1995) or diffusion effects (Weiskoff *et al.*, 1994; Gudbjartsson and Patz, 1995). In this section, we show that magnetic dipole dynamics in the full 3D rotating frame are necessary to accurately simulate diffusion effects, and that surface magnetization decay can be treated in equivalent fashion to diffusion and bulk relaxation along diffusion random-walk pathways.

3.3.1 **Random-Walk Process and Magnetic Dipole Dynamics**

Our algorithm uses a classical continuous random walk, whereby a walker is displaced within the pore space attributed to a given fluid of self-diffusion $D$ and bulk longitudinal and transversal relaxation times $T_{1B}$ and $T_{2B}$, respectively. Following an
initial location randomly determined within the volume occupied by the fluid of interest, at each time step of infinitesimal duration $\delta t$ a vector of normally distributed random numbers $\mathbf{n} = (n_x, n_y, n_z)^T$ is generated with unit variance and zero mean. The walker is then displaced within $\Gamma$ by a differential distance

$$\delta \mathbf{r}_D = \left(6D_{\text{bulk}} \delta t\right)^{1/2} \frac{n}{\|n\|} \quad (3.3)$$

to ensure equivariance of the movement in the 3 dimensions of $\Gamma$. In the presence of velocity drift, $\mathbf{v}$, applied to the walker, an additional drift displacement $\delta \mathbf{r}_v = \mathbf{v} \delta t$ is added to $\delta \mathbf{r}_D$. In so doing, $\delta t$ is dynamically adapted along the walk so that (a) it is smaller than any magnetic field pulse duration, (b) the amplitude of the displacement, $\|\delta \mathbf{r} = \delta \mathbf{r}_D + \delta \mathbf{r}_v\|$, is several times smaller than surrounding geometric features (such as pore throats, wetting film thickness, etc.), (c) the value of the total magnetic field $\mathbf{B} = \Delta \mathbf{B}_0 + \mathbf{B}_1$ can be considered constant during a step, and (d) all walkers are synchronized at the onset and offset of magnetic pulses and at the time of echo acquisition.

Equation (3.1) is solved along the successive segments of the random walk trajectory by defining the evolution matrix $\mathbf{A}$:

$$\mathbf{A} = \begin{bmatrix} \frac{1}{T_2} & -\gamma B_z & \gamma B_y \\ -\gamma B_z & \frac{1}{T_2} & \gamma B_x \\ \gamma B_y & -\gamma B_x & \frac{1}{T_1} \end{bmatrix}, \quad (3.4)$$

and the reduced magnetization

$$\mathbf{M}' = \mathbf{M} + \mathbf{A}^{-1} \cdot \mathbf{M}_0 / T_1, \quad (3.5)$$

so that Eq. (3.1) is integrated as

$$\mathbf{M}'(t) = e^{\mathbf{A}t} \cdot \mathbf{M}'(0), \quad (3.6)$$
where $\mathbf{M}'(0)$ is the reduced magnetization at the onset of each integration interval. As we saw earlier, $\mathbf{B}$ varies with clock time and walker position, whereupon new values for $B_x$, $B_y$, and $B_z$ are used on each random-walk segment. As explained in the next section, $T_1$ and $T_2$ are also locally adjusted to account for the proximity of a relaxing boundary. Consequently, for each step $i$ spanning the time interval $[t, t + \Delta t]$, the magnetic dipole carried by the random walker is subject to a new evolution matrix $\mathbf{A}'$ and longitudinal relaxation time $T_1'$. The resulting magnetization in $\Sigma$ is given by

$$\mathbf{M}' = e^{\mathbf{A}' \omega} \cdot \left\{ \mathbf{M}^{-1} + \left( \mathbf{A}' \right)^{-1} \cdot \mathbf{M}_0 / T_1' \right\} - \left( \mathbf{A}' \right)^{-1} \cdot \mathbf{M}_0 / T_1'. \quad (3.7)$$

The NMR signal is the sum of all $\mathbf{M}$ vectors for all magnetic dipoles, sampled at the same rate. Hydrogen indices weight the magnetization contribution of each walker in the presence of multiple fluid phases with different hydrogen index. It is important to note that $\mathbf{M}$ is continuous but $\mathbf{M}'$ is not in general, especially in the vicinity of fluid boundaries where the updated values of $\mathbf{A}$ and $T_1$ should be used at each step. We remark that the calculation of the onset reduced magnetization via the expression

$$\mathbf{M}'_{\text{onset}} = \mathbf{M}^{-1} + \left( \mathbf{A}' \right)^{-1} \cdot \mathbf{M}_0 / T_1', \quad (3.8)$$

with $\mathbf{A}'^{-1}$ instead of $\mathbf{A}'$ jeopardizes the numerical convergence of the algorithm. Appendix C provides an analytical solution for the matrix exponential of $\mathbf{A}$ as a function of the components $B_x$, $B_y$, and $B_z$ for a given random-walk segment.

### 3.3.2 Local Surface Relaxation

While the walker stays away from a fluid boundary, the magnetic dipole relaxes at its bulk rate, i.e. by accounting for the effective decay created by the cross-interactions between spins. The relaxation times $T_1$ and $T_2$ become equal to the bulk fluid longitudinal and transversal relaxation times, $T_{1B}$ and $T_{2B}$, respectively. When the
walker is located within one step of a fluid boundary of surface relaxivities $\rho_1$ (longitudinal) and $\rho_2$ (transversal), an additional decay applies to the magnetization. The magnetization decay is locally enhanced to include this surface relaxation effect at the microscopic level. If the displacement achieved during the interval $[t, t + \delta t]$ comes within distance $\delta r$ of a fluid boundary, the boundary equation

$$D_{\text{bulk}} \frac{\partial \mathbf{M}}{\partial \mathbf{n}} + \left[ \begin{array}{ll} \rho_2 & \rho_2 \\ \rho_2 & \rho_1 \end{array} \right] \cdot \mathbf{M} = 0$$

(3.9)

governs the behavior of the relaxation, where the unit vector $\mathbf{n}$ describes the normal direction to the surface boundary $\Gamma$. Projected on the orbital plane $(\mathbf{x}', \mathbf{y}')$, Eq. (3.9) is solved for a locally flat boundary either on a square lattice (Mendelson, 1993) or for continuous random walks (Bergman et al., 1995), assuming that the spin has a probability of being instantaneously ‘killed’ when it reaches the boundary. Bergman et al. (1995) derived the analytical solution for the ‘killing’ probability as

$$p_{j,\{j=1,2\}} = \frac{2 \rho_j \delta r}{3 D_{\text{bulk}}} \times 0.96.$$  

(3.10)

In our model, each time the walker reaches a boundary it does not suddenly ‘die’; instead, the magnetization experiences a more physically consistent energy loss which translates in average as a decrease of factor $(1 - p_j)$ over the duration $\delta t$. Since $p_{1,2} \ll 1$, this additional surface decay is equal to $\exp[-\delta t / (p_j / \delta t)]$, and the total relaxation rates $1/T_{j,\{j=1,2\}}$ are for this step equal to $1/T_{jb} + \delta t / p_j$, or equivalently, using Eq. (3.3):

$$\frac{1}{T_j} = \frac{1}{T_{jb}} + \frac{\delta r}{3.84 \rho_j}.$$  

(3.11)
3.3.3 Transfer Probability of Permeable Membranes

The case of permeable barriers between pore volumes can be approached in a similar fashion. The boundary exchange rate \( k_j \) is defined as the proportionality factor between diffusion flux and concentration difference across a boundary \( j \). If bulk and surface relaxations can be neglected, then the macroscopic equation for the magnetization \( M \) within one compartment bounded by permeable membranes (Stanisz et al., 1997; Zientara and Freed, 1980) is given by

\[
\frac{\partial M}{\partial t} = D_{\text{bulk}} \nabla^2 M + \gamma B \times M - \sum_{\text{outwards}} k_j M + \sum_{\text{inwards}} k_j M^{(j)}, \quad (3.12)
\]

where \( M^{(j)} \) is the magnetization within a neighboring compartment \( j \). The sum over outward boundaries acts as a surface sink term whereas the one over inward boundaries acts as a surface source term. Since the surface sink term in Eq. (3.12) acts as the relaxation decay terms in Eq. (3.1), one notices the similarity with an effective surface relaxation term for cases where only surface relaxation and no surface permeability is present:

\[
\frac{1}{T_2} \equiv \sum_{\text{outwards}} k_j. \quad (3.13)
\]

Furthermore, in the fast diffusion limit, the surface decay rate is \( 1/T_{2S} = \rho(S/V) \) (Bownstein and Tarr, 1979), while the boundary exchange rate is \( k_j = P_j(S/V) \), where \( P_j \) is the membrane permeability (Stanisz et al., 1997). It is then straightforward to consider the effect of boundary surface permeability in equivalent fashion to boundary surface relaxation. Surface permeability, however, is not a cause for energy loss, as is surface relaxation. We can therefore use Bergman’s solution from another viewpoint: when the walker comes within one step of distance \( \delta r \) from a permeable boundary \( k \), we define by symmetry with Eq. (3.10) a probability of transfer equal to
\[ g_k = \frac{2 P_k \delta r}{3 D_{\text{bulk}}} \times 0.96. \]  

(3.14)

If \( g_k \) is honored, then the walker crosses the boundary; if not, it bounces back into its original compartment while the clock time is incremented by \( \delta t \). It is remarkable that fluid/rock surface relaxation (Kenyon, 1997) and biological membrane permeability (Stanisz et al., 1997) exhibit the same range of values between 0.5 and 30 \( \mu \text{m/s} \). This suggests that the parallel treatment of either relaxing or permeable boundaries remains valid on the same range of fluids and pore sizes.

### 3.3.4 Discussion

Diffusion random-walks have been used for decades to simulate NMR measurements. Finite differences or finite element methods require many grid blocks, hence large amounts of memory and computation time, to accurately reproduce the geometrical details of microporous media. Diffusion random-walks, on the other hand, readily lend themselves to distributed computer environments thereby considerably reducing computation times.

Previous diffusion/NMR algorithms focused exclusively on some relaxation processes, such that, independently, these formulations seemed incompatible one with another. Most models including the effects of diffusion within inhomogeneous background magnetic fields discard surface effects and used an approximate solution of Bloch’s equations in the \((\hat{x}',\hat{y}')\) rotating frame only, by defining a complex magnetization \( M' = M_x + i M_y \) (Slichter, 1992), which discarded any effects of longitudinal relaxation. Likewise, RF pulses were not accurately described and only \((\pi)_{y}\) pulses could be modeled as a sign change in the phase of \( M' \) with the axis of \( \hat{y}' \) (Weiskoff et al., 1994), which made the method amenable to CPMG sequences.
exclusively. The NMR signal was then considered equal to the sum of the cosine of the spin phase shifts, as mentioned in section 3.2.3, where the phase shifts were equal to the rotation angles $\phi = \gamma B \delta t$ (Weiskoff et al., 1994; Gudbjartsson and Patz, 1995), which matches the rotation described in Eq. (C.1) of Appendix C. As we show in the next section, these calculations performed in the rotating frame give results similar to those obtained in the full rotating frame for CPMG sequences, however small differences can sometimes appear and bias detailed interpretation of these data. Other random-walk models discarded magnetic field influences to concentrate on the analysis of surface decay, through the spin ‘dying’ probabilities mentioned previously. Without notion of magnetization or rotating frame, the NMR signal decay was just deemed equal to the count of ‘surviving’ spins with time. In our approach, all processes are incorporated on equal footing.

3.4 VALIDATION OF THE SIMULATION ALGORITHM

We proceed to validate the pore-scale simulation algorithm for cases where macroscopic analytical results exist, and where traditional spin calculations in the $(\hat{x}', \hat{y}')$ rotating plane do not accurately reproduce NMR signals.

3.4.1 Magnetization of Bulk Fluid

Dispersion of magnetic field strength – and therefore of Larmor frequencies – throughout the volume enhances the precession decay and the formation of echoes due to the $\pi$ RF pulses of a CPMG sequence. When these RF pulses are no longer instantaneous, i.e. when their duration increases, then the measurable echo amplitude decreases. Background field maps can be optimized to maximize the signal-to-noise
ratio. These points are illustrated in Fig. 3.4, where the formation of echoes in 1 cm$^3$ of water is simulated with our random-walk method through spin refocusing between two ($\pi$) RF pulses for different pulse widths and two permanent magnetic field maps. As the duration of the RF pulses increases, the quality of the echoes decreases through lower amplitudes and larger spread. In these tests, the field map shown in Fig. B.2 generates higher echo amplitudes, hence higher signal-to-noise ratios, than that of a homogeneous magnetic gradient. When the spread of Larmor frequencies decreases, e.g., by reducing the sampling volume (Fig. 3.5) or the magnitude of the magnetic gradient, the signal remains maximal. From now on, instead of considering the entire echo shapes of the $M_y$ magnetization signal, the results which follow only use the maximal value of $M_y$ for each echo. The total decay is obtained by considering the envelope formed by these echo peaks.

As shown in Fig. 3.4, even without relaxation decay, the magnitudes of the first few echoes are irregular for a CPMG pulse sequence. Hürlimann and Griffin (2000) quantified the behavior of the amplitudes of the first two echoes with spin dynamic calculations. We show in Fig. 3.6 that similar results can be obtained with our random-walk technique and strongly depend on the duration of the RF pulses. The difference between the results from Hürlimann and Griffin (2000) and our results stems from the fact that we assumed homogeneous magnetic fields in the $z$ direction (Eq. B.1) and that our simulation domain (Fig. B.2) is a subset of the domain used by Hürlimann and Griffin (Fig. B.1). In all cases, the amplitude of the first echo is lower than that of the second echo for $TE < 5$ ms, and becomes larger when $TE$ increases.

Finally, substantial contrasts of longitudinal and transversal relaxation times, i.e. $T_1B/T_2B > 1$, create variations of the apparent measured NMR decay rate, $T_2^{app}$. 

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Random-walk simulations were performed in the magnetic map of Fig. B.2 for two hypothetical bulk fluids with different values of $T_{2B}$ (2 and 4 s) and $T_{1B}$ (from 2 to 40 s). For each such combination, the total simulated decay $M$ was fitted with the mono-exponential model

$$M(t; T_{1B}, T_{2B}) = M_0 \exp\left(-t/T_{2\text{app}}\right) = M_0 \exp\left[-t\left(1/T_{2B} + 1/T_{2D}\right)\right]$$

(3.15)

and the value of $T_{2D}$ was determined knowing that $T_{2\text{app}} = T_{2B}$ when $T_{1B} = T_{2B}$. Results for the apparent decay time are plotted with respect to the $T_{1B}/T_{2B}$ contrast in Fig. 3.7 and remarkably agree with the magnet-dependent trend described in Hürlimann and Griffin (2000).

### 3.4.2 Decay in Inhomogeneous Background Magnetic Field

We then compared the decays generated by the presence of background magnetic gradients between (1) random-walk simulations with Bloch’s equations solved in the full rotating frame, noted formulation A, (2) similar simulations solved in the $(\hat{x}',\hat{y}')$ rotating plane only, noted formulation B, and (3) the analytical decay

$$\exp\left[-t\left(1/T_{2B} + 1/T_{2D}\right)\right],$$

where

$$\frac{1}{T_{2D}} = \frac{(\gamma G TE)^2 D}{12}$$

(3.16)

for a regular CPMG pulse sequence within a uniform background magnetic gradient $G$. Because the $M_y$ signal in formulation A is decreased by large sampling volumes and imperfections in magnetic fields distribution, all its simulated decays were normalized at the time origin. Decays simulated with formulation B needed no normalization. Results for two values of homogeneous gradients, $G = G_z = 12$ G/cm and 29 G/cm, three echo times, $TE = 0.3$, 1, and 3 ms, and two sampling volumes, 1 mm$^3$ and 1 cm$^3$, are plotted in Fig. 3.8 and enlarged at early times in Fig. 3.9. Formulation B yields the
same decays regardless of the sample volume, which exactly match the analytical decays. The more accurate formulation A also perfectly fits the analytical results for the smaller sampling volume, but substantial discrepancy appears for the larger volume. This effect is solely due to the finite duration of the RF pulses and cannot be accounted for with formulation B. For most porous media with sub-millimeter pore size, however, bulk diffusion state at such length scales does not apply, and both formulations A and B yield similar results for CPMG-like sequences.

3.4.3 Surface Relaxation and Fast Diffusion Limit

As long as the diffusion-relaxation problem is controlled by diffusion, i.e., in the fast-diffusion limit \( \rho R/D_{bulk} < 1 \) (\( R \) being the pore radius), the surface decay times \( T_{1S} \) and \( T_{2S} \) are given approximately by Brownstein and Tarr (1979):

\[
\frac{1}{T_j} = \rho_j \frac{S}{V} \quad (j=1,2)
\]

We first test our algorithm in the classic context of an isolated spherical pore of radius \( R \), where \( S/V = 3/R \). Figure 3.10 shows the results of simulations performed with different sphere sizes from 0.4 \( \mu \)m to 4 mm and for different values of surface relaxivity. In all the cases, the simulation decays obtained with both formulations A and B perfectly match the analytical decays as long as \( \rho R/D_{bulk} < 1 \). This is due to the fact no \( \rho_1/\rho_2 \) contrast was enforced, as encountered in natural systems – for example, it is usually observed that \( \rho_2 = 1.5 \rho_1 \) in water-saturated rocks (Kenyon, 1997). If this contrast were to reach several units, however, a behavior similar to the one described in section 3.4.1 for \( T_{1B}/T_{2B} \) contrast can be expected, and differences in apparent decay times would appear between formulations A and B. The deviation from the analytical
expression, Eq. (3.17), is captured by our model precisely at $\rho R/D_{\text{bulk}} = 1$, when the fast-diffusion assumption is no longer verified, and especially at large values of $\rho$.

In what follows, we focus on modeling porous media with dense sphere pack geometries (Schwartz and Banavar, 1988). For this reason, we test the robustness of the previous conclusions in cubic-centered packs of overlapping spheres for which the surface-to-volume ratio $S/V$ can be computed numerically. We define the compaction coefficient $C$ as the ratio between the diameter of the spheres ($2R$) and the size of the period of the cubic-centered pack ($a$), as illustrated in Fig. 3.11. The spheres just touch when $C = 1$, overlap when $C > 1$, and have closed throats when $C$ reaches $\sqrt{2}$, or 1.414. The surface-to-volume ratio of a pore depends on its shape: $S/V = \frac{3}{R}$ for a sphere of radius $R$, $2/R$ for a cylinder of radius $R$, and $1/a$ for a cube of size $a$. In a similar fashion, we define a geometric factor $g$ so that the surface-to-volume ratio of the pore space existing between identical solid spheres of radius $R$ in a compacted cubic-centered arrangement is $S/V = g/R$. This geometric factor is numerically calculated as a function of $C$ and is plotted in Fig. 3.12. NMR decays were then simulated for different combinations of compactions and grain sizes, with an infinitesimal background magnetic gradient. In all the cases, results of formulations A and B exactly overlap. Figure 3.13 compares these simulation results to the analytical exponential decay in the fast diffusion limit:

$$\exp\left[-t\left(1/T_{2B} + \rho g/R\right)\right]$$

(3.18)

Excellent agreement exists between simulated and analytical decays regardless of the degree of grain compaction.
3.5 Simulation of Parametric Multidimensional NMR Maps for Saturated Porous Medium

The previous section demonstrated the ability of our approach to individually reproduce spin dynamics effects, bulk relaxations contrasts, diffusion in inhomogeneous gradients, and surface phenomena in porous media. We now integrate all these factors simultaneously to generate parametric multidimensional NMR maps with the purpose to characterize pore size, wettability, hydrocarbon typing and saturation in the context of oil exploration. The fluids of interest are brine, single- and multicomponent oil, gas, and water-based or oil-based drilling-mud filtrate which invaded into a freshly drilled porous rock formation. Because of the low $T_{1B}/T_{2B}$ contrasts between these fluids, and because the acquisition sequence usually is CPMG-like, it is computationally efficient to consider the traditional formulation B where spin phase shifts are calculated in the rotating plane regardless of longitudinal effects. We insist, however, that the resolution of Bloch’s equations in the full 3-dimensional rotating frame (formulation A) would be required for more exotic RF sequences.

3.5.1 Simulation of Multiple TE and TW Measurement Acquisitions

Multidimensional NMR techniques are based on the simultaneous inversion of suites of CPMG-like sequences with multiple echo times ($TE$) and/or multiple wait times ($TW$) which allow different degrees of spin repolarization between successive CPMG RF sequences. Such a pattern is simulated in Fig. 3.14, which also illustrates the impact of surface relaxation on the NMR $M_z$ build-up and $M_y$ decay.

It is customary to consider that the NMR decay obtained for a fluid after repolarization of duration $TW$ is equal to the decay at full polarization (i.e. starting from $M = M_0$, or $TW \rightarrow \infty$) weighted by $(1 - \exp(-TW/T_1))$. Figure 3.15 shows this
is appropriate for a simple-component fluid such as 7-cp oil with unimodal bulk relaxation time (200 ms at room temperature), but not for a 300-cp multicomponent heavy oil. For a known distribution of bulk relaxations of the multicomponent fluid (e.g., insert of Fig. 3.15), each walker stands for a molecule of one miscible component of that fluid, and is stochastically assigned a bulk relaxation time so that the distribution is respected over the entire population of random walkers. The walker is also assigned a diffusivity which relates to this relaxation time through existing correlations (Lo et al., 2002; Winkler et al., 2005).

3.5.2 Two-Dimensional NMR Maps of Gas/Water and Oil/Water Mixtures in Saturated Rocks

We now use this multi-TE, multi-TW random-walk algorithm to simulate the NMR response of two-phase immiscible fluid in disordered grain packs. The fluid phases are distributed at the pore level based on pore criteria (Toumelin et al., 2004) and drainage/imbibition principles supported by capillary pressure and electrical conductivity calculations (see Chapter 2 of this dissertation). Two examples of rock/fluid systems were simulated to illustrate the methodology in 20%-porosity disordered pack of overlapping spheres exhibiting uniform distribution of sizes, and with homogeneous gradient $G_z = 16$ G/cm.

The first example was simulated for a mixture of 30% water and 70% gas in arbitrary reservoir conditions, whose bulk properties are shown in Table 3.1. Wait times logarithmically varying from 1 ms to 10 s were applied during the simulations of CPMG decay with 0.2 ms echo time, and the corresponding magnetization decays were processed with a $T_1/T_2$ inversion algorithm (Sun and Dunn, 2005). The left panel of Fig. 3.16 shows the resulting intensity $T_1/T_2$ map. The water peak at $T_1 = T_2 = 100$ ms
is affected by surface decay. The small echo time and diffusivity of water make the effect of diffusion in the homogeneous magnetic gradient negligible. The gas peak, however, is affected by this diffusion effect since its diffusivity is very large, thus decreasing its apparent $T_2$ value. In this case, inversion of the $T_1$ dimension efficiently discriminates the signals from the two fluids. We also synthesized magnetization decays for multiple-TE diffusion sequences for $D/T_2$ inversion and mapping, by considering full polarization ($TW \rightarrow \infty$) and values of $TE$ equal to 0.2, 1, 3, 9 and 16 ms. Focusing on the same water/gas mixture saturating our porous rock model, we obtain the $D/T_2$ map shown in the right panel of Fig. 3.16. In this plot, as in subsequent $D/T_2$ maps, the diagonal line characterizes a $D/T_2$ correlation existing for bulk oleic phases in specific conditions of pressure and temperature (Lo et al., 2002). In this plot, water and gas are distinguishable on both the $D$ and $T_2$ dimensions.

Our second example consists of a mixture of 60% water and 40% 7-cp oil in ambient conditions (see Table 3.1) within the same rock model, and illustrates the simulation of wettability effects. The same diffusion sequences were implemented, and the simulation results were inverted into the $D/T_2$ maps presented in Fig. 3.17. The water-wet case (left panel) exhibits a water peak at the intersection of the bulk water diffusivity ($2.10^5$ m$^2$/ms) and the surface relaxation time previously observed in Fig. 3.16 (100 ms). The oil peak, however, can be recognized as such for lying along the $D/T_2$ hydrocarbon correlation line. The $(D, T_2)$ coordinates of that peak along that line allow assessment of oil viscosity and possibly water-wettability. When oil is considered as the wetting phase (right panel of Fig. 3.17), the spread of its $D/T_2$ peak increases along both the $D$ and $T_2$ dimensions, while the relaxation time of the water peak increases because relaxing water/rock surfaces have partially disappeared at the
pore scale and some of the water relaxes in bulk. The next chapter of this dissertation specifically uses the NMR random walk algorithm developed in this chapter to study the combined effects of fluid saturation and viscosity, saturation cycle, and rock wettability, on the quality of $D/T_2$ 2D NMR interpretation.

3.6 Summary and conclusions

By combining magnetic dipole dynamics and random walks, the algorithm described in this chapter consolidates existing NMR numerical simulation methods used in diverse areas of biology and engineering into a single formulation that incorporates both diffusion within inhomogeneous magnetic fields and surface effects, including magnetization relaxivity and membrane permeability. Other than the magnetic dipole approximation, our formulation is constrained by none of the assumptions required for analytical models concerning the statistical distribution of spin phase shifts, spin density, field homogeneity, or fast-diffusion limit. The simulation algorithm advanced in this chapter extends NMR simulation capabilities beyond single-phase periodic media, which are so far the only type of porous medium that can be described with analytical techniques.

We show that the solution of the complete set of Bloch’s equations is necessary to model the magnetic relaxation of molecules with substantial $T_1/T_2$ contrasts and to accurately reproduce echo amplitudes in strongly inhomogeneous magnetic fields and for arbitrary pulse sequences. The same formulation is necessary for the simulation of multicomponent fluids, such as heavy oils, where the distribution of longitudinal relaxation times prevents simple scaling of magnetization decay with wait time. However, when fluids exhibit low $T_1/T_2$ contrasts and when CPMG pulse acquisition
sequences are used, we verify that the classic formulation neglecting $T_1$ effects accurately reproduces surface magnetization decays of complex granular porous media within the fast-diffusion limit.

Suites of longitudinal and transversal magnetizations are generated for mixtures of water, oil and gas saturating the pore space of dense grain packs at different wait times and echo times. These synthetic magnetizations can be subsequently inverted into parametric multidimensional $T_1/T_2$ and $D/T_2$ NMR maps to characterize pore structure, wettability and fluid types, within the assumptions of the model used to distribute the fluid geometries in the pore space. This methodology provides new opportunities to study quantitative relationships between NMR measurements and properties of economic interest that cannot be directly measured in-situ (Kenyon, 1997). The accurate description of the magnetic-dipole equivalent also allows the simulation and optimization of new NMR pulse acquisition sequences for specific applications in porous media.

<table>
<thead>
<tr>
<th>Fluid</th>
<th>Hydrogen index</th>
<th>Bulk relaxation times: $T_1 \approx T_2$</th>
<th>Bulk diffusivity $D_{bulk}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water</td>
<td>1.0</td>
<td>3 s</td>
<td>$2.10^{-5}$ cm$^2$/s</td>
</tr>
<tr>
<td>Gas</td>
<td>0.3</td>
<td>4.5 s</td>
<td>$1.10^{-3}$ cm$^2$/s</td>
</tr>
<tr>
<td>7-cp oil</td>
<td>1.0</td>
<td>0.2 ms</td>
<td>$1.10^{-6}$ cm$^2$/s</td>
</tr>
</tbody>
</table>

Table 3.1: Bulk properties of the fluids used in the numerical simulation of NMR measurements of saturated rocks.
Figure 3.1: Graphical description of the effects of imperfect \((\pi/2)\) and \(\pi\) \(B_1\) pulses on magnetization according to Bloch-Torrey equation (3.1) in the rotating frame. For each case, the magnetization vector progressively evolves from the orange to the red positions. In the absence of relaxation decays, the tip of vector \(M\) continues to describe a radius of the same sphere.
Figure 3.2: Example of $T_1$ MRI pulse sequence synchronizing $B_1$ RF pulses and 3-dimensional pulsed background magnetic gradients. $G_x$, $G_y$, and $G_z$ are the projections of $\nabla B_0$ on the axes of the rotating frame (adapted from Sun et al., 2003).

Figure 3.3 Apparent signal decay during magnetic precession. The projection of $\mathbf{M}$ onto the $y'$ axis gives the amplitude of the signal detected by an NMR tool antenna for that equivalent magnetic dipole.
Figure 3.4: Normalized amplitude of the projections of the mean NMR magnetization simulated by 20,000 walkers in 1 cm$^3$ of water, for a 300-$\mu$s echo-time CPMG sequence, for different $B_0$ maps, and for different values of $t_{90}$ and $t_{180}$. Plain curves: $M_y$ projection (signal); dotted curves: $M_x$ projection (out-of-phase noise); dashed curves: $M_z$ projections. Top row: simulations performed with a homogeneous permanent gradient $dB_y/dz = 20$ G/cm. Bottom row: simulations performed with the field map described in Fig. B.2.
Figure 3.5: Normalized amplitude of the mean $M_z$ magnetization of 20,000 random walkers generating the first three CPMG pulse echoes ($TE = 300 \mu s$) for different volume sizes. Each series of markers represents a different sampling cube size: 10 mm (−), 6 mm (−−), 3 mm (●), 1 mm (○), 0.6 mm (+), 0.3 mm (○) and 0.1 mm (○). The size of the sampling volume affects both the spread and the maximum amplitude (when larger than 1 mm) of the echoes.
Figure 3.6: Amplitudes of the first (dash) and second (plain) CPMG echoes as a function of echo time for 1cm$^3$ of bulk water volume. Curves with square markers (magenta) and circle markers (blue) identify the mean $M_z$ signal simulated with 10,000 random walkers in the approximate background magnetic field map of Fig. B.2, for different $B_1$ pulse widths (square markers: $t_{90} = 10 \mu s$, $t_{180} = 15 \mu s$; circle markers: $t_{90} = 20 \mu s$, $t_{180} = 30 \mu s$). Calculations reported by Hürlimann and Griffin (2000) for the accurate field map of Fig. B.1 are plotted with open triangle markers (green).
Figure 3.7: Relationship between the ratio of apparent to bulk transversal relaxation times, $\frac{T_{2\text{B}}^{\text{app}}}{T_{2\text{B}}}$, and the ratio of bulk longitudinal to bulk transversal relaxation times, $\frac{T_{1\text{B}}}{T_{2\text{B}}}$, for the background magnetic field of Fig. B.2. Two fluids were simulated with the same diffusion coefficient, $D_{\text{bulk}} = 2.5 \, \mu \text{m}^2/\text{ms}$, but with different values for $T_{2\text{B}}$: 2 s for the circles and 4 s for the triangles. The dotted curve represents the best-fit representation of these data using Hürlimann and Griffin’s (2000) equation [33] with $\left\langle n_z^2 \right\rangle = 0.6$. 
Figure 3.8: NMR decay for CPMG pulse acquisition of bulk water in a homogeneous background magnetic gradient $G_z$ for different inter-echo times $TE$ and different resolutions of Bloch’s equations. Open square markers describe the analytical solution, Eq. (3.16); lines: simulation results for 1 mm$^3$ of water; dots: for 1 cm$^3$. Top curves (in red): results of formulation B with $TE = 0.3$ ms; middle curves (in magenta): with $TE = 1$ ms; bottom curves (in blue): with $TE = 3$ ms. For each group of curves, green lines and dots identify the result of the same simulations but performed with formulation A.

Figure 3.9: Enlargement of Fig. 3.8 at early times (within the black boxes drawn at the top left corners of Fig. 3.8 panels) exhibiting the oscillations of the first echoes for full rotating frame simulations (formulation A). Plotting conventions are the same as in Fig. 3.8.
Figure 3.10: Decay curves simulated for water ($D_{\text{bulk}} = 2.5 \, \mu m^2/\text{ms}$, $T_{2B} = 3 \, s$) in a single spherical pore. The pore radius $R$ varies logarithmically from 0.4 $\mu m$ (top panel) to 4 mm (bottom panel), while for each radius the surface relaxivity $\rho$ at the pore wall is equal to 4 $\mu m/s$ (blue, triangles), 20 $\mu m/s$ (green, circles) or 200 $\mu m/s$ (red, squares). Simulation results are plotted in plain curves, while the analytical decays for a sphere (where $1/T_2 = 1/T_{2B} + 3 \rho/R$) are plotted with markers. The radio $\rho R/D_{\text{bulk}}$ is computed within the panels for each combination of $R$ and $\rho$. 
Figure 3.11: Two-dimensional geometrical description of the compaction coefficient $C = 2R/a$ in a compacted cubic-centered sphere pack.

Figure 3.12: Relationship between the geometrical factor $g$ and the compaction coefficient $C$ for a compacted cubic-centered sphere pack.
Figure 3.13: Time decay curves simulated for cubic-centered sphere packs of different grain sizes and different compaction coefficients. In each panel, the simulated time decays (plain curves) are compared to the analytical unexponential time decays of Eq. (3.18) (dot markers). Panels on the same row share the same compaction coefficient, and those on the same column, share the same apparent surface-to-volume ratio. In each panel, the top curves correspond to $\rho = 2 \ \mu m/s$ surface relaxation, and the bottom curves correspond to $\rho = 20 \ \mu m/s$. 
Figure 3.14: Amplitude of the mean $M_z$ and $M_y$ magnetizations simulated for 1-second CPMG pulse acquisitions (1 ms echo time) taking place after different $TW$ wait times, for water in bulk and in a relaxing porous medium (pm) constituted by a grain pack (porosity 17\%, $\rho_1 = \rho_2 = 20 \mu m/s$, pore size 30 $\mu m$). After initial depolarization (for each spin packet $M_z = 0$ and $M_y$ is randomly distributed with zero mean), $M_z$ increases freely for a duration $TW$, which collectively creates a build-up given by $1 - \exp(-t/T_z)$. The CPMG RF pulse is then turned on, $M_z$ is tilted by the $\left(\pi/2\right)_y$ pulse into $M_y$ which becomes non-zero and then decays in the form $\exp(-t/T_z)$ following the refocusing $\left(\pi\right)_y$ pulses.
Figure 3.15: NMR magnetization decays of bulk fluids simulated for different wait times \((TW)\) (left panels), and same decays normalized in amplitude at time \(t = 0\) (right panels). The same legend applies to all panels. For simple fluids with unimodal distribution of bulk relaxation times (top panels), all curves overlap with the canonical form \((1 - \exp(-TW/T_{1b})) \times \exp(-t/T_{2B})\). For multicomponent hydrocarbons (bottom panels), such normalized curves do not overlap. The insert describes the distribution of bulk relaxation times for the 300-cp heavy oil measured in laboratory conditions, and is used as input to the simulation algorithm.
Figure 3.16: $T_1 / T_2$ (left) and $D / T_2$ (right) NMR maps simulated for a two-phase saturation of 70% gas and 30% water in a grain pack exhibiting 20% porosity and uniform grain sizes. The diagonal line in the left-hand panel represents the $T_1 = T_2$ line. The diagonal line in the right-hand panel represents the $D / T_2$ correlation characterizing hydrocarbons in the conditions assumed for the simulations (after Toumelin et al., 2004).
Figure 3.17: $D/T_2$ NMR maps simulated for two-phase saturation of 60% water and 40% 7-cp oil, in water-wet (left-hand panel) and oil-wet (right-hand panel) grain packs exhibiting 20% porosity and uniform grain sizes. The diagonal line in the right-hand panel represents the $D/T_2$ correlation characterizing hydrocarbons in the conditions assumed for the simulations (after Toumelin et al., 2004).
Chapter 4: Numerical Study of the Influence of Saturation History on Diffusion/Relaxation NMR Maps and NMR-Based Petrophysical Estimates

This chapter implements the geometrical rock/fluid framework developed in Chapter 2 together with the NMR random-walk algorithm introduced in Chapter 3 to quantify the influence of saturation history and wettability on NMR measurements. Specifically, we present simulation results for diffusion/relaxation NMR maps at various stages along the same saturation cycles simulated for electrical resistivity in Chapter 2. We use this approach to quantify the impact of saturation history and fluid type on NMR measurements for each of the considered saturation stages. We also study the accuracy of interpretation methods based on diffusion/relaxation NMR maps to assess petrophysical and fluid properties of complex pore-scale models.

4.1 INTRODUCTION

Wettability state and oil viscosity can play a significant role in the NMR response of saturated rocks. This property of NMR measurements has been discussed in recent papers (Freedman et al., 2003) for particular examples of rock systems. However, no systematic study has been published on the reliability and accuracy of NMR methods to assess fluid viscosity and wettability, including the case of mixed wettability. This chapter quantifies the sensitivity of two-dimensional (2D) relaxation/diffusion NMR techniques to petrophysical properties of complex pore-scale distributions of fluids and connectivities, including fluid viscosity and mixed wettability.
Given that measurements are often made on rock samples with uncertain petrophysical factors and hence uncertain corresponding measurement contributions, the work described in this chapter is based on numerical simulation of pore-scale systems. We introduce a general numerical model that includes (a) saturation history and wettability alteration, (b) immiscible fluid viscosities, and (c) rock structure complexity. The geometrical model for saturation history and wettability alteration was previously described in Chapter 2. The present chapter uses the same pore-scale configurations to simulate suites of NMR measurements, and from them the corresponding 2D NMR maps, along the same saturation cycles of successive drainage, imbibition, and wettability alteration. Random-walk simulations are performed within the water-saturated zones (wherein electrical conduction was considered in Chapter 2), but are now also performed within the oil-saturated zones of the pore space for a variety of oil grades. The objectives of this chapter are three-fold: (1) to quantify the importance of the fluid saturation history on the NMR response of saturated rocks; (2) to assess the accuracy of conventional NMR interpretation for fluid typing, wettability detection, and pore-size assessment; and (3) to verify the generality of the previous observations by considering generic rock models with two values of porosity, 20 and 7 p.u.

The first section of this chapter describes the elements of NMR petrophysical interpretation and their current limits of applicability. We then summarize the pore-scale modeling procedure, its assumptions, and limitations. The sections that follow describe simulation results obtained during drainage and imbibition cycles involving water wettability and mixed oil wettability with partial saturations of water and different hydrocarbon types.
4.2 MODEL AND LIMITS OF NMR PETROPHYSICAL INTERPRETATION

4.2.1 Analytical Approximations of NMR Decay and Relaxation Times

Conventional interpretation of NMR measurements performed on saturated rocks is based on the assumptions that (1) the fluid protons within a pore of given size relax independently from protons residing in other pores, and (2) only one fluid is present in each pore. The measured NMR temporal decay $M$ is then expressed as a multiexponential decay of the form

$$M(t) = \sum_{s,f} A_{s,f} \exp\left(-t/T_{2,s,f}\right),$$

where $t$ is time, $s$ is the index of a pore size encountered in the pore space, $f$ is the index of the saturating fluids, $A_{s,f}$ is the partial porosity associated with the pores of size $s$ filled with fluid $f$, and $T_{2,s,f}$ is the apparent transversal relaxation time associated with the same pores. If fluids exhibit substantial contrasts of hydrogen index, the partial porosities in Eq. (4.1) are weighted by their respective fluid hydrogen index values. Let us designate $T_{2B}^f$ as the intrinsic (or bulk) relaxation time of fluid $f$, $\rho_{r,f}$ the surface relaxivity at the interface between rock $r$ and fluid $f$ which dissipates energy depending on the rock/fluid pair, and $(S/V)_s$ the ratio of relaxing surface over volume of the pore of size $s$. $D_B^f$ is the bulk diffusivity of fluid $f$ and $D^f$ its effective diffusivity in the presence of a tortuous porous medium. For a standard CPMG radio-frequency pulsing sequence in the fast-diffusion limit (i.e. where $\rho_{r,f}/(V/S)_s < D_B^f$), the apparent transversal relaxation time is given by the harmonic average (Fukushima and Roeder, 1981):

$$\frac{1}{T_{2,s,f}} = \frac{1}{T_{2B}^f} + \rho_{r,f} \left(\frac{S}{V}\right)_s + \left(\frac{\gamma GT E}{12}\right)D^f.$$ (4.2)
In this equation, $\gamma$ is the proton gyromagnetic ratio, $G$ is an average magnitude of the background magnetic field gradient over the spatial zone of investigation, and $TE$ is the inter-echo time or the interval between two radio-frequency pulses.

### 4.2.2 Limits of the Relaxation Model

The model described above assumes that the protons relax within one pore independently from the surrounding pores. When the bulk and diffusion terms in Eq. (4.2)’s right-hand side are negligible compared to the surface term $\rho_{r,s} \left(S/V\right)_s$, $T_2^{s,f}$ is considered proportional to pore size $\left(V/S\right)_s$. Consequently, the $T_2$ spectrum obtained after one-dimensional (1D) Laplace inversion of Eq. (4.1) is assimilated to the rock’s pore-size distribution. However, this assimilation becomes invalid if the protons diffuse through several pores of strongly contrasting sizes before their NMR signal decays. In such cases, the protons’ NMR response becomes representative of the average size of the pores that are connected within the sample. Known as diffusion coupling, this phenomenon was quantified for the first time by Ramakrishnan et al. (1999) with models of micritized carbonate rocks, which exhibited a combination of (a) low surface relaxivity and (b) high pore-size contrast between intergranular and intragranular porosity regions.

Irreducible water saturation is usually quantified by integrating the area under the $T_2$ spectrum for relaxation times smaller than given $T_2$ cutoffs. Hydraulic permeability can also be estimated from either this irreducible water saturation or the $T_2$ spectrum itself (Kenyon, 1997). When diffusion coupling is present, however, the default $T_2$ cutoffs are inadequate to separate the contributions of irreducible, capillary-bound, and free water components. Substantial errors in the estimation of irreducible saturation and permeability ensue (Toumelin et al., 2003a). Pore-scale geometries
involved with multiphase saturations and mixed wettabilities also affect the predictive abilities of such a surface relaxation model. For instance, in an oil-wet configuration, the model considered by Eqs. (4.1) and (4.2) assumes that the entire pore surface is oil-wet and that water protons within those pores will not be affected by surface relaxation. As detailed in Chapter 2, it is now commonly understood that oil-wet pores remain water-wet in the least accessible pendular rings, thereby giving rise to mixed-oil-wet conditions. Consequently, when water invades oil-wet pores, this water does not systematically relax in bulk mode because it can also be affected by surface relaxation when diffusing across pendular rings. The corresponding NMR response will be markedly different from that predicted by Eqs. (4.1) and (4.2).

4.2.3 Restricted Diffusion

For the case of unbounded diffusion, \( D_f \) is equal to the fluid self-diffusivity \( D_{sf} \). In porous media and in the presence of other immiscible fluid phases, \( D_f \) decreases with time because fluid may be isolated into snapped-off blobs or emulsions, or because pore throats and other immiscible fluids present in the pores restrict free displacement (Latour et al., 1993; see also Fig. 2.2). The asymptotic value of \( D_f \) obtained after very long diffusion times (in the order of \( 10^6 \) ms for water, as illustrated in Fig. 2.2) can reach very low values, down to a small percentage of bulk diffusion for oil-wet cases. As detailed in Chapter 2, these low effective diffusivities originate high electrical resistivity indices. The duration of NMR experiments, however, does not usually exceed \( 10^3 \) ms. In this time frame, \( D_f \) is not expected to decrease by a factor larger than 2 or 3, whereupon the impact of restricted diffusion on water NMR decay remains small in saturated rocks. Light hydrocarbons, however, exhibit values of self-
diffusivity that are higher than that of water. As a consequence, the impact of restricted diffusion within the $10^3$ ms duration of NMR measurements can become substantial.

### 4.2.4 Two-Dimensional NMR

Measurement methods have been developed for improved fluid typing based on special acquisition sequences and 1D relaxation inversion techniques (Chen et al., 2000; Sun and Dunn, 2004). These fluid typing methods, however, remain limited in the presence of heavy oil and to separate light hydrocarbons from water in large pores. For general applications, however, the most promising techniques are based on two-dimensional (2D) diffusion/relaxation inversion of suites of NMR magnetization time decays acquired at different inter-echo times. By varying $TE$, variable emphasis is put on the third term (the diffusion term) of the right-hand side of Eq. (4.2). Proper knowledge of the value of $G$ and 2D Laplace inversion (Song, 2002; Hürlimann and Venkataramanan, 2002; Sun and Dunn, 2005) isolate the diffusion term from the remaining two terms (bulk and surface relaxations) of transverse relaxation times. When the fluids saturating the pore space exhibit low $T_2$ contrasts but high $D$ contrasts, this technique discriminates fluid signals while 1D NMR inversion does not. The main theoretical restriction of the method lies in the accuracy with which $G$ is known to properly quantify diffusion effects (Hürlimann and Venkataramanan, 2002). The present work shows that multiphase fluid saturations also influence the accuracy of $D/T_2$ map interpretation, because of pore-level fluid configurations and because 2D inversion has limited resolution to differentiate signals with close $(D, T_2)$ values.
4.3 NMR SIMULATION PROCEDURE

4.3.1 Summary of the NMR Random Walk Algorithm

Random walkers are displaced within each saturating fluid by infinitesimal steps of duration $\delta t$ and size $\delta r$ related through Einstein’s relation,

$$\delta r^2 = 6D_B \delta t . \tag{4.3}$$

Simultaneously, the NMR magnetization decays are numerically simulated using formulation B of Chapter 3. In this method, for each random-walk step, the magnetization amplitude $M$ of a walker is multiplied by $\exp(-\delta t / T_2)$, where $T_2$ is given by the relation (Section 3.2.2)

$$\frac{1}{T_2} = \frac{1}{T_{2, B}} + \varepsilon \frac{\delta r}{3.84 \rho} . \tag{4.4}$$

In Eq. (4.4), $\varepsilon$ is equal to 1 when the walker is located within one step of a relaxing surface of longitudinal relaxivity $\rho$, and 0 otherwise. The walker spin phase shift acquired during that step is given by

$$\delta \phi = \gamma B \delta t , \tag{4.5}$$

where $\gamma$ is the proton gyromagnetic ratio and $B$ is the value of the background magnetic field exerted by the NMR tool in the rotating frame at the location of the walker. If the walk clock meets a scheduled RF pulse, then the phase shift accumulated until then is reversed. If the clock meets a scheduled acquisition time $t$, then the recorded signal is equal to the mean of the projections $\left<M(t)\cos\left(\int_0^t \delta \phi\right)\right>$ over the entire population of walkers.

4.3.2 Simulation Guidelines

The purpose of the numerical simulations considered in this section is to study the interaction of wettability, oil grade, fluid saturation and saturation history on 2D
NMR responses. To this end, simulations are performed for different values of inter-echo time ($TE = 0.3, 1, 3, 9$ and $16$ ms) assuming the same homogeneous background magnetic field gradient ($G = 16$ G/cm), and for different saturated rock models, resulting in a series of magnetization decays such as the one shown in Fig. 4.1. Specifically, we use the same generic Finney packs (20 and 7 p.u.) as in Chapter 2, and choose two saturation stages about $S_w = 30\%$ and $60\%$ on each water-wet and oil-wet saturation cycle described in Section 2.3. The values of water/rock surface relaxivity (for the water-wet zones) and oil/rock surface relaxivity (for the oil-wet zones) are set equal to $30\, \mu$m/s and $10\, \mu$m/s, respectively, to be representative of sandstones (Kenyon, 1997). We neglect surface relaxivity at the oil/water interface. Four hydrocarbon types are considered: three representative oil grades at ambient conditions ($300$ cp, $7$ cp and $1$ cp) and one gas at downhole conditions.

For each value of $TE$ and each rock/fluid geometry, one set of NMR simulations produces the magnetization decays of all the water/hydrocarbon mixtures. Each of these simulation sets includes one group of random-walkers which diffuse throughout the water-filled pore space, and one group of walkers which diffuse throughout the hydrocarbon-filled pore space for each hydrocarbon type. The contribution of water is therefore identical for all water/hydrocarbon mixtures. The total magnetization decay output for each fluid mixture is an average of the water and hydrocarbon magnetizations, weighted by their respective fluid saturations. Each group of walkers characterizing one fluid is assigned the bulk relaxation and diffusivity of that fluid. Bulk properties are selected to remain consistent with published experimental results (Hirasaki et al., 2002; Lo et al., 2002) and are summarized in
Table 4.1. For ambient conditions, live crude oils are approximately characterized by the correlation
\[ \frac{D_B}{T_{2B}} = 5 \times 10^{-6} \text{ cm}^2/\text{s}^2. \]  
\[
(4.6)
\]

The 1-cp and the 7-cp oil grades are difficult to identify with 1D NMR inversion and interpretation procedures because their bulk relaxations are close to the relaxation time of water affected by surface decay. The 300-cp crude oil exhibits several components that relax at different rates and that describe the \( T_2 \) spectrum shown in Fig. 4.2. In terms of random walk simulation, each walker representing a heavy oil molecule is assigned a value of \( T_{2B} \) which statistically honors this distribution and a value of \( D_B \) in agreement with Eq. (4.6).

### 4.3.3 Inversion and Plotting Conventions

White noise is added to each simulated magnetization decay with amplitude equal to 2% of the first echo amplitude. Time decays obtained for different values of \( TE \) are then simultaneously processed with a \( D/T_2 \) 2D inversion algorithm. Inversion results are plotted as bilogarithmic intensity maps of diffusivity versus relaxation time. On these cross-plots, \( T_2 \) spectra are represented on the vertical axis (with values increasing upward) while the diffusion coefficient is displayed on the horizontal axis (with values increasing to the right). Each plot shows a diagonal reference line which is the fixed linear \( D/T_2 \) oil correlation described by Eq. (4.6). A vertical line at \( D = 2.10^{-5} \text{ cm}^2/\text{s} \) characterizes the response of water. Finally, cumulative distributions of \( T_2 \) and \( D \) are plotted on the right and on the top of the 2D maps. Because these cumulative \( T_2 \) spectra are deprived of diffusion information, they are identical to the \( T_2 \) spectra that would be obtained via 1D inversion of small-\( TE \) magnetization decays.
4.4 **WATER-WET 2D NMR RESPONSE IN THE 20 P.U. ROCK MODEL**

We first consider the water-wet cycles 1 (drainage) and 2 (imbibition) described in Sections 2.3.1 and 2.3.2. The first water saturation stage on cycle 1 is reached at $S_w = 55\%$. Drainage continues, and a second NMR “snapshot” is taken at $S_w = 31\%$. Drainage proceeds until $S_w = 13\%$, when imbibition starts. Then, $S_w$ increases, reaches 30\% again (third NMR simulation stage), and increases to 55\% (fourth stage).

4.4.1 **Water Response from the Simulation of Heavy Oil Saturations**

Figures 4.3 to 4.6 show the $D/T_2$ NMR maps resulting from the simulations described above. The 2D maps are shown clockwise following the saturation history of the model for each case of hydrocarbon grade. Results for partial saturations of heavy oil (Fig. 4.3) are considered in the first place because the distance in $(D, T_2)$ space between the oil signal and the water signal is large enough to avoid overlapping of the oil and water contributions.

During drainage (maps A and B of Fig. 4.3), the $D/T_2$ water peak remains centered at $D = 2.10^{-5}$ cm$^2$/s and $T_2 = 400$ ms, regardless of $S_w$. During imbibition, however, the $T_2$ value of the water response increases to 500 ms at $S_w = 30\%$ (map C) and 600 ms at $S_w = 55\%$ (map D). This change of relaxation time is due to a change of water-saturated pore size. During drainage, oil displaces water from the most accessible pores, generally correlated to be the largest pores. The size of the water-saturated pores is therefore small compared to the size of the oil-saturated pores. During imbibition, water first displaces oil from the most accessible pores. Thus, water occupies pores that are larger during imbibition than those it occupies during drainage. An increase of the total relaxation time of the water peak during imbibition ensues which is associated with a pore size increase factor of 1.5. It is expected that rocks less
homogeneous than the Finney pack would exhibit larger differences of NMR-based pore-size estimates between drainage and imbibition.

In map C, the heavy oil signal appears at very low values of $D$ and $T_2$, consistent with its bulk properties. In the other maps, however, the inversion of these low $T_2$ values occurs off the usual accuracy range of 2D NMR maps (Flaum et al., 2005) and the post-inversion results do not fit Eq. (4.6).

### 4.4.2 NMR Response in the Presence of Other Hydrocarbons

Figure 4.4 shows the $D/T_2$ NMR maps resulting from partial saturations of 7-cp medium oil grade. The behavior of the water peaks during water-wet saturation cycles described in this figure is similar to that described in the previous section for heavy-oil partial saturations. Although the oil peak remains remarkably immobile regardless of saturation history, the increase of water relaxation during imbibition gives rise to a second peak in the projected $T_2$ distribution of case D. Overall, this is the best situation to quantify fluid saturation and types of fluids.

Figure 4.5 shows the results obtained for partial saturation of 1-cp light oil. In all four cases, A to D, the oil peak is correctly centered on its bulk $D/T_2$ properties. In particular, both water and oil peaks are well defined and yield good quantitative fluid saturations and oil type at the high-$S_w$ stages A and D. However, in cases B and C, where $S_w$ is about twice smaller than in cases A and D, the proximity between the oil peak and the water peak biases the inversion of the water peak. If $S_w$ were assessed based only on the amplitude of the two $D/T_2$ peaks, $S_w$ would be underestimated to be 20% or less, instead of 30%. Thus, in the inversion, it is necessary to account for the fact that part of the water signal was inverted as oil signal because of the proximity between the two responses and because of the lack of resolution in the inversion.

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Partial saturations of gas at reservoir conditions are considered in Fig. 4.6. The $D$ range of the plots is shifted to values high enough to include the gas signal. The water peak along the $D = 2.10^{-5}$ cm$^2$/s line continues to exhibit the same behavior as previously observed with heavy oil because no overlap exists between water and gas contributions. After 2D inversion, the gas peak exhibits the correct diffusivity value ($10^{-3}$ cm$^2$/s) and a relaxation time that is close enough to its theoretical value (10 s instead of 4.5 s) to ensure gas recognition. Correct estimation of the fluid saturations from NMR requires knowledge of the gas hydrogen index.

4.5 MIXED-OIL-WET 2D NMR RESPONSE IN THE 20 P.U. ROCK MODEL

In a fashion similar to the water-wet (WW) cases, Figs. 4.7 through 4.9 show, in clockwise order, the 2D NMR maps simulated along the mixed-oil wet (MOW) saturation cycles. At the center of each figure, the corresponding resistivity-index curves obtained previously (Fig. 2.25a) illustrates the position of the NMR maps in the saturation history of the 20 p.u. Finney pack.

4.5.1 NMR Response with Partial Saturations of Heavy Oil

Figure 4.7 first shows the 2D NMR results of simulations performed with partial saturations of water and heavy oil. After wettability alteration several modes of water relaxation appear in map C that contrast with the unimodal water-wet responses described by maps A and B. A mode around $T_2 = 3$ s is always present corresponding to the response of water saturating the oil-wet regions of the pore space at any saturation stage. The $T_2$ value of the remaining mode varies according to the saturation cycle.
By assumption, water in the geometrical model only occupies pendular rings and the least accessible pores when oil-wet drainage starts at $S_w = 13\%$. During drainage, the invading water occupies the most accessible oil-wet pores and reconnects the isolated water-wet zones of the pore space. Consequently, the distributions of water relaxation times are progressively shifted toward higher $T_2$ values as $S_w$ increases. After an additional 20% saturation of water has re-invaded the mixed-oil-wet medium ($S_w = 33\%$), the water signal shown in map C exhibits a continuous distribution of relaxation times down to 200 ms. The low values of this distribution correspond to the relaxation time of water where it remains the wetting phase, while values between 600 ms and 2 s correspond to the relaxation time of water diffusing across the pendular rings and the bulk of the oil-wet pores. As water saturation increases, water protons become increasingly isolated in pendular rings and increasingly connected to oil-wet zones; therefore, the values of relaxation time increase towards bulk relaxation. The slight shading of map D ($S_w = 58\%$) in the vicinity of $D = 10^{-5}$ cm$^2$/s and $T_2 = 200$ ms suggests that small amounts of water protons relax because of surface effects within the tightest water-wet zones, where on average $T_2$ values are twice smaller than those of case C. The low value of $D$ for that peak (half of that of water) also suggests very restricted diffusion, as would occur if the signal originates from pendular rings completely surrounded by oil. Drainage continues up to $S_w = 83\%$, at which point all the pendular rings become reconnected to water-filled pores and no water relaxation time is smaller than 800 ms.

Imbibition then proceeds through growth of the oil wetting films. By creating new divisions within the connected water-filled pore space, this displacement process decreases the relaxation time of part of the saturating water as $S_w$ decreases. In case E
of Fig. 4.7 ($S_w = 58\%$), no snap-off has occurred yet (see Fig. 2.18). The water signal extends continuously from $T_2 = 800$ ms to 3 s as a result of primary drainage. As $S_w$ decreases further, oil films become thick enough to promote snap-offs that create boundaries between (a) water trapped in oil-wet regions and exhibiting bulk relaxation time, and (b) water still connected between the center of the oil-wet pores and the water-wet pendular rings. The marked bimodal water response shown in Map F ($S_w = 29\%$) suggests that the NMR response is sensitive to this snap-off effect.

The ensuing cycle of secondary drainage operates as a two-step process. First, it reinforces the low-relaxation components by connecting the invading water to the pendular rings. Such is the case in map G, where the 300-ms component already observed in map F increases in amplitude. The isolated water contained in snap-offs is then increasingly reconnected to the rest of the saturating water until little surface relaxation impacts the NMR response. This trend is suggested in map H, where the 300-ms water peak has shifted to a $T_2$ value of 1 s.

### 4.5.2 NMR Response with Partial Saturations of 7-cp Oil

In the presence of medium- and light-oil grades, the bulk NMR properties of oil are closer to those of water. This proximity causes a risk of inaccurate 2D inversions that was not present in the case of heavy-oil saturations. Figure 4.8 shows the NMR simulation results for partial saturations of 7 cp medium-oil grade following the same saturation history as in Fig. 4.7. Overall, water peaks exhibit the same behavior as with heavy oil. Oil peaks, however, evolve with saturation history starting from stage F (high value of oil saturation during film-thickening imbibition). From stages A to E of Fig. 4.8, oil peaks remain identically centered on the bulk properties $D = 10^{-6} \text{ cm}^2/\text{s}$ and $T_2 = 200$ ms. The oil-wettability assumption used in stages C to H implies that the
oil NMR signal relaxes faster than bulk oil due to oil/rock surface relaxation. However, because the bulk relaxation time is very low, this additional surface decay has no impact on the oil peak decay time as long as oil films remain thin, i.e., until stage E takes place.

At stage F, where oil films become several microns thick, oil wettability starts affecting the oil NMR response. Two phenomena are then combined: (1) Oil protons mostly experience bulk relaxation in the fully oil-saturated pores because oil viscosity prevents most of these protons from reaching the relaxing pore walls within the 1-s simulation window. The $D/T_2$ response of these protons remains on the crude-oil $D/T_2$ correlation line. (2) Oil protons also diffuse within the thick films and relax at the oil/rock interface. The $D/T_2$ response of these protons appears under the crude oil $D/T_2$ correlation line. At stage F, all the oil phase is continuous inside the pore space, and therefore the $D/T_2$ oil response exhibits continuity between bulk response and surface-affected response.

Once secondary drainage starts, the invading water segregates (a) pores that are fully oil-saturated from (b) pores that are partially saturated and where thick oil films have developed. In map G, the oil signal continues to extend between the bulk oil response and the surface-affected oil response. As shown in map H, these two modes become distinct as water invasion proceeds.

The intensity peak appearing in map G of Fig. 4.8 in the vicinity of $D = 7.10^{-6}$ cm$^2$/s and $T_2 = 300$ ms is also remarkable. A conventional way to assess the water saturation in this simulation case is to apply an oil/water cutoff in the diffusivity spectrum appearing on the top of panel G, and then integrate the surface below the spectrum for values of diffusivity above that cutoff. If such diffusion cutoff is applied
past the $7.10^{-6}$ cm$^2$/s peak, i.e., at diffusivities higher than $10^{-5}$ cm$^2$/s, the water saturation is underestimated to be 20% or less (instead of 31%). Conversely, if the cutoff is applied before the peak, i.e., at diffusivities lower than $3.10^{-6}$ cm$^2$/s, $S_w$ is overestimated to be 45% or more. This suggests that the $D = 7.10^{-6}$ cm$^2$/s peak results from the merging of (1) the signal of the oil protons affected by surface relaxation on the oil-wet surfaces and (2) the signal of the water protons affected by surface relaxation on the water-wet surfaces. This coalescence increases the difficulty of interpreting the NMR map and to quantify fluid saturations.

4.5.3 NMR Response with Partial Saturations of 1-cp Oil

Figure 4.9 shows 2D NMR simulation results where the hydrocarbon phase consists of 1-cp light oil. At this value of viscosity, most oil protons come into contact with the relaxing oil-wet pore walls, while the surface relaxation time is shorter than the bulk oil relaxation time. As a result, the oil peaks shift across the $D/T_2$ crude oil correlation line in most oil-wet cases.

The merging $D/T_2$ peaks occasionally noted with 7-cp oil saturation become frequent with 1-cp oil saturation and bias interpretation results in multiple ways. As remarked previously, in the water-wet case B, the water signal is already absorbed by the light-oil peak, which is the source of uncertainty for the assessment of $S_w$. The same uncertainty arises for the oil-wet case D of Fig. 4.9. By comparing this map against maps D of Figs. 4.7 and 4.8, it is clear that the oil peak centered at $D = 6.10^{-6}$ cm$^2$/s and $T_2 = 500$ ms includes the signal of the water protons that experienced surface decay. Again, disregarding the merging of the oil and water signals leads to errors in the assessment of $S_w$. Stage E of Fig. 4.9 also creates interpretation problems due to oil and water responses merging into a single peak at $T_2 = 800$ ms. Without an
independent measurement of oil saturation, it is impossible to detect the presence of oil solely from the 2D NMR map. Light-oil saturation cases F, G and H (in Fig. 4.9) also exhibit coalescence between (1) the oil response affected by surface relaxation within the thick oil films, and (2) the water response affected by surface relaxation in the water-wet areas of the pores. This behavior is similar to that of the medium-oil saturation cases G and H (in Fig. 4.8). Although it is not obvious from the color scale used in the 2D NMR map of case G, the cumulative diffusivity spectrum confirms that some of the water relaxes at its bulk relaxation rate. Finally, in case C, the water response that is supposed to span the relaxation time interval between 200 ms and 5 s (as shown in Fig. 4.7 with heavy oil) now only spans the interval between 1 and 3 s. Because oil viscosity is the only parameter that changed between Fig. 4.7 and 4.9, the change in the apparent water relaxation time is solely due to the change in oil viscosity.

4.5.4 Impact of Saturation History and Hydrocarbon Type on Water Relaxation Time

The abovementioned variations of $T_2$ values for the water peaks as a function of saturation history and hydrocarbon type have important consequences on the assessment of pore size. The same variations of $T_2$ affect the estimates of irreducible saturation and hydraulic permeability, both traditionally calculated from the $T_2$ distribution of the water affected by surface relaxation. Table 4.2 summarizes the variations of water relaxation time for both water-wet and oil-wet saturation cycles. MOW configuration C (cycle 4, $S_o = 33\%$) is the only case where the surface-affected water relaxation is bimodal. Other cases exhibit either only one value of water $T_2$, or two values one of which is bulk water relaxation. In the latter case, we only consider values of $T_2$ smaller than 3 s.
While saturation history alone influences these values of water relaxation time, interpretation problems also arise in the presence of medium- and light-oil grades. With these oil grades, errors in pore-size estimates can increase to 300% in oil-wet cases because the pore-level fluid configurations change with saturation history. Standard NMR permeability models in $T_2^2$ (Kenyon, 1997), will cause this error in pore-size to bias the calculation of hydraulic permeability by a factor of 4 to 16.

### 4.6 Simulation Results with 7%-Porosity Rock Model

In order to generalize the remarks made previously, we perform similar simulations in the same generic grain pack with 7% porosity. New saturation cycles are designed to yield 20% irreducible water saturation in this 7-p.u. rock model, as described in Section 2.4.4 of Chapter 2. The resistivity index curves for cycles 1, 4, and 5 are reproduced in the central panel of Figs. 4.10 through 4.12. Two-dimensional NMR maps are simulated for partial saturations of the same crude oils as in the previous sections of this chapter, at water saturations close to 30% and 60% along each MOW cycle. The critical water saturation for which the resistivity index suddenly increases during cycle 5 is now close to 60%, and no water saturation below $S_w = 55\%$ can be reached during oil-wet imbibition. Pore configuration F now refers to the endpoint of cycle 5, just a few saturation units below configuration E, to emphasize the effect of water snap-offs on the NMR response at almost constant water saturation.

#### 4.6.1 NMR Response with Partial Saturations of Heavy Oil

Comparison of the $D/T_2$ NMR maps from Figs. 4.7 and 4.10 (both for heavy oil partial saturations) exhibit only a few differences. First, the water response systematically exhibits relaxation times that are smaller in the 7 p.u. rock model than in
the 20 p.u. model. This difference in relaxation times remains consistent with the fact that grains in the 7 p.u. model are overgrown from those of the 20 p.u. model, and therefore the pores are smaller. Second, the $T_2$ distribution for the water signal changes with $S_w$ during oil-wet drainage. In fact, the closer $S_w$ is to its irreducible value, the less water relaxes in bulk mode. The irreducible saturation at which wettability alteration occurs is larger in the 7 p.u. rock model (at $S_w = 20\%$) than in the 20 p.u. model (at $S_w = 13\%$). Consequently, stage C is closer to irreducible water saturation in the 7 p.u. model than it is in the 20 p.u. model. This difference affects the way in which fluids are distributed at stage C. In the 7 p.u. model (map C, Fig. 4.10), most of the water remains in the segments of the pore space where water is the wetting surface, and therefore the corresponding NMR decay also remains centered at $T_2 = 400$ ms. By contrast, in the 20 p.u. model (map C, Fig. 4.7) a large part of the invading water fills oil-wet pores and therefore the corresponding $T_2$ value increases. We observe this $T_2$ increase upon sustained water invasion of the 7 p.u. model (stage D, Fig. 4.10), which confirms that the relaxation of the water peak is only affected by the amount of water that has invaded the pore space after wettability alteration.

For case E, at the onset of imbibition snap-offs, the smallest $T_2$ value of the water $T_2$ spectrum is smaller in the 7 p.u. model than it was in the 20 p.u. model (600 ms versus 300 ms, respectively), which is consistent with the difference of pore size between the two porosity models. At stage F of Fig. 4.10, half of the water saturation is isolated into snap-offs or into small clusters of water-filled pores. In these isolated water regions, proton diffusion is restricted enough to justify a 50%-reduction of $D$ for the 300-ms water peak.
4.6.2 NMR Response with Partial Saturations of 7-cp and 1-cp Oil Grades

The 2D NMR maps resulting from partial saturations of 7-cp medium oil grade at 7 p.u. are shown in Fig. 4.11, and exhibit almost no differences with those simulated for the case of 20 p.u.

Figure 4.12 shows the results obtained for partial saturations of 1-cp light oil grade at 7 p.u. These results are very similar to those obtained with the 20 p.u. rock model. The major differences between the NMR maps simulated for both porosities appear in case E. At this stage, the oil and water signals had completely merged at 20 p.u. while they now appear distinctly at 7 p.u. However, by considering the diffusivity spectra of maps D and E, we find that the correct values of $S_w$ cannot be obtained by applying cutoffs between the apparent oil peaks and water peaks ($S_w$ would read about 70% instead of 54% for map D and 59% for map E). Therefore, some coalescence between water and oil signals remains. Configuration F exhibits a merged oil/water peak similar to that of case C. As noted previously for map G of Fig. 4.9, it is very difficult to quantify fluid saturations solely on the basis of 2D NMR maps.

4.6.3 Impact of Saturation History and Hydrocarbon Type on Water Relaxation Time

Table 4.3 compares water relaxation times obtained during the saturation cycles of the 7 p.u. rock model for the three values of oil viscosity. We observe that the maximum bias due to saturation history occurs during oil-wet saturation cycles using light oil. Conclusions similar to those obtained at 20 p.u. apply to the 7 p.u. results.
4.7 SUMMARY AND CONCLUSIONS

In Chapter 2, electrical rock measurements supported the pore-level model geometry we introduced. In the present chapter, however, no experimental data were available to quantitatively corroborate or reject our results on the saturation-history dependence of NMR measurements. Despite this limitation, our observations emphasize possible reasons for inaccuracies in NMR petrophysical interpretation due to multiphase saturation effects, both in the laboratory and in the field.

Drainage and imbibition effects were incorporated in a quantitative NMR model to numerically assess the effect of wettability and saturation history on the NMR response of two-phase saturated rocks. This approach provided a new way to generate parametric 2D NMR maps based on $D/T_2$ NMR inversions. The saturated water-wet rock models were found to conform well to the standard macroscopic model of Eq. (4.1). Mixed-oil-wet rocks, however, exhibited pore-level distributions of both oil-wet pore walls and water-wet pore corners and pendular rings, which made Eq. (4.1) impractical and inaccurate. The following conclusions stem from the simulation exercises described in this chapter assuming a homogeneous tool gradient of 16 G/cm and a CPMG pulse sequence:

1. The presence of bulk water relaxation is expected in oil-wet rocks. However, when $S_w$ is close to irreducible water saturation, the water mostly fills the water-wet pore corners. As a result, no bulk water relaxation appeared and it became difficult to detect the oil-wet nature of the rock from the NMR signal.
2. Only light oil grades (< 1 cp) were affected by surface relaxation in the presence of oil wettability. The $D/T_2$ correlation line for crude oils must be
determined independently in order to correctly identify the shift of the oil peak as a wettability effect.

3. Surface relaxation affected oil grades heavier than a few cp during oil-wet imbibition, when the oil wetting films became as thick as several microns for film-thickening displacement mechanisms.

4. While saturation history alone already influences the relaxation time of water, the presence of medium- and light-oil grades in oil-wet rocks also biases the result of the water signal $D/T_2$ inversion. The simulation examples showed that pore sizes could be misestimated by a factor of 2 to 4, depending on fluid type, saturation history, and rock facies. If one uses the standard NMR permeability models where permeability is proportional to $T_2^2$, this pore-size uncertainty involves errors in permeability estimates in the order of 4 to 16.

5. Because of the interference between the NMR response of water and that of medium-grade (7-cp) oil, difficulties arose in mixed-oil-wet rocks to apply clear fluid cutoffs. As a result, the absence of clear cutoffs created uncertainties in fluid saturation of up to 20 saturation units.

6. The same problem as described in Conclusion 5 arose with partial saturations of light oil grades (1 cp) in mixed-oil-wet rocks. The oil NMR response overlaps at least partially with the water NMR response, which not only compromises the use of fluid saturation cutoffs, but also at times makes it impossible to detect the presence of light oil from 2D NMR inversion.

7. The similarity of the results obtained for both 20 and 7 p.u. generic rock models supports the generality of the above conclusions.
Thorough analysis of $D/T_2$ maps reveals a plethora of information on the pore/fluid geometry; paradoxically, this plethora of information makes their interpretation complex and sometimes ambiguous. It is therefore desirable to combine 2D NMR techniques with other independent measurements that are sensitive to wettability and fluid saturations.

The methodology presented in this chapter is applicable to the combined study of conductivity and NMR responses of carbonate rock models with complex morphology. This NMR model used an approximation of Bloch Equations that is appropriate to simulate the NMR response for CPMG excitation in the context of the oil industry. Other pulse sequences, including stimulated echoes, DDif (Song, 2000), or CPMG with multiple wait-times (Chen et al., 2000), can be modeled with more accurate NMR formulations (see Chapter 3). The simulation model presented in this chapter can also be used to design new sequences and inversion methods to approach the interpretation of ambiguous pore/fluid configurations.

<table>
<thead>
<tr>
<th>Fluid</th>
<th>Hydrogen index</th>
<th>Peak bulk relaxation time $T_{2B}$</th>
<th>Peak bulk diffusivity $D_B$</th>
<th>Distribution type</th>
</tr>
</thead>
<tbody>
<tr>
<td>Brine</td>
<td>1.0</td>
<td>3 s</td>
<td>$2.10^{-5}$ cm$^2$/s</td>
<td>Sharp peak</td>
</tr>
<tr>
<td>1-cp light oil</td>
<td>1.0</td>
<td>1 s</td>
<td>$5.10^{-6}$ cm$^2$/s</td>
<td>Sharp peak</td>
</tr>
<tr>
<td>7-cp medium oil</td>
<td>1.0</td>
<td>200 ms</td>
<td>$1.10^{-6}$ cm$^2$/s</td>
<td>Sharp peak</td>
</tr>
<tr>
<td>300-cp heavy oil</td>
<td>1.0</td>
<td>40 ms</td>
<td>$2.10^{-7}$ cm$^2$/s</td>
<td>Widely spread (Fig. 4.2)</td>
</tr>
<tr>
<td>Gas</td>
<td>0.3</td>
<td>4.5 s</td>
<td>$1.10^{-3}$ cm$^2$/s</td>
<td>Sharp peak</td>
</tr>
</tbody>
</table>

Table 4.1: Summary of bulk properties for the saturating fluid.
Table 4.2: Evolution of the $T_2$ value of the water peak affected by surface relaxation as a function of saturation history (20 p.u. model).

<table>
<thead>
<tr>
<th>Saturation cycle</th>
<th>Water saturation</th>
<th>Water $T_2$ in the presence of heavy oil</th>
<th>Water $T_2$ in the presence of 7-cp crude oil</th>
<th>Water $T_2$ in the presence of 1-cp crude oil</th>
<th>Water $T_2$ in the presence of gas</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cycle 1</td>
<td>55% 400 ms</td>
<td>400 ms</td>
<td>400 ms</td>
<td>400 ms</td>
<td>400 ms</td>
</tr>
<tr>
<td></td>
<td>31% 400 ms</td>
<td>400 ms</td>
<td>400 ms</td>
<td>400 ms</td>
<td>400 ms</td>
</tr>
<tr>
<td>Cycle 2</td>
<td>30% 500 ms</td>
<td>500 ms</td>
<td>500 ms</td>
<td>500 ms</td>
<td>500 ms</td>
</tr>
<tr>
<td></td>
<td>55% 600 ms</td>
<td>600 ms</td>
<td>600 ms</td>
<td>600 ms</td>
<td>600 ms</td>
</tr>
<tr>
<td>Cycle 4</td>
<td>33% 200 + 700 ms</td>
<td>200 ms + (1)</td>
<td>(2) + 1000 ms</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>58% 200 ms</td>
<td>200 ms</td>
<td></td>
<td>(2)</td>
<td></td>
</tr>
<tr>
<td>Cycle 5</td>
<td>58% 1000 ms</td>
<td>600 ms</td>
<td></td>
<td>(2)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>29% 300 ms</td>
<td>(1)</td>
<td>1000 ms</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cycle 6</td>
<td>31% 300 ms</td>
<td>300 ms</td>
<td></td>
<td>(3)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>62% 1000 ms</td>
<td>(1)</td>
<td></td>
<td>(2)</td>
<td></td>
</tr>
</tbody>
</table>

Notes: (1) Spread of $T_2$ distribution prevents proper quantification. (2) Coalescence of water peak with oil peak prevents identification of water signal. (3) Only bulk water signal appears.

Table 4.3: Evolution of the $T_2$ value of the water peak affected by surface relaxation as a function of saturation history (7 p.u. model).

<table>
<thead>
<tr>
<th>Saturation cycle</th>
<th>Water saturation</th>
<th>Water $T_2$ in the presence of heavy oil</th>
<th>Water $T_2$ in the presence of 7-cp crude oil</th>
<th>Water $T_2$ in the presence of 1-cp crude oil</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cycle 1</td>
<td>65% 300 ms</td>
<td>300 ms</td>
<td>300 ms</td>
<td>400 ms</td>
</tr>
<tr>
<td></td>
<td>32% 300 ms</td>
<td>300 ms</td>
<td>300 ms</td>
<td>400 ms</td>
</tr>
<tr>
<td>Cycle 4</td>
<td>29% 400 ms</td>
<td>400 ms</td>
<td>400 ms</td>
<td>1000 ms</td>
</tr>
<tr>
<td></td>
<td>54% 200 ms</td>
<td>300 ms</td>
<td>300 ms</td>
<td>800 ms</td>
</tr>
<tr>
<td>Cycle 5</td>
<td>59% 300 ms</td>
<td>600 ms</td>
<td>700 ms</td>
<td></td>
</tr>
<tr>
<td></td>
<td>55% 300 ms</td>
<td>300 ms</td>
<td></td>
<td>(1)</td>
</tr>
</tbody>
</table>

Note: (1) The merge of water peak with oil peak prevents identification of water signal.
Figure 4.1: Examples of magnetization time decays simulated in our rock model for different values of inter-echo times.

Figure 4.2: $T_2$ bulk relaxation spectrum measured at ambient conditions for the 300-cp heavy crude oil assumed in the simulations.
Figure 4.3: Parametric $D/T_2$ maps simulated with 300-cp heavy oil during the water-wet saturation cycles (20 p.u. rock model). (A) $S_w = 55\%$ during drainage; (B) $S_w = 31\%$ during drainage; (C) $S_w = 30\%$ during imbibition; (D) $S_w = 55\%$ during imbibition.
Figure 4.4: Same as in Fig. 4.3 but with 7-cp medium oil grade instead of heavy oil.
Figure 4.5: Same as in Fig. 4.3 but with 1-cp light oil grade instead of heavy oil.
Figure 4.6: Same as in Fig. 4.3 but with gas instead of heavy oil.
Figure 4.7: Parametric $D/T_2$ maps simulated with 300-cp heavy oil during MOW saturation cycles (20 p.u. rock model). Saturation history is described in the center panel in terms of resistivity index cycles and hystereses. (A) WW rock, $S_w = 55\%$ during drainage; (B) WW rock, $S_w = 31\%$ during drainage; (C) MOW rock after wettability alteration, $S_w = 33\%$ during drainage; (D) MOW wet rock, $S_w = 58\%$ during drainage; (E) MOW rock, $S_w = 58\%$ during imbibition; (F) MOW rock, $S_w = 29\%$ during imbibition; (G) MOW rock, $S_w = 31\%$ during secondary drainage; (H) MOW rock, $S_w = 62\%$ during secondary drainage.
Figure 4.8: Same as in Fig. 4.7 but with 7-cp medium oil grade instead of 300-cp heavy oil.
Figure 4.9: Same as in Fig. 4.7 but with 1-cp light oil grade instead of 300-cp heavy oil.
Figure 4.10: Parametric $D/T_2$ maps simulated with 300-cp heavy oil during MOW saturation cycles (7 p.u. rock model). Saturation history is described in the right panel in terms of resistivity index cycles. (A) WW rock, Sw=65% during drainage; (B) WW rock, Sw=32% during drainage; (C) MOW rock after wettability alteration, Sw=29% during drainage; (D) MOW wet rock, Sw=54% during drainage; (E) MOW rock, Sw=59% during imbibition (just at the onset of water snap-offs); (F) MOW rock, Sw=55% during imbibition (half of the water content is trapped as snap-offs).
Figure 4.11: Same as in Fig. 4.10, but with 7-cp medium oil grade instead of 300-cp heavy oil.
Figure 4.12: Same as in Fig. 4.10, but with 1-cp light oil grade instead of 300-cp heavy oil.
Chapter 5: Two-Dimensional Pore-Scale Simulation of Wide-Band Electromagnetic Dispersion in Saturated Rocks

This chapter introduces a new approach to quantify frequency dispersion of dielectric and electrical conductivity of saturated rocks in the kHz-GHz range. The approach is based on pore-scale two-dimensional numerical simulation of electromagnetic (EM) scattering for specific geometries, distributions, and connectivity of pores. We solve Maxwell’s equations assuming two-dimensional pore maps of brine and rock grain pixels. The discrepancy between the internal fields and internal currents calculated for a homogeneous scatterer and those calculated for a given pore map is minimized to yield the effective isotropic electrical conductivity and dielectric constant for the corresponding rock/fluid model. This minimization is performed independently for each frequency and is successfully implemented and validated for pore/grain models saturated with a single-phase fluid with variable conductivity.

We show that existing effective medium theories fail to predict dielectric dispersion due to pore connectivity. Moreover, we show that the accuracy of the well-established Complex Refractive Index Method in the GHz range is determined by the percolation efficiency of the rock under consideration. Pore connectivity information is available from modal contributions present in dielectric dispersion regardless of pore and grain shape distribution. Such modal contributions in dielectric dispersion have so far been neglected in the interpretation of wide-band EM measurements of saturated rocks. The simulation method introduced in this chapter provides a systematic method to assess the sensitivity of a multitude of pore-scale properties on the macroscopic wide-band dielectric dispersion of saturated rocks.
5.1 INTRODUCTION

5.1.1 Maxwell-Wagner Interfacial Polarization Process

The complex electrical impedance measured across a saturated rock is in some ways analogous to a parallel resistor/capacitor model. Geometrically normalized measurements of conductance and capacitance yield the effective conductivity $\sigma_{\text{eff}}$ and dielectric permittivity $\varepsilon_{\text{eff}}$ of the rock sample, both real quantities. Electrical conductivity quantifies dissipation of energy whereas dielectric permittivity quantifies energy storage. If the rock sample is regarded as a conductor of complex conductivity $\bar{\sigma}^*$ subject to monochromatic excitation of frequency $f$ and radian frequency $\omega = 2\pi f$, $\bar{\sigma}^*$ can be expressed in terms of the measured values of $\sigma_{\text{eff}}$ and $\varepsilon_{\text{eff}}$ with the expression

$$\bar{\sigma}^* = \sigma_{\text{eff}} - i\omega\varepsilon_{\text{eff}}, \quad (5.1)$$

where the $e^{-\text{int}t}$ time harmonic convention is adopted for the exciting electric field and $t$ is time. Similarly, if the rock sample is regarded as a capacitor of complex dielectric permittivity $\bar{\varepsilon}^*$ under the same conditions, $\bar{\varepsilon}^*$ is equal to

$$\bar{\varepsilon}^* = i\bar{\sigma} / \omega = \varepsilon_{\text{eff}} + i\sigma_{\text{eff}} / \omega. \quad (5.2)$$

The dielectric constant $\kappa$ of the medium is the ratio of effective dielectric permittivity to that of vacuum, $\varepsilon_0 = 8.854 \times 10^{-12}$ Farad/m. Conductivities and permittivities are nearly constant over the entire kHz-GHz frequency range for pure, charge-free isolating rock, bulk hydrocarbons, and bulk water. In the case of rock-fluid mixtures, electric charges accumulate at the interface between brine and rock (or oil). Within these charged surfaces, brine polarizes in the form of a macroscopic dipole, which can create frequency-dependent macroscopic polarization. At low values of frequency, macroscopic dipoles reach equilibrium before the incident field has notably changed,
hence no macroscopic polarization occurs. When frequency increases, the orientation of macroscopic dipoles cannot follow the applied field due to the viscosity of the fluid, thereby resulting in energy storage, increased dielectric permittivity, and reduced electrical conductivity. This behavior, summarized by Bona et al. (1998, 2001, 2002), is known as the Maxwell-Wagner phenomenon, and describes the complex effective permittivity of the composite medium as a function of frequency in a Debye-relaxation fashion:

\[
\tilde{\varepsilon}^*(\omega) = \tilde{\varepsilon}^*(\omega \rightarrow \infty) + \frac{\Delta \tilde{\varepsilon}^*}{1 + i\omega \tau} \tag{5.3}
\]

In this equation, \(\Delta \tilde{\varepsilon}^*\) is the difference between the asymptotic values of the composite permittivity at zero and at infinite frequencies, and \(\tau\) is the dielectric relaxation time of the equivalent dipole formed by the brine pores. The relaxation time \(\tau\) depends on both the shape factor and isotropic orientation of the pores, and the permittivities of rock and brine (Sillars, 1937). Variants of Eq. (5.1) exist with adjustable exponents introduced to match experimental data. Other models adapt Eq. (5.3) for distributions of pore geometries (Lysne, 1983) that include several inflection points in a single dielectric dispersion curve. These types of models correctly describe measured variations of the frequency-dispersion of permittivity with brine salinity.

5.1.2 Dielectric Mixing Laws and Other Polarization Models

Dielectric mixing laws based on effective medium theory and polarization averaging (Sihvola, 2002) also yield sigmoidal frequency dispersion curves. Starting from Maxwell-Garnett’s mixing formula, strictly valid for isolated inclusions, a family of models was developed to describe the behavior of dense composites, including Bruggeman’s, coherent potential, Looyenga’s, Sen-Scala-Cohen’s (Sen et al., 1981) and Mendelson-Cohen’s (1982) effective medium approximation (EMA). Symmetry
between the components is variably enforced in these models. In similar fashion to Maxwell-Wagner type models, effective-medium models account for (a) contrasts of electrical properties between the components and (b) eccentricities and anisotropic distributions of brine-filled zones (or, similarly, of grains and resistive oil blobs), regardless of pore or grain size. Sihvola (2002) also describes a family of power-law dielectric models where the effective complex permittivity of the mixture taken to some power, \( (\varepsilon^*)^{1/N} \), is equal to the volumetric average of \( (\varepsilon^*)^{1/N} \) of each component.

These models include the popular complex refractive index method (CRIM) with \( N = 2 \), but are not accurate for frequencies lower than 10-100 MHz.

Another model worth mentioning is the Stroud-Milton-De (SMD) model (Stroud et al., 1986), based on Bergman’s analytic model for a 2-component composite. In this approach, the effective complex permittivity of the mixture is described as a function of its porosity and DC conductivity, and fits laboratory measurements remarkable well for a variety of saturated rock samples at frequencies above 10 MHz. However, the same analytical model has not been validated below 10 MHz, has not been rigorously adapted to describe the behavior of multiphase fluid saturations, and does not account for clay electrical double-layers. The main geometrical assumption implicit in the SMD model is that the contact area between the grains that form the rock skeleton is small compared to the surface offered by the rock/fluid interface.

The analytical models summarized above shed much theoretical insight on the relaxation processes taking place in saturated rocks; unfortunately, they scarcely provide practical and quantitative petrophysical information beyond the scope of fitting or justifying measured trends. Their physical consistency is also sometimes
questionable (Sihvola, 2002), e.g., for neglecting the electromagnetic (EM) coupling between brine bodies within rocks, and for neglecting the electric/magnetic duality of Maxwell’s equations. In this chapter, we show that geometrical Maxwell-Wagner polarization can be accurately reproduced when solving Maxwell’s equations in detailed rock/fluid geometries at the pore scale. This approach circumvents some of the conceptual deficiencies of analytical methods implicit in conventional effective-medium theories of dielectric dispersion.

5.1.3 Objective and Methodology

Remote-sensing electromagnetics, as used for instance in borehole geophysics, explicitly solves Maxwell’s equations to propagate the response of dilute concentrations of electrical charge carriers (dilute ionic fluids included in large-scale porous media) subjected to a prescribed excitation. Our objective is (a) to adapt these numerical simulation methods at the pore scale and show their reliability to reproduce geometrical dielectric polarization due to specific pore geometries, and (b) to quantify the influence of pore/grain information on dielectric dispersion neglected by dielectric mixing laws. We specifically target our analysis to the range between 1 kHz and 1GHz, which corresponds to the frequency band of field measurements acquired with open-hole logging resistivity and induction (10-200 kHz), logging-while drilling propagation (2 MHz) and EM propagation (1 GHz) instruments.

We introduce a numerical framework consisting of two-dimensional (2D) digital pore maps that distribute sub-μm brine and rock/oil pixels of variable complex conductivities included in realistic pore and throat geometries. Frequency-dependent dispersions of upscaled effective conductivity, $\sigma_{\text{eff}}$, and dielectric constant, $\kappa_{\text{eff}}$, for these pore maps are estimated based on Maxwell’s equations and EM propagation
principles. The electric fields induced by a monochromatic EM excitation are calculated within the pore maps via Maxwell’s equations. These fields and the corresponding internal currents are subsequently compared to those that would be excited by the same incident plane wave in a homogeneous cylindrical scatterer of given conductivity and dielectric constant. The conductivity and dielectric constant of the homogeneous cylinder that minimize the misfit between the internal fields and electrical currents in the pore map and in the homogeneous medium become the best-fit effective properties of the pore map. We compare dielectric and conductivity dispersions calculated for a variety of grain/pore configurations against the predictions of Mendelson and Cohen’s (1982) EMA and quantify the effects of pore shape and connectivity.

Without loss of generality, the developments presented in this chapter assume macroscopic isotropy of the rock models when using an isotropic homogeneous cylinder to calculate the effective values of $\sigma_{\text{eff}}$ and $\kappa_{\text{eff}}$. Electrical anisotropy can be readily incorporated with analytical models of EM scattering due to a homogeneous and anisotropic cylinder to estimate the corresponding tensors of effective conductivity and dielectric permittivity.

5.2 EM SCATTERING AND INVERSION OF EFFECTIVE CONDUCTIVITY AND DIELECTRIC PERMITTIVITY

5.2.1 Scatterer Geometry

The geometrical configuration adopted for the pixel-based scatterer is compatible with an existing fast analytical solution of EM scattering due to a homogeneous dielectric and lossy cylinder on a wide frequency range (kHz-GHz).
Pekonen et al. (1999) apply similar principles to simulate the MHz-range response of 2D pixel-based purely dielectric mixtures bounded by a waveguide. These authors compute the effective dielectric constant of the medium from the reflection and transmission coefficients at the scatterer boundaries. The main disadvantage of the waveguide method is that it remains accurate only below 80 MHz (Pekonen et al., 1999), whereas our problem demands high numerical accuracy for frequencies as high as 1 GHz.

To circumvent the above limitation, we introduce a new estimation approach based on the cylindrical scatterer shown in Fig. 5.1. Without restriction on frequency, the medium is described as a disc populated with square pixels of contrasting conductivities and dielectric constants of grain and fluids representing the pore map. As summarized below, the frequency-domain solution of EM scattering from a homogeneous cylinder (in three dimensions) can be written as an expansion of cylindrical modes (Balanis, 1989). We consider transverse-magnetic (TM) excitation such that the vector components of the incident electric field are in the same plane defined by the cross-section of the 2D scatterer. This strategy ensures scattering results akin to general 3-dimensional (3D) scattering.

The presence of corners, vertices, and irregular shapes on the boundary of the disc-shaped scatterer can cause significant fringe effects on the internal electric field. To mitigate this problem, we choose a circular boundary to define the spatial extension of the pore map. In addition, a high-resolution pore map is necessary to attenuate boundary effects at low frequencies for the case of resistive pixels. As shown in Fig. 5.2, at the nm- to \( \mu \)m-scale resolution used in our models, pore maps with less than 400x400 pixels resolution entail substantial boundary fringing below 10 MHz for a
homogeneous distribution of resistive pixels and 1 S/m background water. These numerical artifacts bias the inversion of effective properties of the scattering medium. In what follows, we show that spatial discretizations of the scattering medium larger than 400x400 pixels enable reliable estimations of effective properties of a homogeneous disc in the entire kHz-GHz range.

5.2.2 Numerical Solution of Maxwell’s Equations on the Detailed Pore Map

We assume that the individual pixel conductivities as well as the conductivity of the lossy brine background are isotropic. Equation (5.1) defines the complex effective conductivity for each pixel. Similarly, the complex effective conductivity of the water background is given by

$$\bar{\sigma}_b^* = \sigma_b - i \omega \varepsilon_0 k_b,$$  \hspace{1cm} (5.4)

where $\sigma_b$ is the brine effective conductivity and $\kappa_b$ is its dielectric constant. If $\mu_0 = 1.257 \times 10^{-6}$ H/m is the vacuum magnetic permeability, the wave number $k_b$ of the background is defined as

$$k_b^2 = i \omega \mu_0 \bar{\sigma}_b^*.$$  \hspace{1cm} (5.5)

The pore map is regarded as a complex scatterer where each element interacts with an incident wave, and where the cross-coupled response (or cross-scattering) of all the elements gives rise to the overall EM response of the saturated rock. The Method of Moments (MoM) (Wang, 1991) follows this approach and takes into account the cross-interactions between scattering pixels. We selected this method to solve Maxwell’s equations in the detailed heterogeneous pore map for several reasons: (a) it is formulated in the same frequency domain as the fast analytical homogeneous solution used for effective property inversion; (b) it explicitly honors the scatterer boundaries and does not require implementing special boundary conditions such as those of finite-
difference and finite-elements methods; (c) it accurately and efficiently handles large contrasts in material electrical properties (as encountered at the water/grain interface); and (d) it allows large discretization grids in conjunction with Fast-Fourier transformation (FFT) and an iterative solver such as the Stabilized Bi-Conjugate Gradient (Sleijpen and Fokkema, 1993).

Appendix D describes the practical implementation and benchmarks of accuracy of the 2D FFT-MoM technique used to compute the electric fields within the pore map. All the calculations are performed in the \((x, z)\) 2D Cartesian coordinate frame described in Fig. 5.1. The algorithm numerically solves the general integral equation for the electric field \(\mathbf{E}\) at location \(\mathbf{r} = (x, z)\) given by

\[
\mathbf{E}(\mathbf{r}) = \mathbf{E}_b(\mathbf{r}) + \int_{V_{\text{scat}}} i \omega \mu_0 \mathbf{\tilde{G}}(\mathbf{r} - \mathbf{r}') \cdot \Delta \sigma^*(\mathbf{r}') \cdot \mathbf{E}(\mathbf{r}') \, dV, \tag{5.6}
\]

where \(\mathbf{E}_b\) is the background field normalized by the \(e^{-i\omega t}\) time-harmonic variation imposed by a TM incident plane wave that forms a counter-clockwise angle \(\phi\) with the \(x\) axis:

\[
\mathbf{E}_b(\mathbf{r}) = \begin{bmatrix} -e^{i k (-x \cos \phi + z \sin \phi)} \sin \phi \\ 0 \\ -e^{i k (-x \cos \phi + z \sin \phi)} \cos \phi \end{bmatrix}. \tag{5.7}
\]

The scatterer consists of rock and fluid pixels of effective complex conductivity \(\sigma^*\) occupying the volume \(V_{\text{scat}}\). We solve Eq. (5.6) as the Riemann sum of the scattering due to all the pixels forming \(V_{\text{scat}}\). For each pixel, \(\Delta \sigma^*\) is the electrical conductivity contrast tensor between the scatterer and the water background. The tensor \(\Delta \sigma^*\) is assumed isotropic at the pixel level and, following Eqs. (5.1) and (5.4), becomes the complex scalar \(\Delta \tilde{\sigma}^* = \tilde{\sigma}^* - \tilde{\sigma}_b^*\). Finally, in Eq. (5.6) \(\mathbf{\tilde{G}}(\mathbf{r}, \mathbf{r}')\) is the dyadic Green’s tensor for the electric field. This tensor quantifies the cross-interaction of two scatterers
located in the \((x, z)\) plane of the pore map at positions \(r\) and \(r'\), respectively, and is defined as the solution of the dyadic wave equation
\[
\nabla \times \nabla \times \bar{G}(r, r') - k_b^2 \bar{G}(r, r') = \bar{I} \delta(r - r'),
\]
i.e.,
\[
\bar{G}(r, r') = \left( I + \frac{1}{k_b^2} \nabla \nabla \right) g(r, r').
\]
In Eq. (5.9), \(g\) is the scalar Green’s function that satisfies of the wave equation with a point source excitation,
\[
\nabla^2 g(r, r') + k_b^2 g(r, r') = -\delta(r - r').
\]
In the process of discretizing Eq. (5.6), \(\bar{G}(r, r')\) is integrated on the rectangular area of each pixel of the pore map using the analytical expressions derived by Gao et al. (2005).

### 5.2.3 Inversion of Effective Conductivity and Dielectric Permittivity

From the viewpoint of EM propagation, we define the effective conductivity and dielectric constant of the composite pore map as the conductivity \(\sigma_h\) and dielectric constant \(\kappa_h\) of a homogeneous and isotropic scatterer reproduces as closely as possible the scattered field due to the pore map. These conditions include angle of incidence, frequency and amplitude of the exciting EM wave, and scatterer shape. Hence, the estimation of \(\sigma_h\) and \(\kappa_h\) is consistent with Maxwell’s equations and can be approached as a minimization problem.

From Eq. (5.6), it follows that the electrical field propagated to any location in space is a weighted function of the currents \(J\) inside the scatterer, i.e.,
\[
J = \Delta \sigma^{-1} E.
\]
Therefore, if one seeks to minimize the discrepancy between the electric fields scattered by the pore map and the fields scattered by a homogeneous scatterer
regardless of the position where the fields are evaluated, then the same minimization should hold for the internal currents $J$ within the scatterers.

If the pore map is considered as the scatterer, $\Delta \vec{\sigma} = \vec{\sigma}^* - \vec{\sigma}_b^*$ varies for each pixel. If the scatterer is homogeneous of real conductivity $\sigma_h$ and dielectric constant $\kappa_h$, then we define its complex conductivity as $\vec{\sigma}_h^* = \sigma_h - i\omega \varepsilon_0 \kappa_h$ and the conductivity contrast with respect to the background becomes $\Delta \vec{\sigma} = \vec{\sigma}_h^* - \vec{\sigma}_b^*$ for the entire scatterer. We minimize the discrepancy of internal currents $J$ over the entire scatterer by minimizing the cost function

$$\Psi = \left\| \vec{\sigma}^* - \vec{\sigma}_b^* \right\|_2 = \left\| \vec{\sigma}^* \vec{E} - \vec{\sigma}_h^* \vec{E}_h - \vec{\sigma}_b^* \left( \vec{E} - \vec{E}_h \right) \right\|_2,$$

where $\vec{E}$ is the total electric field at a given pixel of complex conductivity $\vec{\sigma}^*$, and $\vec{E}_h$ is the electric field analytically calculated for the homogeneous scatterer of complex conductivity $\vec{\sigma}_h^* = \sigma_h - i\omega \varepsilon_0 \kappa_h$. Because the pore map does not exceed 1 mm², this analytical value is identical across the entire disc and we calculate it close to the disc center. The $L_2$ norm adopted for the cost function $\Psi$ above enforces the quadratic misfit over the entire surface of the pore map. Therefore, the values of $\sigma_h$ and $\kappa_h$ for which $\Psi$ reaches its minimum correspond to the effective, upscaled electrical properties $\sigma_{\text{eff}}$ and $\kappa_{\text{eff}}$ of the pore map for this frequency and this angle of excitation.

It is desirable to choose a reference scattering geometry which allows fast computation of the internal electric field $\vec{E}_h$. The analytical mode expansion used to describe EM scattering from a homogeneous infinite cylinder offers this possibility. This is why earlier we adopted the disc shape to describe the EM scattering due to complex pore maps. Appendix E provides detailed calculations of $\vec{E}_h$ for the case of a homogenous and isotropic infinite cylinder (i.e., a disc extended in 3 dimensions along its axis) illuminated by an EM plane wave. A similar approach could be used to
estimate effective anisotropic electrical properties of the pore map using semi-analytical scattering models for homogeneous anisotropic cylinders (Monzon and Damaskos, 1986; Wu and Yasumoto, 1997) and derive an effective conductivity tensor and an effective permittivity tensor for the pore map. Appendix F describes the practical implementation of the minimization of Eq. (5.12) with a disc-shaped, homogeneous and isotropic 2D scatterer. In Appendix F we show that the choice of the cost function

$$
\Psi_3 = \|\hat{\sigma}^* E - \hat{\sigma}_b^* E_b\|_{L_2} + \|\hat{\sigma}_b^*\| \times \|E - E_b\|_{L_2}
$$

(5.13)

provides the widest range of accuracy, including rock conductivities as low as 1 mS/m.

We note that the approach described above for the estimation of $\sigma_{\text{eff}}$ and $\kappa_{\text{eff}}$ is performed frequency by frequency independently. As shown in the next sections, our estimation method does not require the explicit enforcement of the Kramers-Kronig relationships (Landau and Lifschitz, 1960) to obtain smooth dielectric dispersion curves.

5.3 COMPARISON WITH EFFECTIVE-MEDIUM APPROXIMATION

5.3.1 Effective Medium Approximation with Depolarization Factor $l$

We first validate our estimation approach by comparing inversion results against the predictions of Mendelson and Cohen’s (1982) EMA (subsequently adapted by Feng and Sen, 1985, to the case of multiphase fluid saturations). This analytical model assumes an incremental refinement of the rock/water mixture where infinitesimal amounts of rock are added to the rock/water mixture of a previous step, and where the new complex conductivity of the mixture is estimated by averaging the electric fields and the electric displacements throughout the entire volume. At each
step, the rock grains added to the mixture are oblong spheroids randomly oriented and
individually characterized by the same geometric depolarization factor, \( l \). The EMA
then yields a relationship between the porosity \( \phi \) of the saturated rock and the complex
dielectric constants of water, \( \varepsilon_w^* \), rock grains, \( \varepsilon_{\text{grain}}^* \), and mixture, \( \varepsilon^* \), (Mendelson and
Cohen, 1982; Sen, 1984; Kenyon, 1984) given by:

\[
\ln \phi = \frac{3l(1-l)}{1+3l} \ln \left( \frac{\varepsilon_w^*}{\varepsilon^*} \right) + \ln \left( \frac{\varepsilon_w^* - \varepsilon_{\text{grain}}^*}{\varepsilon_w^* - \varepsilon_{\text{grain}}^*} \right) \\
+ \frac{2(1-3l)^2}{(1+3l)(5-3l)} \times \ln \left( \frac{(5-3l)\varepsilon_w^* + (1+3l)\varepsilon_{\text{grain}}^*}{(5-3l)\varepsilon^* + (1+3l)\varepsilon_{\text{grain}}^*} \right).
\]

(5.14)

In 3 dimensions, a depolarization factor \( l \) is defined in each principal direction
of the ellipsoidal inclusions. For example, if \( a, b, \) and \( c \) are the semi-axes of the
ellipsoid in the principal directions \( x, y, \) and \( z, \) respectively, the depolarization factor
along the \( x \) direction is given by

\[
l_x = \frac{abc}{2} \int_0^\infty \frac{du}{(u+a)^2 \sqrt{(u+a^2)(u+b^2)(u+c^2)}}.
\]

(5.15)

The value of \( l \) to be used in Eq. (5.14) is the highest value among \( l_x, l_y, \) and \( l_z, \)
because it corresponds to the largest dimension opposing the incident waves, and it is
the one which affects the dielectric dispersion of the composite. Simple expressions for
\( l \) exist for the cases of oblate and prolate ellipsoidal inclusions (Landau and Lifshitz,
1960; Mendelson and Cohen, 1982). When these inclusions are spherical, \( l = 1/3; \)
increasing values of ellipsoid eccentricity cause the value of \( l \) to increases toward the
limiting value of 1.

In 2 dimensions, \( l \) is given by the expression (Sihvola, 2005)

\[
l = \frac{\sqrt{e}}{1+\sqrt{e}},
\]

(5.16)
where \( e \) is the eccentricity of an elliptic inclusion, i.e., the ratio of the lengths of the semi-axes of that ellipse. In the comparisons that follow, ellipses of water are randomly distributed in an insulating solid host with semi-axes equal to 4 pixels by 48 pixels, thereby involving a constant eccentricity \( e = 12 \) and a depolarization factor \( l = 0.776 \) for each inclusion. Figure 5.3 shows the resulting pore maps grouped as 4 cases with 8\% porosity (cases A to D) and 4 cases with 20\% porosity (cases E to H).

### 5.3.2 Low-Porosity Simulation Cases

We first consider the 8\%-porosity pore maps shown in Fig. 5.3. Each map includes a distribution of 401x401 pixels with a resolution of 1 \( \mu \text{m}^2/\text{pixel} \). In these simulations, inclusions of water have the properties \( \sigma_w = 1 \text{ S/m} \) and \( \kappa_w = 70 \). The insulating host is assigned two possible dielectric constants, \( \kappa_{\text{host}} = 2 \) and 10, which bound realistic values for rock (4.5 for quartz and 7.5 for calcite). All the simulations are performed for one angle of incidence and include two frequency samples per decade. Simulations are also performed at a rate of one frequency per decade with a second incident angle perpendicular to the first one, when \( \kappa_{\text{host}} = 2 \). These latter simulations exhibit possible anisotropy effects due to the geometry of the pore maps.

Figure 5.4 shows an example of internal currents distributed within pore map B for two cases of perpendicular plane-wave TM excitation at 100 MHz. The electrical parameters in this case are \( \sigma_w = 1 \text{ S/m} \), \( \kappa_w = 70 \), and \( \kappa_{\text{host}} = 2 \). At 100 MHz, the out-of-phase dielectric effects are more important than the in-phase conductivity effects. Consequently, the internal currents induced across the scatterer are normal to the incoming electric field, i.e., parallel with the incoming TM wave according to the nomenclature of Fig. 5.1. Varying the scale of the current amplitudes in Fig. 5.4 emphasizes two main phenomena. First, the distribution of low-current amplitudes
(middle panels) shows the directionality of the internal currents and describes how the currents bypass the ellipsoidal inclusions that block the passage of the incident waves. Second, the distribution of high-current amplitudes (right-hand panels of Fig. 5.4) show that electrical current becomes maximum in the brine inclusions that are normal to the incident waves (parallel to the incident electric fields), while the amplitude of currents decreases in the inclusions parallel to the incident wave.

The solution of Mendelson and Cohen’s (1982) EMA given by Eq. (5.14) is plotted in Fig. 5.5 with a depolarization factor of \( l = 0.82 \) for both values of \( \kappa_{\text{host}} \). These EMA dispersions fit very well an average of the simulation results for maps sharing the same value of \( \kappa_{\text{host}} \) on the entire frequency band. Two conclusions stem from this result: First, the scattering that appears between (a) the different pore map realizations and angles of incidence and (b) the corresponding EMA sigmoid suggest that analytical mixing rules capture an average trend for given porosities, material electrical properties, and \( l \) values. Second, the difference between this best-match value of \( l \) (0.82) and the theoretical one (0.776) is small, and is possibly due to the fact that some ellipses touch each other (Fig. 5.3) and form clusters with overall eccentricities larger than 12.

The anisotropy observed between the open and closed markers of Fig. 5.5 is emphasized in Fig. 5.6, where the intervals between electrical properties calculated for each angle of incidence are represented as grayscale surfaces. It is notable that the pore map which exhibits the largest anisotropy for dielectric constant (map B) is not the one which exhibits the largest anisotropy for conductivity (map A). Visual inspection of both pore maps in Fig. 5.3 does suggest some anisotropy effects for the case of map B (in a top left-bottom-right pattern), but not for the case of map A.
Next, we quantify the sensitivity of dielectric dispersion to brine conductivity with pore map A. Starting with the anisotropic results shown in Fig. 5.5 with \( \kappa_{\text{host}} = 2 \) and \( \sigma_w = 1 \) S/m, Fig. 5.7 shows simulation results for \( \sigma_w = 0.1 \) and 10 S/m. The corresponding EMA results (still with \( l = 0.82 \)) are plotted for each value of brine conductivity. Results confirm the robustness of our estimation algorithm.

Figure 5.8 shows the Argand plot constructed with the results described in Fig. 5.7. Given a sample impedance \( Z = R + iX \), where \( R \) is the resistance and \( X \) is the reactance, an Argand plot describes the evolution of -X with respect to \( R \) for increasing values of frequency. Normalization of \( Z \) by sample length and cross section, gives rise to the complex resistivity \( \rho^* = \rho' - i\rho'' \), where \( \rho' \) and \( \rho'' \) are the in-phase and out-of-phase resistivities, respectively. Previously, we only considered the rock sample as a parallel admittance between the conductivity \( \sigma_{\text{eff}} \) and the dielectric permittivity \( \varepsilon_{\text{eff}} = \varepsilon_0 \kappa_{\text{eff}} \). The normalized admittance resulting from this configuration is \( \tilde{\sigma}^* = \sigma_{\text{eff}} + i\omega \varepsilon_0 \kappa_{\text{eff}} \), which is also the reciprocal of \( \tilde{\rho}^* \). By equating \( \tilde{\sigma}^* \) to \( \tilde{\rho}^* \), one obtains

\[
\rho' = \frac{\sigma_{\text{eff}}}{\left(\sigma_{\text{eff}}^2 + (\omega \varepsilon_0 \kappa_{\text{eff}})^2\right)^{\frac{1}{2}}} \quad \text{and} \quad \rho'' = \frac{-\omega \varepsilon_0 \kappa_{\text{eff}}}{\left(\sigma_{\text{eff}}^2 + (\omega \varepsilon_0 \kappa_{\text{eff}})^2\right)^{\frac{1}{2}}},
\]

which are the quantities plotted in Fig. 5.8. For the three tested values of brine conductivity, the Argand plot obtained from our simulations agrees very well with the EMA results, and, furthermore, exhibits the characteristic convex curvature of saturated rocks (Lima and Sharma, 1992).

At 8% porosity, therefore, our numerical estimation procedure is in several ways justified by the EMA. The simulations indicate that the EMA describes the average behavior of water/rock mixtures, but does not account for the geometrical features that entail variations of \( \sigma_{\text{eff}} \) and \( \kappa_{\text{eff}} \) from one pore map to another.
5.3.3 High-Porosity Simulation Cases

We now consider the case of high-porosity pore maps E to H ($\phi = 20\%$) shown in Fig. 5.3. Figure 5.9 shows the dielectric constant and conductivity calculated for these pore maps with $\sigma_w = 1 \text{ S/m}$, $\kappa_w = 70$, and one angle of incidence. Estimated frequency dispersion curves still exhibit sigmoidal shapes and occasionally reach values of dielectric constant higher than any mixture constituent (for maps G and H at the lower frequencies). EMA results for $l = 0.82$ still agree well with the simulation results for $\sigma_{\text{eff}}$ in the frequency spectrum, but not for $\kappa_{\text{eff}}$ below 10 MHz. Between 10 kHz and 10 MHz, the value $l = 0.875$ better fits the simulated values of $\kappa_{\text{eff}}$. The same value of $l$, however, does not fit the conductivity data. Thus, we conclude that at 20% porosity it is not possible to reproduce the wide-band electrical dispersion of these 2D rock models with a single value of $l$ and the EMA theory. Such a discrepancy between EMA and numerical simulations is due to the heavy clustering and partial overlap of pore eccentricities within models E to H. Isolation of inclusions is a central assumption of mixing laws, which explains why the EMA does not perform well in the presence of such clusters. In spite of this problem, it is remarkable that the conductivity dispersions properly match the EMA results for the case of 20% porosity.

5.4 Study of Wide-Band Dispersion for Different Rock Geometries

We now construct pore maps that describe distributions of both water inclusions in a rock host and grain inclusions in a water host. The distributions include a variety of aspect ratios, pore geometries, and degrees of connectivity between the water zones. Figure 5.10 shows the constructed 2D rock models. In analogy with the previous section, pore maps exhibit porosity values of 8% (maps I to M) and 20%
In all cases, rock pixels are assigned quartz properties \((\kappa = 4.5)\) whereas water pixels are assigned arbitrary brine properties \((\kappa = 78 \text{ and } \sigma = 1 \text{ S/m})\).

### 5.4.1 Low-Porosity Cases

Pore maps I to K consider inclusions of water ellipses with different eccentricities (1, 4, and 16) in a rock host. Figure 5.11 shows the calculated frequency dispersion curves of effective dielectric constant and conductivity calculated for these pore maps. The curves shown in Fig. 5.11 closely follow the behavior previously noted in Section 5.3.2. Conductivity dispersion curves appear as smooth sigmoids, with conductivity values increasing with increasing values of water inclusion eccentricity. This behavior is consistent with the fact that high-eccentricity pores offer better conductive pathways to electrical conduction than low-eccentricity pores for the same value of porosity. In these cases, depending on the value of frequency, rock model K is 10 to 20 times more conductive than rock model I.

As predicted by effective-medium theories, dielectric dispersion curves for maps I to K also exhibit enhanced values of low-frequency dielectric constant for increasing values of eccentricity. This behavior is due to the fact that larger shape factors in opposition to the incident EM wave increase the capacitance of the water/rock mixture. As noted in Section 5.3.2, these dispersion curves do not individually describe a sigmoid shape: they exhibit several inflection points, or modes. In case K, for instance, two inflection points appear around 500 kHz and 50 MHz, spanning two frequency decades. Lysne’s (1983) model assumes that a distribution, rather than a single value of aspect ratios, is responsible for the distribution of modes in the frequency spectrum of the dielectric constant. For the case of 8% porosity, however, maps I, J and K exhibit very little clustering between water inclusions. This
behavior rules out pore clustering as the sole origin of such a wide distribution of modes in the dielectric spectrum. Instead, we speculate that dielectric spectra are also influenced by other phenomena not included in standard analyses, such as pore connectivity and percolation. The exact nature of the EM interactions (or coupling) between brine-filled pores varies for each realization of rock/water mixture.

By contrast, maps L and M of Fig. 5.10 regard the rock phase as grain inclusions within a water host. In map L, the grains are roughly isotropic and are organized into a tight and homogeneous arrangement. The water films coating each side of the rock grains simultaneously exhibit individually high eccentricities (in the order of 25, since their size is approximately 2 pixels thick and 50 pixels wide), and collectively good interconnections. The corresponding simulation results (Fig. 5.11) yield flat frequency dispersion curves for both conductivity and dielectric constant. This result suggests that the distribution between stored and dissipated energy through the rock model is identical regardless of frequency. The high value of mixture conductivity (more than 1/10th of the brine conductivity) reflects the very high degree of connectivity between brine zones across the pore map. It is remarkable that, even as a flat dispersion, the values obtained for the dielectric constant are higher than those obtained for the other 8%-porosity rock models. Such a result suggests that, even if the brine films are well connected, they store energy at frequencies as high as 1 GHz. The high connectivity between films prevents any additional build-up of capacitance for decreasing values of frequency.

In map M, rock grains exhibit substantial anisotropy. Because the brine phase is continuous across the pore map, the effective conductivity is relatively high (Fig. 5.11). Both rock models K and M entail similar ranges of effective dielectric constant.
at low and high values of frequency. Such a behavior is expected given the similarity
of eccentricities of the inclusions for the two pore maps (water for K, rock for M).
However, the transition between the two asymptotic values differs greatly in the two
cases. As seen previously, model K exhibits a wide distribution of modes while its
brine inclusions remain relatively well isolated. Model M, on the other hand, entails a
clear unimodal sigmoid with a single inflection point at 10 MHz, while the rock grains
it includes do not share a single form factor. This observation reinforces the statement
that multimodal dispersions of dielectric constant are not necessarily due to
distributions of inclusion shapes and, reciprocally, that distributions of inclusion
shapes are not necessarily responsible for multimodal dispersions of dielectric
constant. A key factor in understanding the behavior of frequency dispersion of the
dielectric constant seems to be pore arrangement and degree of connectivity. This
factor is often neglected in the interpretation of wide-band EM measurements.

5.4.2 High-Porosity Cases

Rock models N to P described in Fig. 5.10 also include elliptic brine inclusions
randomly oriented in a rock host with increasing form factors for the case of 20%
porosity. By contrast, models Q and R are constructed with grain ellipses randomly
distributed in a brine host. Concerning cases N to P, Fig. 5.12 shows that the amplitude
of both dielectric and conductive dispersion curves increases with increasing values of
eccentricity of the brine inclusions. Two important remarks can be made about the
behavior of these dispersion curves: First, the dielectric constant spectrum does not
exhibit more modes than for the case of 8% porosity, while grouping of pore bodies
into clusters becomes substantial. Second, the low-frequency asymptotic value of
conductivity remains very low (around 0.002 S/m) for models N and O while it
increases tenfold (above 0.01 S/m) for model P. This difference can be attributed to the different degree of percolation of the brine phase across the pore maps: percolation is reached in map P, but not in maps N and O.

Pore maps Q and R do not exhibit enough spatial resolution to accurately reproduce the geometry of zones where non-cemented elliptic grains are close one to another without overlapping (Fig. 5.13). Thus, rock models Q and R can be regarded as cemented packs of elliptic grains. Figure 5.12 shows that the corresponding EM dispersions exhibit minor differences between the two models: the EM effect of grain shape is negligible in such cemented rocks geometries. This behavior is remarkable given that differences of grain shape are visually noticeable between the two pore maps. The spectra of Fig. 5.12 also suggest that the dielectric behavior of models Q and R is intermediate between that of models N and O on the entire frequency band. The conductivity behavior of models Q and R is also intermediate between that of models N and O at high frequencies. At frequencies below 10 MHz, however, the behavior of electrical conductivity falls between that of models O and P. Based on these observations, we conclude that the quantitative interpretation of wide-band EM dispersion of complex conductor/insulator mixtures requires the use of both frequency dispersion curves.

5.4.3 CRIM Dielectric Constant in the GHz Range

The CRIM volumetric model is a well-established asymptotic mixing rule for the dielectric constant of saturated rocks in the GHz range. The volumetric mixing rule is given by

\[
\sqrt{\kappa_{\text{CRIM}}} = \sum_{\text{component } i} \phi_i \sqrt{\kappa_i},
\]  

(5.18)
where $\phi_i$ is the fractional volume assigned to phase $i$ in the mixture. Comparison of CRIM dielectric constants with the simulated values of $\kappa_{\text{eff}}$ in the GHz range in Figs. 5.4, 5.9, 5.11 and 5.12 shed insight to the conditions of validity of the CRIM. Given the properties of the constituents in each case, $\kappa_{\text{CRIM}}$ can be assessed for all the simulated cases. In Fig. 5.5, $\kappa_{\text{CRIM}} = 4$ for $\kappa_{\text{host}} = 2$, and 13 for $\kappa_{\text{host}} = 10$. In Fig. 5.9, $\kappa_{\text{CRIM}} = 8$ for $\kappa_{\text{host}} = 2$ and 18 for $\kappa_{\text{host}} = 10$. In Fig. 5.11, $\kappa_{\text{CRIM}} = 7$, and finally in Fig. 5.12 $\kappa_{\text{CRIM}} = 12$. These CRIM results agree well with all the simulated cases of Fig. 5.5, and with all those of Fig. 5.9. In Fig. 5.11, however, cases K and M’s results agree better with CRIM predictions than for other models. The same conclusion can be drawn for case P in Fig. 5.12. We note that the best agreements between CRIM and simulation results occur when water-filled pores exhibit large eccentricities and weak to moderate degrees of pore connectivity.

5.5 SUMMARY AND CONCLUSIONS

We introduced a new method to calculate wide-band dispersion curves of electrical conductivity and dielectric constant for explicit rock model geometries without the use of dielectric mixing laws. This method accurately describes the kHz-GHz EM polarization of arbitrary pore structures with conductivities above $10^{-3}$ to $10^{-2}$ S/m. We successfully validated the new method by comparing the statistical distribution of our estimation results against results predicted by effective medium theory. Our numerical approach lends itself to the quantitative analysis of the EM response of explicit complex pore/throat/fluids geometries. However, the accuracy of our method is limited by the resolution and precision of the discretization mesh used to describe relevant geometrical features of the saturated rock.
The following conclusions stem from the work reported in this chapter:

1. Eccentricities of inclusions within a rock mixture determine the amplitude of the dielectric constant and conductivity dispersions for the mixture. However, the exact behavior of the dielectric constant between its low-frequency (kHz) and high-frequency (GHz) asymptotes depends on additional information about the characteristics of the pore map. Our simulations indicate that the degree of connectivity between brine-filled pore bodies could have as much impact on the dielectric spectrum as their shape factors.

2. When pore bodies are connected across the rock model, the shape of the dielectric dispersion curve approaches that of a symmetrical sigmoid. Isolated pores involve distributions of modes in the dielectric dispersion curve regardless of shape factor distributions. Therefore, the shape of dielectric dispersion curves could be used to indirectly assess the presence of non-connected pore structures.

3. The effective medium approximation (EMA) introduced to describe dielectric dispersion of dense rock/brine aggregates only describes the average wide-band polarization of rocks of equal porosity and pore eccentricity. In general, the wide-band electrical behavior of each rock departs from an average sigmoid curve by a factor of 2 for relatively low values of pore eccentricity (12 in our simulations). More pronounced scattering effects can be expected for larger values of pore eccentricity.

4. In the presence of substantial cementation, grain shape information can be lost and, consequently, the presence of elongated grains in the rock fabric can have negligible impact on the rock’s dielectric dispersion curve. Wide-band
dielectric models must therefore incorporate both pore and grain geometries to make accurate predictions of effective dielectric dispersions. Standard geometrical mixing laws exclusively incorporate either pore or grain information that is insufficient to accurately predict dielectric dispersion.

5. Our 2D simulations suggest that the dielectric spectrum can generally not be predicted from low-frequency conductivity and porosity, as proposed by the SMD model (Stroud et al., 1986) for frequencies higher than 10 MHz.

6. For the 2D examples used in this work, the validity of the CRIM results at 1 GHz was associated with the presence of large eccentricities and moderate connectivity between the pore bodies. Errors of at least 30% in the prediction of rock dielectric constant with the CRIM are expected due to variations of pore connectivity.

In this chapter, we emphasized that 2D simulations of EM scattering are closely related to simulations of 3D EM scattering when the excitation is in the form of TM polarization. This is because TM polarization causes the induced electrical currents to cross boundaries of electrical conductivity. Such is not the case when the 2D scatterer is excited with transverse-electric plane waves. The assumption of 2D EM scattering allowed us to simulate frequency dispersion curves with relatively modest computer resources. Specifically, the FFT-MoM method allowed us to simulate frequency dispersion of 2D pore maps as large as 1 megapixel in a desktop workstation. By contrast, computer resources necessary to model frequency dispersion curves of 3D pore maps are not currently available on desktop computers. Remarkable 3D EM scattering phenomena not accessible with our 2D simulations include cross-
polarization effects due to directional patterns in the spatial distribution of pore inclusions.

Figure 5.1: Description of the model geometry: incident transverse-magnetic (TM) polarized plane wave illuminating the 2-D scattering medium at an angle $\phi$ with respect to the $x$ axis. $E$: incident electric field; $H$: incident magnetic field; $k$: wave (propagation) vector. $(\rho, \theta)$ are the polar coordinates of a point within the scatterer, with respect to the incident plane wave and the scatterer center, and $(E_{\rho}, E_{\theta})$ are the polar projections of the electrical field vector at that point.
Figure 5.2: Illustration of the impact of frequency and map resolution on the boundary fringing distorting the internal electric fields computed within a resistive homogeneous disc. All maps include 255x255 pixel resolution except for that of the bottom right panel (501x501 pixel resolution). Electric excitation is in the form of an incident TM wave illuminating the disc in a top-right, bottom-left direction.
Figure 5.3: Pore maps used to compare frequency dispersion predicted by effective-medium theory against the estimation procedure described in this chapter. The pore maps consist of 4x48 pixels water ellipses (black) embedded in rock host (gray). A-D: 8% porosity. E-H: 20% porosity.
Figure 5.4: Graphical description of internal current amplitudes within pore map B (Fig. 5.3) at 100 MHz for two perpendicular angles of incidence and at different scales. The arrows indicate the directions of plane-wave incidence.
Figure 5.5: Frequency dispersion of effective dielectric constant (top panel) and electrical conductivity (bottom panel) for pore maps A to D shown in Fig. 5.3. Open and black markers: results for $\kappa_{\text{host}} = 2$ for two perpendicular angles of incidence. Gray markers: results for $\kappa_{\text{host}} = 10$ for one angle of incidence. Solid curves: EMA results, Eq. (5.14), for a depolarization factor $l = 0.82$. 

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Figure 5.6: Anisotropic dispersions of effective dielectric constant (top panel) and electrical conductivity (bottom panel) for pore maps A to D (Fig. 5.3, for $\kappa_{host} = 2$). For each pore map, a grayscale surface represents the interval of effective properties calculated in Fig. 5.5 for the two angles of incidence.
Figure 5.7: Frequency dispersions of effective dielectric constant (top panel) and electrical conductivity (bottom panel) for pore map A (Fig. 5.3, $\kappa_{\text{host}} = 2$) for three magnitudes of water conductivity. Markers: simulation results (starting with the ones previously plotted in Fig. 5.5 for $\sigma_w = 1$ S/m). Plain curves: EMA results.
Figure 5.8: Argand plot of the simulation results described in Fig. 5.7 (markers) together with the corresponding EMA results (plain curves). The insert enlarges the scale of the main plot for values of $\rho'$ smaller than 700 $\Omega$.m.
Figure 5.9: Frequency dispersion of effective dielectric constant (top panel) and electrical conductivity (bottom panel) for pore maps E to H shown in Fig. 5.3. Simulation results for $\kappa_{\text{host}} = 2$ are identified with open markers and for $\kappa_{\text{host}} = 10$ with gray markers, all for one angle of incidence. EMA results are identified with plain curves for $l = 0.82$ and with dashed curves for $l = 0.875$. 

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Figure 5.10: Pore maps used for the analysis of dielectric dispersion curves. Black pixels represent water; gray pixels represent rock matrix. Maps I to K: 8% porosity. Maps N to R: 20% porosity.
Figure 5.11: Frequency dispersions of effective dielectric constant (top panel) and electrical conductivity (bottom panel) for pore maps I to M shown in Fig. 5.10.
Figure 5.12: Frequency dispersion of effective dielectric constant (top panel) and electrical conductivity (bottom panel) for pore maps N to R shown in Fig. 5.10.
Figure 5.13: Illustration of the loss of geometric information due to finite-pixel resolution for two near-touching ellipses with an eccentricity of 10 represented with infinite (left) and finite (right) pixel resolution.
Chapter 6: Generalization of the wide-band EM Model for Multiphase-Saturated Rocks and Complementarity with NMR Measurements

This chapter generalizes the electromagnetic methodology introduced in the previous chapter to combine the interpretation of electrochemical effects and multiphase fluid saturations. The complementary nature of wide-band electromagnetics (WBEM) and NMR for general petrophysical characterization is illustrated with two specific applications. We first emphasize the WBEM characterization of microporous rock facies as the result of flat dielectric dispersion and numerical upscaling. Multiphase saturation and clay distribution are also included in the numerical WBEM model and exhibit characteristic trends of rock wettability. These two applications, morphology probing through frequency scanning and wettability recognition, constitute two key areas of complementarity between NMR and WBEM for improved petrophysical assessment of pore size distribution, hydraulic permeability, wettability, and fluid saturation.

6.1 INTRODUCTION

A number of experimental and theoretical studies suggest the sensitivity of WBEM to various petrophysical factors, including porosity, brine salinity, fluid saturation and wettability, clay content, surface roughness, and even pore surface-to-volume ratio. Given the complexity of the different phenomena under consideration, practical models are designed to fit measured dielectric dispersions to ad-hoc models whose parameters are marginally supported by quantitative petrophysical concepts.
The ability to extract quantitative petrophysical information from dielectric spectra remains a subject of research.

Therefore, to assess whether accurate and reliable petrophysical interpretations are possible with WBEM measurements requires an analysis that (a) incorporates pore structure, pore connectivity, multiphase saturation and electrochemical effects, and (b) quantifies the contributions of each factor in the measured WBEM dispersions. However, extracting explicit petrophysical information directly from WBEM responses is a difficult task. Myers (1991), for instance, illustrated the non-uniqueness of WBEM measurements when a decrease of either water saturation, porosity, or brine salinity yielded similar responses. As showed earlier in Chapter 4, 2D NMR interpretation can eliminate these ambiguities in most cases if the rock wettability is known. Conversely, it seems that WBEM measurements could provide independent wettability assessment when 2D NMR measurements alone might not. Likewise, the interpretation of NMR measurements could be biased by unaccounted rock morphology, while WBEM measurements provide additional information on rock connectivity and overall morphology. It is therefore appropriate to introduce a general WBEM pore model for specific applications wherein WBEM interpretation would either benefit from robust NMR interpretation, or provide independent support when NMR interpretation is ambiguous. The objective of this chapter is twofold: (a) to introduce an integrated methodology to predict WBEM dispersions of saturated rocks, and (b) to establish two specific domains of application for WBEM techniques to yield petrophysical information unavailable from other in-situ measurements.

We first discuss the low-frequency electrical behavior of saturated rocks which do not strictly honor the Maxwell-Wagner polarization studied in Chapter 5. Previous
attempts to relate WBEM dispersions to specific petrophysical properties are reviewed to emphasize the need for a general quantitative model. Next, we generalize the framework described in Chapter 5 to include low-frequency phenomena and multiphase saturations at the pore scale. The complementary nature of WBEM and NMR measurements is then illustrated with two focal points. A first application targets the use of WBEM rock measurements to characterize the effects of rock morphologies. Specifically, the upscaling concepts mentioned in the conclusion section of Chapter 5 are applied to characterize the WBEM response of microporous carbonate rocks, where NMR fails to quantify pore-size distributions. The second application of WBEM-NMR integration deals with the characterization of wettability effects and multiphase saturations in sandstones. Chapter 4 emphasized the need of an independent technique to assess wettability for a more reliable and accurate petrophysical interpretation of 2D NMR maps; we show that WBEM measurements can contribute to solving this interpretation problem.

6.2 **WIDE-BAND ELECTROMAGNETIC MEASUREMENTS OF SATURATED ROCKS**

6.2.1 **Origins of Wide-Band Dispersion**

As summarized by Sen and Chew (1983), two main phenomena influence the dispersion of conductivity and dielectric permittivity in saturated rocks at frequencies in the kHz-GHz range. The first effect is due to the Maxwell-Wagner phenomenon in the MHz range, where various geometrical effects create the sigmoid-type dispersions of conductivity and dielectric constant discussed in Chapter 5. The Maxwell-Wagner effect arises in the presence of bimodal lossy and dielectric compounds where no surface electrical charges (zeta potentials) are present. Ions concentrate along the edges
of elongated pores and create local capacitors in the pore structure whose effective capacitance and conductivity depend on frequency. This behavior solely depends on structural aspect ratios regardless of size.

The second main electromagnetic phenomenon appearing in rocks consists of substantial enhancements of the dielectric constant as frequency decreases below the MHz range. In the early 1980s, when WBEM studies for petrophysical applications were in vogue, this low-frequency enhancement was regarded as measurement noise and spurious electrode polarization effects. Subsequent quantification of electrode polarization exhibited strong negative power laws of dielectric constant at kHz-range frequencies. This power-law effect has no connection with Maxwell-Wagner polarization and is due to the presence of static electric charges at the interface between rocks (in particularly clay minerals) and brine. Several models have been derived to quantify the latter effect, although none of them entirely captures the complexity of the phenomenon.

To understand the origin of low-frequency enhancement of the measured dielectric constant, let us recall fundamental postulates of electromagnetism: when an electric field $E$ of radian frequency $\omega$ illuminates a lossy material of conductivity $\sigma^*(\omega)$ and dielectric permittivity $\varepsilon^*(\omega)$, it generates a current density $J = \sigma^* E$ and an electric displacement field $D = \varepsilon^* E$ through that material. In general, both $\sigma^*$ and $\varepsilon^*$ are complex numbers and can be written in terms of their real and imaginary parts as $\sigma^* = \sigma' - i\sigma''$ and $\varepsilon^* = \varepsilon' + i\varepsilon''$, where $i^2 = -1$ (the minus sign in $\sigma^*$ is consistent with the expressions that follow). As in the case of any causal physical mechanism, $\varepsilon'$ and $\varepsilon''$ are coupled through the Kramers-Kronig relationship (Landau and Lifschitz, 1960):
\[ \varepsilon'(\omega) = 1 + \frac{2}{\pi} \int_0^\infty \frac{\omega \varepsilon''(\omega)}{\omega^2 - \omega_0^2} d\omega_0. \]  

(6.1)

This relationship is generally used to verify the compatibility of experimental measurements with a complex expression of the dielectric constant (Milton et al., 1997). A similar relation holds between \( \sigma' \) and \(-\sigma''\). With the \( e^{-\text{lost}} \) convention for the time-harmonic electric field of radian frequency \( \omega \), the total density current \( \mathbf{J} \) generated through the material is given by

\[ \mathbf{J} = \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t} = (\sigma^* - i\omega\varepsilon^*) \mathbf{E} = \tilde{\sigma}^* \mathbf{E}, \]  

(6.2)

where \( \tilde{\sigma}^* \) is the total effective complex conductivity of the material. The above total current density can also be expressed in terms of the real effective conductivity \( \sigma_{\text{eff}} \) and permittivity \( \varepsilon_{\text{eff}} \) used in Chapter 5:

\[ \mathbf{J} = \left( \sigma_{\text{eff}} - i\omega\varepsilon_{\text{eff}} \right) \mathbf{E}, \]  

(6.3)

so that

\[ \sigma_{\text{eff}} = \text{Re}\left( \sigma^* - i\omega\varepsilon^* \right) = \sigma' + \omega\varepsilon'', \]  

(6.4a)

\[ \varepsilon_{\text{eff}} = \text{Re}\left( \varepsilon^* + i\sigma^*/\omega \right) = \varepsilon' + \frac{\sigma''}{\omega}, \]  

(6.4b)

and the dielectric constant is \( \kappa_{\text{eff}} = \varepsilon_{\text{eff}} / \varepsilon_0 \). When static charges are negligible at the rock/brine interface, the current \( J \) and displacement \( D_E \) are in phase with \( E \), and both \( \sigma^* \) and \( \varepsilon^* \) remain real. However, if the surface of an obstacle to the propagation of \( E \) is electrically charged, then an ionic double layer develops at that interface. The current density \( J \) is constrained to follow the direction of this charged surface away from the direction of \( E \), depending on the size of the obstacle. Such a behavior is responsible for substantial out-of-phase conductivity, \( \sigma'' \), which from Eq. (6.4b) implies an enhancement of the measured dielectric constant at low frequencies.
6.2.2 Power-Laws, Double-Layers, and Fractal Geometries

If $\sigma''$ varies slightly at low values of frequency, a power-law of exponent (-1) is straightforwardly obtained from Eq. (6.4b) between dielectric constant and frequency. The power law becomes a linear relationship between $\kappa_{eff}$ and frequency on a bilogarithmic scale. This very intuitive approach may justify the systematic power-law behavior experimentally observed in clay-bearing rocks (Knight and Nur, 1987; Bona et al., 1998 – see Fig. 6.1), although to date there is no conclusive physical explanation that justifies it. Different models and approaches have been used to quantify such low-frequency behavior of the dielectric constant. All these models are considered as multiscale (or, in some extent, fractal) systems.

The basic element of such multiscale constructions is the electrochemical double layer (EDL) that develops outside a charged rock surface. Sodium cations in brine solution concentrate at the surface of negatively charged rocks to enforce electrical neutrality of the rock/fluid system. According to the Stern model, a fixed layer of charged cations ensues that is adsorbed to the rock surface. A second, diffusive layer of charges extends into the pore brine with a negative exponential profile of cation concentration. The ions in this EDL migrate under the excitation of time-varying electric field, and the EDL as a whole behaves in the form of a dipole with complex electrical properties that depend on frequency, ion mobility, pore brine salinity, surface charge, and surface geometry (Fixman, 1980; Lima and Sharma, 1992; Lesmes and Frye, 2001). Computation of the EDL potentials proceeds from the combined solution of the electrical and diffusion potentials with boundary conditions specific to the EDL (Lacey and White, 1981; Chew and Sen, 1982; Cao et al., 1994).
Thevanayagam (1987) proposed an approach that posits the fractal nature of the observed power-laws between $\kappa_{\text{eff}}$ and $\omega$. Such a model is intended to capture the effective electrical properties at each rock scale. Brine chemistry and electrical properties are assumed to vary at each scale (bound fluid, clay-bound double layer, free fluid). Starting from the smallest scale, effective electrical properties are computed at each scale from (a) the brine properties at that scale and (b) the effective properties of the next smaller scale through nested mixing-laws. Thevanayagam recognized the necessity of incorporating EDL effects at the smallest scale; however, he used arbitrary values of brine conductivity and dielectric constant at each scale. In essence, Thevanayagam’s (1987) approach complements Sen et al.’s (1981) self-similar models using stepwise iterations of compounds whose electrical properties vary from scale to scale, instead of infinitesimal dilution of compounds that remain self-similar at all scales.

Rather than using arbitrary values of brine conductivities at each fractal level, Lima and Sharma (1992) incorporated fundamental electrochemical double-layer calculations around spherical clay grains based on Fixman’s (1980) model to quantify the effective conductivity and dielectric constant for the clay zones. These values were then upscaled with Sen et al.’s (1981) self-similar, infinite-dilution mixing law by regarding brine as the host of the mixture, rock as spherical grain inclusions, and clay as either spherical pellets or as shells coating the rock grains. In Thevanayagam’s model, the latter approach constitutes a 2-step fractal process with a different mixing law. Lima and Sharma (1992), however, made no mention of power-law effects in their work. The EDL low-frequency dielectric enhancement takes the form of a sigmoid which converges at frequencies lower than 1 kHz and to high values of dielectric
constant, depending on the clay geometry and surface charge. It can be argued that, if the sigmoid extends along several decades of frequency and if it is truncated before reaching its low-frequency asymptote, then that dielectric constant trend behaves in similar fashion to a power law. This assumption is very plausible considering the measurements of Lesmes and Frye (2001). Their measurements of dielectric constant in saturated samples of Berea sandstone exhibit an increase of $\kappa_{\text{eff}}$ as $\omega$ decreases from 1 kHz to 0.1 Hz that exactly matches a power law of exponent (-1). Below 0.01 Hz, however, these measurements of $\kappa_{\text{eff}}$ do converge to static values. Such a behavior suggests that the observed power laws may be formed by truncated high-amplitude sigmoids which would converge out of the measurement range. In turn, this result supports the assumption of an EDL origin for the so-called dielectric low-frequency power law.

### 6.2.3 WBEM for Quantifying Petrophysical Properties

Previous studies examined the influence of specific petrophysical properties of interest on WBEM measurements, including clay presence, multiphase saturations, rock wettability, and pore size; however, such studies failed to quantify the influence of the same petrophysical properties on WBEM measurements. In this section, we summarize the most relevant previous studies and their limitations.

Because electrochemical and geometrical phenomena affect the dielectric response of saturated rocks, Myers (1991, 1996) considered the dispersion of dielectric constant measured in the 20 MHz – 200 MHz range as the sum of (1) a clay term, where clay cation exchange capacity appears, (2) a geometric term, and (3) a vuggular porosity term. For that frequency range, Myers (1991, 1996) showed that terms (1) and (2) are sufficient to fit the dielectric dispersion of sandstones saturated with two fluid
phases, while terms (2) and (3) are appropriate to fit the dielectric measurements of single-phase heterogeneous carbonates. The fitting parameters, however, are deprived of petrophysical meaning and are yet to be quantitatively related to rock morphology and macroscopic petrophysical properties, such as hydraulic permeability (Myers, 1996).

Bona et al. (1998) used a similar superposition concept to fit partial-saturation dielectric rock measurements under the form of (1) a power-law term added to (2) a Maxwell-Wagner sigmoid term, but on a broader 100 Hz – 100 MHz frequency range. As shown in Fig. 6.1, Bona et al. (1998)’s measurements of water-wet Berea samples clearly exhibit power-law behaviors below 1 MHz. By contrast, the measurements performed on samples treated to be oil-wet at similar water saturations reach sigmoid-like asymptotic behavior at values of dielectric constant much smaller than for the case of water-wet samples. Although Bona et al. (1998) did not advance quantitative methods to calculate fluid saturation, they did emphasize the fact that WBEM measurements performed in the kHz-MHz range could be used to characterize rock wettability in the laboratory with no need for the prohibitively long equilibrium times associated with standard Amott wettability tests.

The complex refractive index method (CRIM) discussed in Chapter 5 is known to quantify partial fluid saturations reasonably well in the GHz range; the uncertainties associated with this method are lower than those of low-frequency Archie-based conductivity calculations. However, CRIM and similar models do not account for heterogeneous carbonate pore structures and are inaccurate to quantify fluid saturations in these conditions (Myers, 1996). CRIM also serves as a starting point for Seleznev et al. (2005) to derive a mixing law that corrects for the same geometrical parameters and
that fits dielectric measurements in geometrically challenging carbonate rocks between 100 MHz and 1 GHz. Such ongoing efforts suggest that more quantitative morphologic details can be incorporated in the interpretation of WBEM measurements to improve the estimation of petrophysical properties.

Beyond their observation of power-law behaviors in the sub-MHz range, Knight and Nur (1987) also observed a correlation between measured dielectric constant and rock surface-to-volume ratio for partially saturated rocks in the range of 60 kHz – 4 MHz. However, their results lend themselves to ambiguous interpretation. The largest dispersions of dielectric constant (correlated with the highest surface-to-volume ratios) also happened to be measured in samples that exhibited ultra-low permeability (< 1 mD), low porosity (< 8%), and clay content. Furthermore, these measurements were made in deionized water, which displaces the frequency range of pore geometrical effects below 1 MHz. Eventually, the correlation measured by Knight and Nur (1987) between dielectric dispersion and rock surface-to-volume ratio has no clear physical origin and is inconclusive.

In his comprehensive review of wide-band electrical phenomena in rocks in the mHz-MHz range, Olhoeft (1985) cited oxidation-reduction reactions as a common phenomenon taking place at the brine/rock interface. When surface reactions take place in a diffusion-limited (by opposition to kinetics-limited) fashion, the electrical response of the compound generally depends on the size of metallic bodies in the mixture. In rocks, these bodies can consist of pores coated with metallic deposits, or of metallic inclusions embedded in the rock matrix. To illustrate this argument, Olhoeft noted that suspensions of 1-mm metallic particles exhibit a 10-Hz relaxation mode in their wide-band dielectric spectrum, while suspensions of 10-μm particles exhibit a 100-kHz
mode. An adaptation of double-layer models would provide similar results, although a macroscopic model that incorporates both kinetics- and diffusion-limited reactions in saturated rocks is yet to be proposed. The possibility of inferring pore size information from WBEM measurements becomes very attractive to validate NMR pore-size estimates.

Among the various directions of investigation possible, we choose to generalize the geometrical model of Chapter 5 to capture the combined effects of rock morphology, presence of clay, wettability, and fluid saturation at the pore scale.

6.3 **GENERALIZED 2D WBEM NUMERICAL FRAMEWORK**

6.3.1 **Pore/Fluid/Clay 2D Geometry**

The 2D geometrical model developed in Chapter 5 only incorporates interfacial WBEM effects arising from the accumulation of charges at the boundaries between brine and rock with no zeta potential. Most of the pore maps used in that chapter were synthesized to exhibit single-eccentricity pores, which is not a realistic rock representation. In this chapter, pore maps consider more complex rock/pore structures and are extracted from rock digital pictures at different rates of magnification. Figure 6.2 shows an example of a digitized picture of a 24%-porosity sample, which is converted into a disc-shape binary pore map. This new rock model exhibits explicit distributions of pores and throats larger than the pixel resolution of the rock image.

Clay-equivalent pixels are then arbitrary distributed throughout the pore map, as illustrated in Fig. 6.2 where clay pixels represent 3% of the rock volume. At each frequency, clay pixels are assigned effective electrical properties following Lima and Sharma’s (1992) treatment of an ionic double-layer around a spheroid clay grain (see
the next section). If the grains are larger than the pixel resolution, then several pixels form one clay-coated grain and each pixel is assigned the same electrical properties. On the other hand, if the grains are smaller than the pixel resolution, then one pixel represents a group of clay-coated grains that span a surface equal to that pixel. Thus, the pore-level numerical framework described previously upscales the response of the clay-bearing rock regardless of mixing laws.

Because TM polarization is used to excite the EM field and because the 2D pore map is assimilated to a cross section of 3D rock geometry, multiphase saturations can also be distributed in the pore map as they would appear on a 2D cross-section of a 3D saturated rock. Chapter 2 introduced 3D pore-to-pore drainage/imbibition heuristics to distribute fluid phases in the pore space. Here, 2D pixel-based fluid distributions are designed to resemble a cross-section through a rock where 3D drainage and imbibition take place. Figure 6.3 illustrates this concept and emphasizes the pixel-based structure of such a 2D model for a water-wet rock. In this model, a layer of 1 to 2 water pixels is preserved at the rock surface, while oil is assumed to invade the pore structure starting from the outside of the disc.

Wettability is a key element in our geometrical model. As shown in Fig. 6.1, large enhancements of the dielectric constant are measured at low frequencies in water-wet rocks with low values of water saturation. Both geometrical and electrochemical reasons could be invoked to explain this enhancement. Given the low value of water saturation present in the samples considered in Fig. 6.1 ($S_w = 20-22\%$), a substantial number of thin wetting films of brine develop in water-wet pores drained by oil. These films exhibit very high eccentricity, but they are also very well connected in the presence of uniform water-wettability throughout the rock. In Chapter 5, pore models
L and M (Fig. 5.9) exhibited similar high eccentricities and connectivities of brine bodies, with moderate dielectric enhancement at low frequencies (Fig. 5.10). Such a behavior suggests that the extremely high values of dielectric constant measured at low frequencies in water-wet rocks are not necessarily due to geometrical effects, but could be mostly due to the dual fractal/EDL phenomenon developed at clay surfaces in water-wet conditions. In strongly oil-wet conditions, these EDLs are inhibited because no cations are in contact with the charged clay surface. The activation of EDLs in the magenta pixels of Fig. 6.3 characterizes the water wettability of the rock model depicted in Fig. 6.3. Section 6.5 will use these principles to construct water-wet (WW) and oil-wet (OW) multiphase pore models.

### 6.3.2 Quantitative Incorporation of Electrical Double Layers

Following de Lima and Sharma (1992), we adapt the effective values of conductivity and dielectric constant for the wet clay ionic double layers from Fixan’s (1980) model. In this method, clay particles are represented as spheres of radius $a$ and consist of a resistive core and a counter-ion surface charge density $\beta$ (in units of $1/m^2$). Ions in the double-layer of diffusivity $D$ displace around the insulating sphere and build up a stationary charge. The corresponding diffusion time $\tau$ is given by the ratio

$$\tau = \frac{a^2}{2D},$$

(6.5)

while the double-layer efficiency $\delta$ is defined by the dimensionless ratio

$$\delta = \frac{\beta}{aC},$$

(6.6)

where $C$ is the density of cations in the bulk water (in $1/m^3$). The complex conductivity associated with this double-layer $\tilde{\sigma}_{DL}$ can be written as a function of the pore water conductivity, $\tilde{\sigma}_w$, as follows:
\[ \sigma_{DL}^* = \frac{\delta \sigma_w^*}{1 - \delta Y}, \]  

(6.7)

where \( Y \) stands for the frequency-dependent build-up due to the time oscillation of charges around the insulating grain, and is given by

\[ Y = -\frac{1 + (1-i)\sqrt{\omega \tau}}{2 + 2(1-i)\sqrt{\omega \tau} - 2i\omega \tau}. \]  

(6.8)

From the above expressions, it follows that the values of real effective conductivity and dielectric constant for the clay particle and its EDL can be approximated by the equations

\[ \sigma_{eff} = \sigma_{\omega} \text{Re} \left( \frac{\delta}{1 - \delta Y} \right) + \omega \varepsilon_\omega \kappa_{\omega} \text{Im} \left( \frac{\delta}{1 - \delta Y} \right), \]  

(6.9a)

and

\[ \kappa_{eff} = \kappa_{\omega} \text{Re} \left( \frac{\delta}{1 - \delta Y} \right) - \frac{\sigma_{\omega}}{\varepsilon_\omega} \text{Im} \left( \frac{\delta}{1 - \delta Y} \right) + \kappa_{\text{grain}}. \]  

(6.9b)

The practical use of Eqs. (6.9) requires quantification of \( \beta \) and \( C \) in Eq. (6.6).

As noted by Glover et al. (1994), \( \beta \) depends on ion surface adsorption, brine pH, as well as electrolyte concentration. However, it is reasonable to assume a constant clay surface charge density in the order of 10-20 \( \mu \text{C/cm}^2 \), as measured by Sonon and Thomson (2005) in smectites. Hence, in the remaining sections of this chapter we assume a conservative value of \( \beta = 11 \mu \text{C/cm}^2 \). It must be pointed out that values as high as 100 \( \mu \text{C/cm}^2 \) have been reported for kaolinites (Kanket et al., 2005), which would make the impact of clays on the electrical response of rocks more important than what is shown below.

The brine cationic density \( C \) is linked to the brine electrical properties. Stroud et al. (1986) invoke existing correlations between \( \sigma_w \) (in S/m), \( \kappa_w \), temperature \( T \) (in \( ^\circ \text{C} \)) and salinity \( X \) (in kppm) through the equations

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By dividing $X$ by the molecular atomic mass of the dissolved salt and multiplying the result by the elementary charge one obtains the expression for $C$.

Using the above equations (6.5)-(6.10) for $a = 100$ nm and NaCl dissolved salt, we simulate the wide-band dispersions of effective conductivity and dielectric constant for clay particles and brine salinities equal to 40 and 4000 ppm. Figure 6.4 shows the corresponding simulation results and exhibits two important features. First, clay effective conductivity is negligible at 4000 ppm salinity (less than 1% of brine conductivity), while it can be substantial at 40 ppm salinity (up to 86% of brine salinity). Conductivity dispersion remains approximately flat in the kHz-GHz range for these values of clay size and surface charge. Second, the contribution of the ionic double-layer in the effective dielectric constant of the charged clay is negligible at 4000 ppm brine salinity ($\kappa_{\text{eff}} \approx \kappa_{\text{grain}}$) while it becomes substantial at lower salinities ($\kappa_{\text{eff}} \approx \kappa_w$ at 40 ppm). These frequency dispersions are flat above 300 kHz, but do exhibit a power-law behavior below 100 kHz.

Using the DC limit of Eq. (6.9a) constitutes a possible way to quantify electrical DC conduction through clay exchange cation from specific values of clay geometry and brine salinity. This approach makes it possible to assign specific values of $\sigma_{\text{clay}}$ in the DC-conductivity random-walk model of Chapter 2 (Section 2.2.2).
6.3.3 Simulation of Generic Rock WBEM Single-Phase Response

We now use the wide-band effective clay properties of the previous section at the pixel level in the pore map of Fig. 6.2. The pixels labeled as ‘clay’ in that pore map are successively assigned the electrical properties of (a) rock, (b) 0.1 S/m brine, and (c) 100-nm clay in 0.1 S/m brine background. Figure 6.5 shows the corresponding dielectric dispersions for the three cases and emphasizes the influence of rock texture in the MHz range. In that figure, the conductive paths created by brine in case (b) decrease the capacity of the rock model to store energy compared to case (a). The amplitude of the dielectric dispersion at low frequencies is lower in case (b) than in case (a). In case (c), where the presence of 3% dispersed clay is simulated over the entire frequency range, the dielectric dispersion is similar to that simulated for case (b) at 10 MHz, but diverges exponentially below this frequency. All cases (a) to (c) are associated with similar dielectric behavior above 10 MHz.

If we vary brine salinity in the clay-free configuration (a), then the simulated dielectric response (Fig. 6.6) exhibits the same scaling with brine conductivity as the one observed in Chapter 5 (Fig. 5.7). On the other hand, if brine salinity is varied in the 3%-clay rock model, then the scaling of dielectric constant with conductivity disappears and the dispersion shown in Fig. 6.7 ensues. We also note that high brine salinity preserves rock texture information in the MHz range while double-layer phenomena are prominent at frequencies below 1 MHz. By contrast, low brine salinities induce a dielectric response where both effects overlap in an indistinguishable manner.

This model can therefore reproduce Myers’ (1996) results on the basis of explicit pore geometries. We now adapt the same general model for the qualitative
simulation of dielectric dispersions in complex microstructures and for different states of fluid wettability.

6.4 COMBINING NMR WITH WBEM MEASUREMENTS TO ASSESS ROCK MORPHOLOGY: EXAMPLE OF COUPLED MICROPOROUS ROCK

As mentioned earlier in Section 4.2.2, the presence of diffusion coupling in microporous carbonate rocks with low surface relaxivity prevents NMR measurements from correctly quantifying pore-size distributions, bound fluid volumes, and hydraulic permeability. This section shows that WBEM measurements have the potential to reduce ambiguities on such complex rock morphologies. In this example, a WBEM geometric model is built on the basis of rock images and two-step EM upscaling in the absence of double-layer effects.

6.4.1 Problem Geometry

We synthesized a carbonate rock model from core data, core pictures, and NMR measurements of a micritized rock sample exhibiting diffusion coupling (Sample A from Toumelin et al., 2003a). This sample includes both dissolution vugs and abundant micritized intragranular porosity. The image analysis reported by Toumelin et al. (2003a) indicates the presence of secondary-porosity vugs (amounting to 10 of the 24% porosity of the sample, with pores sizes in the 15 μm range), primary-porosity macropores (4% porosity, 5-15 μm range), and micritized intragranular micropores (10% porosity, sub-micron range). Irreducible water saturation at 60 psi (414 kPa) in air was equal to 52% and assumed to fill the micritized porosity. Micritized grains in the range of 2-μm diameter agglomerate into packs of approximately 50 μm which form microporous grains (Fig. 6.8). Finally, calcite volumes in the range of 50-100 μm
are present in the sample, so that approximately 1/3 of the volume can be considered calcite-cemented while the rest of the rock matrix exhibits microporosity.

6.4.2 Uncertainty of NMR Caused by Diffusion Coupling

We constructed a 3D rock model to reproduce the rock structure described above. Grain objects similar to those illustrated in Fig. 2.5 are intended to reproduce the geometry of microporous micrite packs, whereas calcite volumes were considered as solid grains. Given the relatively high macroscopic homogeneity of the microporous grains shown in the left-hand panel of Fig. 6.8, we kept considering the Finney pack (see Chapters 2 and 4) as the skeleton of the rock model. That pack was sized and overgrown until porosity, grain size, and pore size fitted primary intergranular porosity data. Grains were then removed from the pack to match vug size and porosity. Subsequently, two-thirds of the Finney pack grains were made microporous with a compacted cubic-centered structure until they matched intragranular data and resembled the pore structure shown in Fig. 6.8. We adopted a homogeneous value of rock/water surface relaxivity equal to 1 μm/s to match the measured $T_2$ spectrum with the $T_2$ distribution simulated at full brine saturation via the random-walk technique described in Chapter 4. Figure 6.9 shows the good match between measured and simulated $T_2$ spectra, and illustrates the discrepancy existing between the NMR spectrum and the actual pore-size distribution. The pore-size-based NMR spectrum of Fig. 6.9 is obtained from simulations where diffusion coupling was disabled between intragranular microporosity and intergranular porosity.

6.4.3 WBEM Simulation Results

Following the dual-porosity structure shown by the high-resolution images of Fig. 6.8, Figure 6.10 shows an equivalent 2-scale 2D rock model amenable to the
simulation of WBEM measurements. This figure comprises two disks with two different spatial resolutions that constitute the two steps of the upscaling method. The left disk of Fig. 6.10 forms a 501x501-pixel map of a low-resolution rock model (1 pixel = 0.5 μm) and captures the general dual porous structure of the micritized carbonate sample (10% intergranular and 15% intragranular porosities). However, its low spatial resolution neglects the sub-micron micropores and microthroats existing within the microporous grains. This is why we also used a higher-resolution micromodel (map L of Fig. 5.9) that explicitly enforced the presence of 100-nm brine layers between micrite grains, as shown in the right disk of 501x501-pixel resolution (1 pixel = 50 nm). Once the dispersions of isotropic conductivity and dielectric constant are computed for the high-resolution micromodel, they are assigned to the grain pixels in the low-resolution rock model. The effective conductivity and dielectric constant obtained for the low-resolution model constitute the effective properties of the coupled micritized rock.

Figure 6.11 illustrates the distribution of the electric current strength calculated at frequencies below 1 MHz within the low-resolution rock model after 2-step upscaling. The incorporation of the microscale model in the 2-step upscaling process plays a fundamental role in the effective response of the coupled rock model. Figure 6.12 compares the wide-band dielectric dispersions calculated for the coupled model, with and without 2-step upscaling, with the frequency dispersions calculated for the generic model of Fig. 6.2. In the absence of upscaling, the dielectric response of the coupled macromodel (left disc of Fig. 6.10 only) is similar to that shown in Fig. 6.6 for the generic rock, except for the amplitude of the dielectric constant. That amplitude is larger in the generic model than in the coupled macromodel because eccentricities and
dead-ends are more prominent in the generic model. Once the micromodel (right disc of Fig. 6.10) is incorporated as the first step of the upscaling, the dielectric dispersion of the coupled model becomes remarkably flat. The presence of a water layer between all micrite grains effectively connects all the pores of the macromodel and eliminates the geometric dielectric enhancement of the rock. Existence of dead ends where electrical storage occurs in disconnected water zones is therefore the key to dielectric enhancement. Given these simulation results, it is likely that a rock exhibiting strong diffusion coupling will also exhibit high electrical conductivity and abnormally constant electromagnetic dispersion. Therefore, special emphasis can be placed on WBEM measurements to characterize abnormal heterogeneous rock morphologies and refine the estimation of petrophysical properties performed with NMR measurements.

6.5 COMPLEMENTING NMR WITH WBEM MEASUREMENTS TO ASSESS WETTABILITY AND FLUID SATURATIONS

6.5.1 Uncertainties of 2D NMR Interpretation Caused by Wettability

As emphasized in Chapter 4, $D/T_2$ NMR maps are sensitive to rock structure and saturating fluids. However, situations arise where the geometry of the fluids in the pore space and the lack of spatial resolution of 2D NMR inversion cause ambiguities in the interpretation of NMR maps. Figures 6.13 to 6.15 describe cases simulated with a saturation model similar to the one introduced in Chapter 4 (see Toumelin et al., 2004). In Fig. 6.13, rock wettability alteration causes a shift of the light-oil peak toward lower $T_2$ values (due to oil/rock surface relaxivity), and a shift of the water peak toward larger $T_2$ values (due to a decreasing water/rock surface). However, in the mixed-oil-wet NMR maps described in Fig. 6.13, no $D/T_2$ peak appears at the bulk water
response, as in cases F or G of Fig. 4.9 and case C of Fig. 4.12. Therefore, it is not straightforward to identify the presence of partial oil-wettability from NMR measurements. Figure 6.14 illustrates a possible water-wet interpretation for what is actually representative of a mixed-oil-wet case. In this case, a wrong wettability assumption has three adverse consequences: (a) it neglects the presence oil wettability, (b) the oil peak characterizes an oil grade slightly thicker than the actual value (2 cp instead of 1 cp), and (c) the water peak characterizes pores that appear four times larger than the actual size (with a main relaxation time equal to \( T_2 = 400 \text{ ms} \) instead of 100 ms). In turn, inaccurate interpretations of pore size bias the estimation of both bound fluid volume and hydraulic permeability (see Chapter 4).

On the other hand, cases such as the one simulated in Fig. 6.15 for the case of a heavier oil grade are likely to exhibit no shift in water signal upon wettability alteration. The higher value of oil viscosity prevents oil/rock surface relaxation from affecting the oil response when oil is the wetting phase. As a result, there is a marginal difference between water-wet and mixed-oil-wet NMR simulation results. Chapter 4 describes additional examples where the 2D NMR maps are unable to correctly predict wettability type and fluid saturation because no clear cutoffs can be applied to cumulative spectra of diffusivity or relaxation time, or because the \( D/T_2 \) peaks of water and light hydrocarbons coalesce.

### 6.5.2 WBEM Simulation Results

As mentioned earlier, electrical double-layer effects fully develop in water-wet cases, possibly enhanced by fractal surface roughness, while they are inhibited in oil-wet cases. We now illustrate the ability of our numerical model to capture this behavior. Following the methodology developed in Section 6.3.1, we populate the pore
map of Figs. 6.2 and 6.3 with wetting and non-wetting fluid pixels to describe the progressive drainage of a water-wet rock by oil (Fig. 6.16). By contrast, Fig. 6.17 models the progressive drainage of an oil-wet rock by water.

Figure 6.18 shows the wide-band dispersions of dielectric constant simulated for all the pore maps of Figs. 6.16 and 6.17, and for two values of brine conductivity, $\sigma_w = 0.1$ and 1 S/m. Each panel of Fig. 6.18 groups the simulation results by brine conductivity or wettability type. Several remarks stem from this comparison. First, the scaling of the dielectric constant with conductivity remains present in the EDL-free OW cases regardless of fluid saturation. This scaling disappears in the WW cases. Second, each panel of Fig. 6.18 shows that the hierarchy of the dielectric dispersion curves with respect to water saturation or brine conductivity is enforced in the GHz range. For instance, the values of dielectric constant simulated for low values of water saturation are smaller than those simulated for higher values of water saturation, which honors CRIM results. Likewise, the dielectric dispersion sigmoids of the bottom right-hand panel of Fig. 6.18 exhibit a shift to the left (lower frequencies for same values of dielectric constant) when conductivity decreases. Such a behavior is consistent with the notion of conductivity scaling mentioned earlier. However, when frequency decreases in the MHz range where EDL effects become important, this curve hierarchy disappears as dispersion curves intersect and change order.

The simulation results described in Fig. 6.18 exhibit a low-frequency power-law behavior for the dielectric constant of WW rock models. This power-law behavior is remarkable given the small amount of clay pixels (as low as 3% of the total number of rock pixels) and the small value of surface charge ($\beta = 11 \ \mu\text{C/cm}^2$ – see Section 6.3.2) considered in the model. Simulation results agree very well with the measured
trends of dielectric constant of WW rocks (Fig. 6.1). Dielectric dispersions obtained from simulations and experiments exhibit both (a) low-frequency convergence in OW cases, (b) low-frequency exponential behavior in WW cases, and (c) dual inflection in the MHz-range in some WW cases. Quantitatively, the absolute values of simulated and measured dielectric constants differ by a factor approximately equal to 20. It is likely that larger values of clay surface charge, clay amount, or a more accurate double-layer model, would reduce this discrepancy. However, the relative wide-band behavior of WW dielectric dispersions is identical for both simulations and measurements. In the 1-MHz range, between the two inflection points of the dielectric dispersion curves, both simulations and measurements yield values of dielectric constant equal to 10 times the value of their respective high-frequency asymptotes. In the 10-kHz range, this enhancement factor becomes approximately equal to 30 for both simulations and measurements.

It is also important to note that water/oil EM measurements in general, and water-wet dielectric low-frequency enhancements in particular, are insensitive to oil viscosity. The only assumption formulated on the saturating oil was to assign it a dielectric constant equal to 2 over the entire kHz-GHz frequency spectrum.

6.6 SUMMARY AND CONCLUSIONS

We reconciled fractal and double-layer concepts to explain the low-frequency dielectric behavior of saturated rocks. A generalized 2D pore-scale EM model ensued, which incorporates the simultaneous dielectric effects of pore geometry, charged clays and minerals, wettability, and fluid saturations. Despite quantitative limitations due to the spatial resolution of the pore map and the double-layer model, we obtained very
encouraging results when modeling explicit rock WBEM measurements independently from mixing rules or fitting parameters:

First, simulations qualitatively reproduced WBEM measurements for partially saturated rocks. They characterized wettability trends in clay-bearing sandstones, even for clay concentrations as low as 3%, and regardless of oil grade. Wide-band EM techniques can therefore help to determine in-situ sandstone wettability and complement NMR estimates which are ambiguous when oil viscosity exceeds a few cp.

Second, the flat dielectric dispersion simulated in coupled microporous rocks makes WBEM a viable technique to characterize complex rocks where NMR interpretation fails to correctly predict pore size distribution, bound fluids, and hydraulic permeability. One can envisage a generalization of WBEM measurements to detect the presence of complex pore inhomogeneity, including micritized, oolitic, or vuggy carbonate rocks. Chapter 5 also emphasized a possible role of WBEM measurements to quantify pore connectivity. However, WBEM measurements have no immediate sensitivity to pore size. The only theoretical counter-example occurs when EDL develops as pore surface coating; only in that particular case pore size affects the dielectric response of the double-layer.

A comprehensive WBEM model needs to be reliable in the presence of charged clay presence to perform quantitative petrophysical assessments. Clays usually form dia- or para-magnetic impurities causing internal magnetic fields which make NMR interpretation unreliable for petrophysical estimates (see Section 3.2.2). Consequently, WBEM techniques can improve the reliability of NMR techniques for the case of clayey sands.
Figure 6.19 summarizes the different sensitivities that are required to perform accurate petrophysical assessments for a general rock model. Pore size and connectivity are vital to assess hydraulic permeability in both clean and clayey sands. NMR measurements usually provide pore size distribution but not pore connectivity, unlike WBEM measurements. It is also necessary to identify a variety of fluids to perform adequate fluid typing. NMR measurements detect medium and light oil grades quite well, but are riddled by acquisition problems in the presence of gas (variable hydrogen index and high diffusivity) or heavy oil grades (low relaxation times). Oil grades whose relaxation times and diffusivities are close to those of water within confining rocks also cause NMR interpretation problems. WBEM measurements, on the other hand, are independent of hydrocarbon type; therefore, they allow wettability assessment but not fluid typing. Figure 6.19 emphasizes the sensitivity level of NMR and WBEM techniques for each of these criteria. Likewise, Fig. 6.19 indicates that a combination of the two measurement techniques permits a full coverage of the sensitivity domain required to perform accurate petrophysical assessments.
Figure 6.1: Wide-band dispersions of dielectric constant measured on four 22%-porosity Berea samples treated to exhibit different wettabilities and saturated with different brine salinities. OW: oil-wet samples; WW: water-wet samples. The conductivity of deionized water is $1.57 \times 10^{-3} \text{ S/m}$ at 100 Hz, and that of saline brine (75.8 g/l NaCl) is 9.5 S/m. After Bona et al. (1998), data courtesy of Nicola Bona.
Figure 6.2: Sandstone micrograph (left panel; white: grain; black: pore space) and corresponding digital pore map (right panel; white: grain; blue: pore space) scattered with arbitrary clay inclusions (magenta pixels). The scale on the pore map axes is given in pixels, with a pixel resolution equal to 5 μm.

Figure 6.3: Graphical example of two-phase fluid distribution within the pore map of Fig. 6.2. Colors are coded identically to Fig. 6.2; non-wetting hydrocarbons are identified with red pixels. The local enlargement shown in the right-hand panel exhibits the pixel-based construction of the 2D model.
Figure 6.4: Frequency dispersions of effective conductivity (left panel) and dielectric constant (right panel) simulated for $a = 100$ nm clay particles. Dotted lines indicate the bulk dielectric constant of quartz and water.

Figure 6.5: Frequency dispersion of dielectric constant simulated for the rock model shown in Fig. 6.2 assigning three different textures to its magenta pixels. Brine conductivity is equal to 0.1 S/m.
Figure 6.6: Frequency dispersion of dielectric constant simulated for the rock model of Fig. 6.2 (no clay double-layers) and for three different values of brine salinity.

Figure 6.7: Frequency dispersion of dielectric constant simulated for the rock model of Fig. 6.2 (with the clay double-layers characterized in Fig. 6.4) and for three different values of brine salinity.
Figure 6.8: High-resolution Scanning Electron Microscope (SEM) images of a carbonate sample exhibiting diffusion pore coupling at 140X (left panel) and 1400X (right panel) magnifications (Toumelin et al., 2003a)

Figure 6.9: Comparison between the NMR $T_2$ spectrum measured in 100% water-saturated coupled micritized carbonate rock, and the $T_2$ spectra simulated in the corresponding 3D rock model. Coupled (decoupled) simulations assume presence (absence) of diffusion coupling between the intragranular micropore space and the intergranular pore space.
Figure 6.10: Representation of the two-step 2D model of a rock designed to replicate the rock structure shown in Fig. 6.8.

Figure 6.11: Distribution of internal current amplitudes within the low-resolution microporous rock model below 1 MHz. The arrow shows the direction of polarization of the incident electric field.
Figure 6.12: Comparison between the dielectric dispersions obtained for 1 S/m brine with the generic model of Fig. 6.2 and with the coupled model of Fig. 6.10.

Figure 6.13: $D/T_2$ NMR maps inverted for 80% water saturation and 20% 1-cp oil saturation assuming water-wet (left panel) and mixed-oil-wet (right panel) rock models. O: oil $D/T_2$ response; W: water response. The arrows show the displacement of the oil and water peaks due to wettability alteration.
Figure 6.14: Two different interpretations of the same $D/T_2$ NMR map. Right-hand panel: simulated mixed-oil-wet results (same as the right panel of Fig. 6.13). Left-hand panel: interpretation of the same NMR map under the assumption of water wettability.

Figure 6.15: $D/T_2$ NMR maps inverted for 30% water saturation and 70% 7-cp oil saturation assuming water-wet (left-hand panel) and mixed-oil-wet (right-hand panel) rock models.
Figure 6.16: Fluid distribution in water-wet rock models with clays and 3 values of water saturation, $S_w$. White pixels: grain; blue pixels: brine; magenta pixels: clay; red: oil.

Figure 6.17: Fluid distribution in oil-wet rock models for 3 values of water saturation $S_w$. White pixels: grain; blue pixels: brine; red pixels: oil.
Figure 6.18: Frequency dispersions of dielectric constant simulated for the pore maps of Figs. 6.16 (water-wet cases, WW) and 6.17 (oil-wet cases, OW), for two values of brine conductivity. Top left-hand panel: all simulation results for $\sigma_w = 1 \text{ S/m}$; top right-hand panel: for $\sigma_w = 0.1 \text{ S/m}$; bottom left-hand panel: all water-wet geometries; bottom right-hand panel: all oil-wet geometries.
Figure 6.19: Pie-chart representation of the complementary domains of sensitivity of NMR and WBEM measurements. The colors (green, yellow and red) quantify the sensitivities (good, moderate, and poor, respectively) of each measurement technique used independently.
Chapter 7: Summary, Conclusions, and Recommendations

This final chapter summarizes the main results and contributions of the work presented in the dissertation. We also recapitulate the conclusions and elaborate on possible future extensions of the research.

7.1 SUMMARY

The main thrust of this dissertation was to introduce new pore-scale models that can simulate the sensitivity of NMR and WBEM measurements to pore structure, grain morphology, fluid saturations, saturation history, and wettability. These models were developed through the multiphysics integration of (a) drainage, imbibition, and wettability phenomena, (b) diffusion and NMR magnetization decays in porous media, and (c) remote-sensing electromagnetics. We successfully benchmarked these pore-scale models with conventional petrophysical models for DC resistivity, NMR relaxation, and wide-band dielectric responses. Our new numerical models allowed the simulation of petrophysical cases for which standard mixing laws become invalid, such as for DC conductivity and NMR measurements in inhomogeneous rocks and mixed-oil wettability cases, and for WBEM measurements in clayey rocks. The simulation work emphasized situations where NMR or WBEM measurements could not individually provide accurate petrophysical assessments, but where the joint interpretation of both methods exhibited more accuracy than an interpretation taken separately.

We developed two classes of pore-scale models to simulate the DC electrical conductivity, NMR, and WBEM response of saturated rocks. The first model class
consisted of 3D, dense, grain-pack skeletons saturated with a two-phase fluid. Specific intragranular features modeled the effects of microporosity and clay exchange cations, while the two fluid phases were explicitly distributed in the ensuing pore-space following Kovscek’s model (1993), with strict adherence to capillary and saturation history. The mean-square-displacement of random walkers diffusing throughout the conductive pore zones yielded the resistivity formation factor and the resistivity index. Bloch’s equations were subsequently solved along random-walk trajectories in both water-filled and oil-filled pore space to simulate NMR magnetization decay as a function of fluid type, rock surface relaxation, and NMR pulse sequences. A series of such decays were then inverted into parametric 2D NMR maps along saturation cycles taking place in the rock model.

The second model class was based on 2D digital pore maps, in which pixels were assigned contrasting electrical properties for quartz grains, clay, and fluids. The calculation of the frequency dispersions of effective conductivity and the dielectric constant for each pore map made use of a new methodology. First, we solved Maxwell’s equations for the electric fields within the disc-shaped scatterer for a given frequency and angle of incidence. Next, we computed the effective upscaled conductivity and the dielectric constant of the pore map as the properties that characterize a homogeneous cylinder in which the internal electric fields and the associated current densities most closely match those calculated within the pore map under the same electromagnetic plane-wave excitation. Finally, we independently repeated the process for distinct frequencies between 10 kHz and 1 GHz. Dispersions of conductivity and dielectric permittivity ensued for each pore map as functions of
brine salinity, grain/pore eccentricity, pore connectivity, fluid saturation, clay content, and wettability.

The main technical contributions stemming from this dissertation are summarized as follows:

1. Integration of pore-level fluid distributions with previously well-established random-walk techniques for DC conductivity and NMR in single-phase.
2. Development of a pore-scale model capable of reproducing DC rock resistivity according to saturation history, rock wettability preference, and rock morphology.
3. Development of a petrophysically oriented NMR formulation that includes the combined effects of bulk relaxation, surface relaxation, and inhomogeneous magnetic fields for arbitrary pulse sequences.
5. Quantification of saturation history effects on the NMR response of both water-wet and mixed-oil-wet rocks.
7. Quantitative integration of NMR and WBEM data to improve the petrophysical assessment of pore structure in micritized rocks.
8. Quantitative integration of NMR and WBEM data to improve the petrophysical assessment of wettability, fluid saturation, and fluid type in sandstones.
7.2 CONCLUSIONS

The simulation results reported in the dissertation provided the following conclusions:

1. The relation between Archie’s cementation exponent \( m \) and rock facies is not evident. The dependence of formation factor on porosity canceled any conduction enhancement offered by the presence of intragranular microporosity. Decreasing brine salinities, however, consistently enhanced the DC conductivity of clay rocks and thus reduced the apparent cementation exponent \( m^* \).

2. Variations of the resistivity index as a function of saturation history, wettability, and saturation were accurately reproduced for the cases of water-wet and mixed-oil-wet systems. For water-wet systems, Archie’s saturation exponent \( n \) was predicted to be equal to 2 for homogeneous rocks. Lower values were obtained when imbibition occurred through growth of the water films. Values of \( n \) lower than 2 were also produced for rock exhibiting intragranular porosity. For oil-wet rocks, values of \( n \) during drainage were consistently observed to be between 3 and 4 for homogeneous rocks and down to 2 for microporous rocks. Under the assumption that oil imbibition occurs through oil film growth, \( n \) increased to 10 or more below a critical water saturation in the range of \( S_w = 0.4 \) to 0.7, consistent with published data. That critical water saturation was found to increase when porosity decreases or when microporosity increases.

3. Under the assumed conditions (16 G/cm magnetic field tool gradient, \( TE = 0.2 \) to 16 ms, CPMG pulse sequence), only light oil grades characterized by
viscosities < 1 cp, exhibited obvious 2D NMR shift when wettability was altered. As oil viscosity increased, changes in wettability state had a decreasing impact on NMR oil response. In the presence of oil grades more viscous than a few cp, the increasing relaxation time of the water signal was the only evidence of wettability alteration.

4. Saturation history and fluid distribution affected the NMR response of saturated rocks. Despite substantial improvements over 1D $T_2$ inversion, $D/T_2$ 2D NMR maps involved uncertainties in fluid saturations of up to 20 saturation units when the $D/T_2$ response of oil was close to that of water. The pore size estimated from the water $T_2$ spectrum also varied by as much as 400% because of different pore-scale geometries during successive saturation cycles.

5. Even in homogeneous rocks, it was shown that mixed-oil wettability could create different patterns of $D/T_2$ 2D NMR responses depending on the fluid saturation history. In particular, the locations of the water peak in the $D/T_2$ maps changed during the saturation cycles; that peak described part of the interval between the 2D NMR response of bulk water and the 2D NMR response of water affected by surface relaxation.

6. Dielectric mixing laws only describe average wide-band polarizations of rocks of equal porosity and pore eccentricity. In our simulations, the wide-band electrical behavior of each rock departed from an average sigmoid curve by a factor of 2 for relatively moderate values of pore eccentricity. We expect more pronounced scattering effects for larger values of pore eccentricity.

7. Because they scan the rock structure in a wide frequency range, WBEM measurements are more sensitive to pore connectivity and hydraulic
permeability than NMR measurements. Unlike existing mixing laws, our simulations showed that shape and amplitude of WBEM dielectric dispersions depend on pore structure and connectivity more than on pore eccentricity. Dielectric dispersions with several inflection points suggest the presence of unconnected porosity, and not necessarily the presence of different pore eccentricities. By contrast, smooth dielectric sigmoid dispersions were observed in the presence of good pore connectivity throughout the sample, even in the absence of a single value of pore eccentricity. Flat dispersions characterized rock models where diffusion coupling between intergranular and intragranular pore spaces biased NMR measurements.

8. In our work, the validity of the dielectric CRIM results at 1 GHz was associated with the presence of large eccentricities and moderate connectivity between the pore bodies. Errors of at least 30% in the prediction of the rock dielectric constant with CRIM are expected due to variations of pore connectivity.

9. WBEM measurements are sensitive to rock wettability. This was illustrated by 2D numerical simulations in which the low-frequency dielectric enhancement of clay double-layers was activated at the contact of water-wet surfaces, while it was deactivated at the contact of oil-wet surfaces. The simulation results showed that our model captured the relevant mechanisms of WBEM dispersions in saturated rocks, combining pore geometric effects in the MHz-range and wettability/EDL/power-law effects below that range. We expect that higher resolution grids, more accurate double-layer models, and possibly 3D extensions of the numerical model will quantitatively reproduce WBEM measurements to accurately assess wettability and brine saturation.
10. The WBEM determination of wettability and, to a certain degree, fluid saturations can constrain 2D NMR interpretation. Therefore, they make the determination of wettability, fluid saturations and fluid types more robust with respect to abnormal rock morphologies, 2D NMR inversion resolution, and clay presence.

7.3 **RECOMMENDATIONS FOR FUTURE RESEARCH**

The numerical models developed in this dissertation were based on several assumptions. First, the model geometry needs to be representative of the pore scale phenomena taking place in the real rock. For instance, if the imbibition mechanism in an oil-wet rock does not respect Kovscek’s film-growth assumption, then different fluid distributions would ensue. In turn, this new fluid geometry would impact the simulated values of the resistivity index and NMR decay rates. The 3D model also assumed no residual oil saturation upon complete wettability alteration; this assumption becomes inaccurate in the presence of irreducible oil saturation. In this case, one must enforce selective wettability alteration according to criteria to be defined, such as a pore wall curvature criterion. We also described the oil blobs as single spheres concentric with the pore units, thereby defining a single curvature value for all the water/oil interfaces in that pore. More accurate calculations of fluid interface curvatures (e.g., Gladkikh and Bryant, 2003) could be used to define a different interface curvature for each pore throat inlet and each pendular ring.

We calculated the pseudo-capillary pressure curves of Section 2.3 from the inverse of the throat-size thresholds that parameterize drainage and imbibition cycles. This calculation is overly simplified and does not account for contact angle, or local grain curvature. It might be necessary to use pore network models based on the same
grain-pack skeleton (Gladkikh and Bryant, 2003) to obtain accurate values of capillary pressure as a function of water saturation. Such models used at a pre-processing stage would also yield relative permeability curves.

Most of the analyses performed to validate the 3D model considered homogeneous grain packs. It is desirable to extend this model to more complex rock structures and fully develop the interplay between rock morphology, fluid saturation, and wettability. A sensitivity analysis of the impact of grain arrangements and intragranular morphology would be particularly helpful to assess the origin of abnormal conductivity and NMR behavior in carbonate rocks. The example of resistivity index calculated for a microporous rock model in Chapter 2 matched the trends that were measured by Sweeney and Jennings (1960), suggesting that their data set could include microporous carbonates. Unfortunately, few reports of such measurements include sufficient geological and petrographical information to quantitatively calibrate the 3D model. Much work remains to reproduce the variety of resistivity index curves measured by Fleury (2002) in carbonates, and to assess their 1D and 2D NMR responses.

Numerical algorithms exist to extract grain features from 3D CT scans of real rock samples (Saadatfar et al., 2005). A validation of the simulation models developed in this dissertation could extract the equivalent grain packs for a series of samples, and then compare two-phase measurements and simulations for both resistivity and NMR data.

The 2D WBEM model could also be improved. From the results shown in Chapter 6, this model captures the relevant physics of dielectric polarization. However, the analytical model that we used to reproduce double-layer polarization around
charged clay surfaces (Lima and Sharma, 1992) assumed individual spherical grains. The electromagnetic interaction appearing between two such grains in contact is implicit in Maxwell’s equations at the pore scale. However, the spatial distribution of the charges is not accurately calculated when the clay particles touch each other. Other existing electro-chemical models (e.g., Glover, 1994) incorporate parameters neglected in Lima and Sharma’s (1992) model, including pH, into the net clay surface charge. The existence of (possibly fractal) roughness at the surface of certain sandstones is also known to enhance the clay dielectric power-law effect in the kHz range. It would be desirable to develop an effective model that captures this fractal roughness as a frequency-dependent conductivity and dielectric permittivity to be assigned to the appropriate pixels of the pore maps. Finally, the anisotropy of a pore/fluids map can be calculated by considering the analytical response of a homogeneous anisotropic cylinder during the inversion process, thus yielding anisotropic effective conductivity and dielectric dispersions of 2D rock/fluid models.

Also, it would be desirable to conduct a rigorous validation of the model by comparing its behavior to actual measurements. This procedure would proceed as follows: (1) perform WBEM measurements on samples exhibiting a variety of porosities, absolute permeabilities, saturations, salinities, clay content, and roughness (as could be measured by Brunauer-Emmett-Teller (BET) adsorption); (2) digitize some of their cross sections to serve as 2D pore maps; (3) quantify the clay content in the sample through cation-exchange-capacity (CEC) measurements.

We also recommend extending the 2D WBEM framework into three dimensions. This conversion would be computationally costly, although manageable on parallel computing platforms, and could improve the accuracy of the model to
quantitatively reproduce measured values of conductivity and the dielectric constant. That 3D model would take the form of a cylinder, and its homogeneous properties would be inverted from those of a finite homogeneous cylinder. However, we expect no major change between the dielectric dispersions calculated with a 2D model and those calculated with a 3D model because the incident electrical plane wave is already transverse to the 2D pixel plane.

Two additional types of preprocessing tasks could be performed to make the 3D diffusion grain-pack model more universal. First, the random-walk technique allows the incorporation of a displacement bias, such as a local velocity drift. The NMR response of the fluid(s) saturating the grain pack can, therefore, be modeled with the help of an appropriate fluid velocity map when that fluid is in motion. The latter map could be created from Lattice-Boltzmann simulations, or from the steady-state resolution of Stoke’s equation on a finite-element mesh of the pore volume. Another option concerns the simulation of clay effects on NMR measurements. Both the DC conductivity model and the WBEM model include the effect of the explicit distribution of clays. However, the NMR model requires an accurate calculation of the distortions created by paramagnetic or diamagnetic clays on the tool background magnetic field $B_0$. The calculation of these internal fields can be approached as a magnetostatic problem that could also be discretized and solved with finite elements on the entire bulk volume of the rock/fluid model.

Last, an extension of the 3D model to three immiscible fluid phases could incorporate distinct distributions of an aqueous phase (WBM or native brine), an oleic phase (OBM or native oil), and a gaseous phase.
Appendix A: Geometrical Equations for Random-Walker Positioning Within the Delaunay Tessellation

A.1 TETRAHEDRA BOUNDARIES

Let us consider one tetrahedron, $\Omega$, resulting from the Delaunay tessellation. $\Omega$ defines the pore unit between grains 1, 2, 3 and 4. The four planes that define the four faces of $\Omega$ are $\{(\Pi_i) | i = 1..4\}$, and the pore center of $\Omega$ is point $C$. Each plane $\Pi_i$ is characterized by its coefficients $Q_{i(x,y,z)}$ in the Cartesian equation

$$\Pi_i: Q_{ix}x + Q_{iy}y + Q_{iz}z + 1 = 0. \quad (A.1)$$

Plane $\Pi_1$ contains Apices 2,3,4 of cell $\Omega$ and separates $\Omega$ from its neighboring cell $N_1$; likewise, $\Pi_2$ contains Apices 1,3,4 of $\Omega$ and separates it from $N_2$, etc. For each plane $\Pi$ containing the three tessellation apices (grain centers) of non-null coordinates $(x_k, y_k, z_k) | k \in \{1,2,3\} | (x_k, y_k, z_k) \neq (0,0,0)$, the coefficients $Q_i$ are defined by the linear system:

$$\begin{bmatrix} x_1 & y_1 & z_1 \\ x_2 & y_2 & z_2 \\ x_3 & y_3 & z_3 \end{bmatrix} \begin{bmatrix} Q_x \\ Q_y \\ Q_z \end{bmatrix} = \begin{bmatrix} -1 \\ -1 \\ -1 \end{bmatrix}. \quad (A.2)$$

To determine whether the random walker of coordinates $(x, y, z)$ is located within tetrahedron $\Omega$, a comparison is made for each face $(\Pi_i)_{i=1..4}$ of the sign of Eq. (A.1) estimated at $(x, y, z)$ and the corresponding sign for a point known to be within $\Omega$ and opposite to $\Pi_i$ – for instance Apex $i$. If both results have same sign, then both points lie on the same side of $\Pi_i$, and the walker remains within $\Omega$. Otherwise, the walker has crossed $\Pi_i$, moved toward the neighboring tetrahedron $\Omega' = N_i(\Omega)$, and similar tests are now performed for the new cell.
A.2 THROAT CENTERS

Assuming that face $\Pi$ connects the centers of grains 1, 2 and 3, then the throat of $\Pi$ is characterized by its center $c = (x_0, y_0, z_0)$ and size $r_0$, such that the disc centered on $c$ of radius $r_0$ is the largest disc that can be drawn on the plane $\Pi$ between the three grains which form its apices. These apices are located at the coordinates $\{(x_k, y_k, z_k) | k \in \{1, 2, 3\}\}$, the grains radii are given $\{|R_k | k \in \{1, 2, 3\}\}$, $(x_0, y_0, z_0)$ and the $r_0$ is the solution a system of four equations with four unknowns, given by

$$\begin{align*}
(x_1 - x_0)^2 + (y_1 - y_0)^2 + (z_1 - z_0)^2 &= (R_1 + r_0)^2, \\
(x_2 - x_0)^2 + (y_2 - y_0)^2 + (z_2 - z_0)^2 &= (R_2 + r_0)^2, \\
(x_3 - x_0)^2 + (y_3 - y_0)^2 + (z_3 - z_0)^2 &= (R_3 + r_0)^2, \\
Q_x x_0 + Q_y y_0 + Q_z z_0 + 1 &= 0.
\end{align*}$$

(A.3)

After performing simple algebraic steps one obtains the equivalent system:

$$\begin{align*}
(x_1 - x_0)^2 + (y_1 - y_0)^2 + (z_1 - z_0)^2 &= (R_1 + r_0)^2, \\
x_0 \Delta x_{12} + y_0 \Delta y_{12} + z_0 \Delta z_{12} &= R_0 \Delta R_{12} + B_{12}, \\
x_0 \Delta x_{13} + y_0 \Delta y_{13} + z_0 \Delta z_{13} &= R_0 \Delta R_{13} + B_{13}, \\
x_0 Q_x + y_0 Q_y + z_0 Q_z &= -1.
\end{align*}$$

(A.4)

where $\Delta x_{mn} = 2(x_n - x_m)$, $\Delta y_{mn} = 2(y_n - y_m)$, $\Delta z_{mn} = 2(z_n - z_m)$, $\Delta R_{mn} = 2(R_n - R_m)$, and $B_{mn} = R_m^2 - R_n^2 + (x_n^2 + y_n^2 + z_n^2) - (x_m^2 + y_m^2 + z_m^2)$. A more convenient representation of the last three equations is the linear system

$$\begin{bmatrix}
\Delta x_{12} & \Delta y_{12} & \Delta z_{12} \\
\Delta x_{13} & \Delta y_{13} & \Delta z_{13} \\
Q_x & Q_y & Q_z
\end{bmatrix}
\begin{bmatrix}
x_0 \\
y_0 \\
z_0
\end{bmatrix}
= \begin{bmatrix}
B_{12} \\
B_{13} - r_0 \Delta R_{13} \\
-1
\end{bmatrix}.$$

We make use of a standard Newton-Raphson algorithm (Press et al., 1992) to iteratively solve for the value of $r_0$ that satisfies the above system of equations. This is
performed by successively evaluating $c = (x_0, y_0, z_0)$ from the matrix product for a
given $r_0$, and then by computing the residual
\[
\left| (x_1 - x_0)^2 + (y_1 - y_0)^2 + (z_1 - z_0)^2 - (R_1 + r_0)^2 \right|.
\] (A.6)

The pore throat is open when the solution for $r_0$ is positive. Moreover, the
throat center $c$ may be located outside of the triangular face of the tetrahedron,
depending on the grain geometrical arrangement and radii. We also considered that the
throat is closed if $c$ is too far from the tetrahedron, i.e., if $c$ is located outside $\Omega$ and its
distance to a face $\Pi'$ of $\Omega$ (other than $\Pi$) is larger than $r_0$, i.e.,
\[
\frac{|Q'_x x_0 + Q'_y y_0 + Q'_z z_0 + 1|}{\sqrt{Q'^2_x + Q'^2_y + Q'^2_z}} > r_0.
\] (A.7)

In the case where $\Omega$ is relatively flat, i.e., when three of the four grains are close from
alignment, the Newton-Raphson algorithm may not converge. When this situation
occurs we diagnose that the throat is also closed.

A.3 PORE CENTERS

In similar fashion for the treatment of throat centers, the pore defined within
tetrahedron $\Omega$ is characterized by its center $C = (x_0, y_0, z_0)$ and radius $R_0$ such that
the sphere of center $C$ and radius $R_0$ is the largest sphere that can be centered between
the grains. As a result, $C$ is the intersection of the four spheres centered on the apices
of $\Omega$, \( \{(x_k, y_k, z_k) | k \in \{1, 2, 3, 4\}\} \), with radii equal to \( \{R_k | k \in \{1, 2, 3, 4\}\} \). The
coordinates $(x_0, y_0, z_0)$ and $R_0$ can then be found from the solutions of the system of
equations
\[
\left\{(x_0, y_0, z_0, R_0) | (x_k - x_0)^2 + (y_k - y_0)^2 + (z_k - z_0)^2 = (R_k + R_0)^2 | k \in \{1, 2, 3, 4\}\right\}
\]
Equivalently, the system of equations can be written as
\[
\begin{align*}
\begin{cases}
(x_1 - x_0)^2 + (y_1 - y_0)^2 + (z_1 - z_0)^2 = (R_1 + R_0)^2 \\
\Delta x_{12} \Delta y_{12} \Delta z_{12} \quad \begin{bmatrix} x_0 \end{bmatrix} = \begin{bmatrix} B_{12} \end{bmatrix} - R_0 \begin{bmatrix} \Delta R_{12} \end{bmatrix} \\
\Delta x_{13} \Delta y_{13} \Delta z_{13} \quad \begin{bmatrix} y_0 \end{bmatrix} = \begin{bmatrix} B_{13} \end{bmatrix} - R_0 \begin{bmatrix} \Delta R_{13} \end{bmatrix} \\
\Delta x_{14} \Delta y_{14} \Delta z_{14} \quad \begin{bmatrix} z_0 \end{bmatrix} = \begin{bmatrix} B_{14} \end{bmatrix} - R_0 \begin{bmatrix} \Delta R_{14} \end{bmatrix} 
\end{cases}
\end{align*}
\]  
(A.8)

The location of the pore center \( C = (x_0, y_0, z_0) \) and the radius \( R_0 \) are obtained upon convergence of the Newton-Raphson algorithm used to solve the above system of equations. However, depending on the grain positions and radii, \( C \) may not be defined (e.g. when the Newton-Raphson algorithm does not converge). This situation occurs in the cases where \( \Omega \) is almost flat and a larger grain hides a smaller grain from the rest of the tetrahedron, thereby effectively creating several pore bodies within \( \Omega \) (see Fig. A.1). In such a situation, the pore center from which fluid blobs are grown is defaulted to the center of mass of the open-throat centers. The radius then becomes the largest distance between \( C \) and the grain surfaces.

A.4 UNIDIRECTIONALLY FRACTURED GRAINS

Micro-fractured grains are considered split by a slit fracture of aperture \( h \) along one homogeneous direction of angles \( \theta_x \) (\( \theta_y \)) with the \( x \) (\( y \)) direction of the Cartesian grid, respectively (see Fig. A.2). Let \( C = (x_0, y_0, z_0) \) be the center of the microfractured grain, and \( (\Pi'_1) \) and \( (\Pi'_2) \) the two planes that define the limits of the fracture. Let \( C_{\Pi'_1} = (x_1, y_1, z_1) \) and \( C_{\Pi'_2} = (x_2, y_2, z_2) \) be the corresponding projections of \( C \) on the planes \( (\Pi'_1) \) and \( (\Pi'_2) \), respectively. These two planes are defined by the equations

\[
\begin{align*}
(\Pi'_1): f_{\theta_x, \theta_y}(x, y, z) - f_{\theta_x, \theta_y}(x_1, y_1, z_1) &= 0 \\
(\Pi'_2): f_{\theta_x, \theta_y}(x, y, z) - f_{\theta_x, \theta_y}(x_2, y_2, z_2) &= 0 \\
\forall(x', y', z')
\end{align*}
\]  
(A.9)

\[
f_{\theta_x, \theta_y}(x', y', z') = x' (\cos \theta_y \sin \theta_x) + y' (\cos \theta_x \sin \theta_y) - z' (\cos \theta_x \cos \theta_y),
\]  
(A.10)
and \( \Pi' \) and \( \Pi'' \) intersect the normal vectors \( \mathbf{CC}_{\Pi'} \) and \( \mathbf{CC}_{\Pi''} \) at \( C_{\Pi'} \) and \( C_{\Pi''} \), respectively. The projections coordinates are then given by

\[
\begin{align*}
x_{1,2} &= x_0 \pm \frac{h \cos \theta_y \sin \theta_x}{2 \sqrt{\cos^2 \theta_y \left(1 - \cos^2 \theta_x\right) + \cos^2 \theta_x}} \\
y_{1,2} &= y_0 \pm \frac{h \cos \theta_x \sin \theta_y}{2 \sqrt{\cos^2 \theta_y \left(1 - \cos^2 \theta_x\right) + \cos^2 \theta_x}} \\
z_{1,2} &= z_0 \mp \frac{h \cos \theta_x \cos \theta_y}{2 \sqrt{\cos^2 \theta_y \left(1 - \cos^2 \theta_x\right) + \cos^2 \theta_x}}
\end{align*}
\]  

(A.11) (A.12) (A.13)

The grain center \( C = (x_0, y_0, z_0) \) is located within the slit pore space. If both equations for \( \Pi' \) or \( \Pi'' \) evaluated at \( P = (x, y, z) \) have the same sign when evaluated at \( (x_0, y_0, z_0) \), whereupon \( P \) belongs to the slit pore space; otherwise, the walker moves toward the solid semi-spheres defined by the grain.
Figure A.1: An example of tessellation cell where the strong heterogeneity of grain sizes prevents a clear definition of pore center. Left: grains forming the tessellation cell and complementary pore space. Right: pore space within the elementary tetrahedron of the cell.

Figure A.2: Graphical representation of grains which are either solid (in blue) or fractured (in red) along a slit of thickness $h$ at an angle with respect to the reference frame pictured in the bottom-right corner.
Appendix B: Approximation of the Static Magnetic Field Map Enforced by a Wireline Borehole Logging NMR Tool

Due to the inside-out design of their permanent magnet, borehole NMR logging tools exert magnetic fields which are much more inhomogeneous than those of laboratory spectrometers. Figure B.1 shows an example of such logging tool field map (Hürlimann and Griffin, 2000). In this figure, the origin of the system of coordinates coincides with the location of the NMR antenna, while the x axis designates the radial distance between the RF antenna and the rock formation. The grayscale intensity represents the amplitude of the field variation $\Delta B_0$ from the sweet spot located at the center of the green square (where $B_0 = 541.2$ Gauss and $t_{180} = 29.2 \ \mu s$). White dashed lines describe the locations where walkers are in resonance with the antenna, $\|\Delta B_0\| = 0$.

For the purpose of the simulations performed in this chapter, we used a rough approximation of the field map focusing on the central cm² area of Fig. B.1 (green square) under the assumption that $\Delta B_0$ remains in the $z$ direction and is described by the elliptical form:

$$\Delta B_0 = \left( -\frac{x}{c} - 0.5 \right)^2 + \left( \frac{y}{c} - 0.5 \right)^2 \times 30 \ \hat{z} \quad [\text{Gauss}],$$

(B.1)

where $c = 1$ cm and $x$ and $y$ are the Cartesian locations of the random walker in the framework $\Gamma$. Figure B.2 shows the resulting field map of the amplitude of $\Delta B_0$. 

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Figure B.1: Static magnetic field map in the plane perpendicular to the axis of an NMR borehole logging tool, adapted from the one described by Hürlimann and Griffin (2000) (courtesy of Martin Hürlimann).
Figure B.2: Magnetic field map representing Eq. (B.1) as an approximation of Fig. B.1 for the highlighted zone surrounding the sweet spot (green square in Fig. B.1).
Appendix C: Analytical Calculations of the Evolution Matrix
Exponentials in Bloch’s Equations

The total magnetic field applied to the walker \( \mathbf{B} = \Delta \mathbf{B}_0 + \mathbf{B}_1 \) is either
\( \mathbf{B} = \Delta \mathbf{B}_0 = \Delta B_y \hat{z} \) between RF pulses, \( \mathbf{B} = B_x \hat{x} + \Delta B_y \hat{z} \) during \( x' \)-pulses, or
\( \mathbf{B} = B_y \hat{y} + \Delta B_y \hat{z} \) during \( y' \)-pulses. This approach makes no approximation on the magnetic pulses quality because the actual dispersion of Larmor frequencies is honored across the walker population and the walker diffusion is fully accounted for during the enforcement of \( \mathbf{B}_1 \). In what follows, we provide analytical solutions for the matrix exponential in Eqs. (3.4) and (3.7) depending on the walk clock time.

**Between ** \( \mathbf{B}_1 \) **pulses**, the only magnetic field present is the background field, and the effective relaxation times for that step are either equal to the bulk relaxation times or given by Eq. (3.11). It then follows that

\[
A\Delta t = \begin{pmatrix}
-\frac{\Delta t}{T_2} & \gamma B_z \Delta t & 0 \\
-\gamma B_z \Delta t & -\frac{\Delta t}{T_2} & 0 \\
0 & 0 & -\frac{\Delta t}{T_1}
\end{pmatrix}, \text{ and therefore}
\]

\[
e^{A\Delta t} = \begin{pmatrix}
e^{-\frac{\Delta t}{T_2}} \cos(\gamma B_z \Delta t) & \frac{e^{-\frac{\Delta t}{T_1}}}{\gamma} \sin(\gamma B_z \Delta t) & 0 \\
g^{-\frac{\Delta t}{T_1}} \sin(\gamma B_z \Delta t) & \frac{e^{-\frac{\Delta t}{T_1}}}{\gamma} \cos(\gamma B_z \Delta t) & 0 \\
0 & 0 & e^{-\frac{\Delta t}{T_1}}
\end{pmatrix}.
\]

**During ** \( \mathbf{B}_1 \) \( (\pi / 2)_x \) **pulses**, \( A\Delta t \) takes on the form:
The three eigenvalues $\lambda_i$ of $\mathbf{A}\Delta t$ are found by solving the characteristic polynomial:

$$P_3(\lambda) = \det(\lambda \mathbf{I} - \mathbf{A}\Delta t) = \lambda^3 + \lambda^2 \left( \frac{2\Delta t}{T_2} + \frac{\Delta t}{T_1} \right)$$

$$+ \lambda \left( \frac{2(\Delta t)^2}{T_2T_1} + \frac{(\Delta t)^2}{T_2^2} + (\gamma B_x \Delta t)^2 + (\gamma B_x \Delta t)^2 \right)$$

$$+ \left( \frac{(\Delta t)^3}{T_2^2T_1} + \frac{(\Delta t)^3 (\gamma B_x)^2}{T_2} + \frac{(\Delta t)^3 (\gamma B_x)^2}{T_1} \right)$$

Using Cardan’s method, we obtain

$$\lambda_1 = \sqrt[3]{s-q} - \sqrt[3]{s+q} - \frac{a}{3}$$

$$\lambda_2 = \frac{1}{2} \left( \sqrt[3]{s+q} - \sqrt[3]{s-q} \right) - \frac{a}{3} + \frac{i\sqrt{3}}{2} \left( \sqrt[3]{s+q} + \sqrt[3]{s-q} \right)$$

$$\lambda_3 = \frac{1}{2} \left( \sqrt[3]{s+q} - \sqrt[3]{s-q} \right) - \frac{a}{3} - \frac{i\sqrt{3}}{2} \left( \sqrt[3]{s+q} + \sqrt[3]{s-q} \right)$$

(C.3)

with

$$p = \frac{1}{3} \left( b - \frac{a^2}{3} \right); \quad q = \frac{1}{2} \left( c - \frac{ab}{3} + \frac{2a^3}{27} \right); \quad s = \sqrt{q^2 + p^3},$$

and

$$a = \left( \frac{2\Delta t}{T_2} + \frac{\Delta t}{T_1} \right); \quad b = \left( \frac{2(\Delta t)^2}{T_2T_1} + \frac{(\Delta t)^2}{T_2^2} + (\gamma B_x \Delta t)^2 + (\gamma B_x \Delta t)^2 \right);$$

$$c = \left( \frac{(\Delta t)^3}{T_2^2T_1} + \frac{(\Delta t)^3 (\gamma B_x)^2}{T_2} + \frac{(\Delta t)^3 (\gamma B_x)^2}{T_1} \right)$$

(C.4)

A matrix of eigenvectors corresponding to these eigenvalues can be calculated as
\[
U = \begin{bmatrix}
\frac{\gamma B_z \Delta t}{\lambda_1 + \frac{\Delta t}{T_2}} & \frac{\gamma B_z \Delta t}{\lambda_2 + \frac{\Delta t}{T_2}} & \frac{\gamma B_z \Delta t}{\lambda_3 + \frac{\Delta t}{T_2}} \\
1 & 1 & 1 \\
\end{bmatrix},
\]

\[
A\Delta t = \begin{bmatrix}
-\frac{\Delta t}{T_2} & \gamma B_z \Delta t & -\gamma B_z \Delta t \\
-\gamma B_z \Delta t & -\frac{\Delta t}{T_2} & 0 \\
\gamma B_z \Delta t & 0 & -\frac{\Delta t}{T_1} \\
\end{bmatrix}.
\]

Upon replacing \( B_z \) with \( B_y \) in Eq. (C.4), it is readily found that the eigenvalues of this last matrix are identical to those of Eq. (C.3). The corresponding eigenvectors are included in matrix \( U \) as

\[
U = \begin{bmatrix}
\frac{\gamma B_z \Delta t}{\lambda_1 + \frac{\Delta t}{T_2}} & \frac{\gamma B_z \Delta t}{\lambda_2 + \frac{\Delta t}{T_2}} & \frac{\gamma B_z \Delta t}{\lambda_3 + \frac{\Delta t}{T_2}} \\
1 & 1 & 1 \\
\end{bmatrix}.
\]

The computation of \( e^{A\Delta t} \) follows directly from the above expressions.
Appendix D: Numerical Solution of the Electric Field Integral Equation with a 2D FFT-MoM-biCGstab(L) Method

D.1 Principle

The objective is to solve the integral equation for the electric field:

\[
E(r) = E_b(r) - i \omega \mu \int_{V_{\text{scat}}} \bar{G}(r, r') \cdot [\Delta \sigma(r')] \cdot E(r') \, dr'
\]  

To this end, we discretize the scattering volume, \(V_{\text{scat}}\), and cast the integral equation (D.1) into the matrix form

\[
E = E_b + A \cdot \Delta \sigma \cdot E.
\]  

In Eq. (D.1), \(E(r)\) and \(E_b(r)\) are 3-component complex-valued vectors. The matrix equivalent of Eq. (D.2) describes the column vectors \(E\) and \(E_b\) with the 3 components of the original vectors as indexed entries for all the elements that discretize \(V_{\text{scat}}\).

Solving the linear system (D.2) by direct methods becomes computationally impractical when more than a few hundreds discretization elements are involved. Thus, Eq. (D.2) has to be solved iteratively by minimizing the cost function

\[
\|E - A \cdot \Delta \sigma \cdot E - E_b\|_i,
\]

where the norm includes all the elements involved in the discretization. A Bi-Conjugate Gradient Stabilized method (Sleijpen and Fokkema, 1993) of order 1 proved to be an efficient solver for this problem when the background was more conductive than the scatterer (which is the case when the background medium becomes the saturating brine).

We make use of the Fast-Fourier-Transform (FFT) to compute the matrix product \(A \cdot \Delta \sigma \cdot E\) included in Eq. (D.2). As detailed below, the elements of matrix \(A\) are integrals of the projections of the Dyadic Green’s tensor. From the definitions of Eqs. (5.8)-(5.10), it follows that \(\tilde{G}(r, r') = \bar{G}(\|r - r'\|)\), whereupon \(\bar{G}\) is translation
invariant. Matrix $A$ is therefore block-Toeplitz, which allows certain manipulations of its entries without the need to numerically compute and store the full matrix $A$.

D.2 IMPLEMENTATION IN 2D SCATTERING PROBLEMS

The integration domain $V_{scat}$ of Eq. (D.1) is partitioned into a Cartesian grid consisting of $N_x$-$by$-$N_z$ square cells. Each square cell is identified with the symbol $V_n$. The 2D-FFT MoM method is implemented in three steps:

First, the matrix equation $\mathbf{E} - A \cdot (\Delta \sigma \cdot \mathbf{E}) = \mathbf{E}_b$ is projected onto each coordinate axis, $k = x, y, z$, to yield the projections

$$\mathbf{E}^k - \sum_{l=x,y,z} A^{kl} \cdot \left[ \sum_{p=x,y,z} (\Delta \sigma)^{lp} \cdot \mathbf{E}^p \right] = (\mathbf{E}_b)^k, \quad k = x, y, z,$$

where $A^{kl}$ is a family of $N_x$-$by$-$N_z$ matrices, $A^{kl} = \left( a_{mn}^{kl} \right)$, which include only the terms of components $kl = xx, xy, \ldots, zz$ of $A$, and whose elements are equal to

$$a_{mn}^{kl} = -i\omega \mu \int_{V_n} \mathcal{G}^{kl}(\mathbf{r}_m, \mathbf{r}') d\mathbf{r}' \cdot \mathbf{E}^l. \quad (D.4)$$

These elements are computed with the analytical expressions reported by Gao et al. (2005). In Eq. (D.3), the vectors $\mathbf{E}^k$ and $(\mathbf{E}_b)^k$ consist of $N_x \times N_z$ complex entries.

Second, a $N_x$-$by$-$N_z$ matrix $\mathbf{J}$ is constructed to store the complex current contrasts (i.e. the electrical currents multiplied by the conductivity contrasts $\Delta \sigma$) for each scattering cell. The projections of $\mathbf{J}$ onto the $x, y, z$ axes are designated as

$$\mathbf{J}^l = \sum_{p=x,y,z} (\Delta \sigma)^{lp} \cdot \mathbf{E}^p = \left( j_{mn}^l \right), \quad l = x, y, z.$$

Explicitly, for a 2D medium the contrast of internal current within each cell $(m, n)$ is a function of the complex conductivity contrasts and the total electric fields in that cell, i.e.,

$$j_{mn}^l = \Delta \sigma_{xx}(m,n) \ E_x^l(m,n) + \Delta \sigma_{xy}(m,n) \ E_y^l(m,n) + \Delta \sigma_{xz}(m,n) \ E_z^l(m,n). \quad (D.6)$$
Third, each matrix $A^{kl}$ is block-Toeplitz because of the translational invariance of both the Green’s function $g$ and the tensor $\tilde{G}$. Using the method proposed by Fang et al. (2003), the circulant matrix $C^{kl}$ of $A^{kl}$ can be written as

$$C^{kl} = \left[ \left( c^{kl} \right) \mathbf{R} \left( c^{kl} \right) \mathbf{R}^2 \left( c^{kl} \right) \ldots \mathbf{R}^{M_l-1} \left( c^{kl} \right) \right],$$

where $\mathbf{R} = \left[ \mathbf{e}_2 \mathbf{e}_3 \ldots \mathbf{e}_{-(N_y-1)} \mathbf{e}_{-(N_y)} \mathbf{e}_{-1} \right]$ is a permutation of the identity matrix and $\mathbf{e}_k$ is the $k$-th column of the identity matrix. For a one-dimensional geometry of length $N$, $\left( c^{kl} \right)$ becomes a vector with $N$ entries. In two dimensions, the same vector consists of $M_x$ vectors with $M_z$ entries each. The expression for $\left( c^{kl} \right)$ can be formally written with the following $M_x$-by-$M_z$ matrix:

$$c^{kl} = \begin{bmatrix}
  a^{kl}_{m=n=0} & a^{kl}_{m=0,n=1} & \ldots & a^{kl}_{m=0,n=N_y} & 0 & \ldots & 0 & a^{kl}_{m=0,n=-N_y} & \ldots & a^{kl}_{m=0,n=-1} \\
  a^{kl}_{m=1,n=0} & a^{kl}_{m=1,n=1} & \ldots & a^{kl}_{m=1,n=N_y} & 0 & \ldots & 0 & a^{kl}_{m=1,n=-N_y} & \ldots & a^{kl}_{m=1,n=-1} \\
  \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
  a^{kl}_{m=N_x,n=0} & a^{kl}_{m=N_x,n=1} & \ldots & a^{kl}_{m=N_x,n=N_y} & 0 & \ldots & 0 & a^{kl}_{m=N_x,n=-N_y} & \ldots & a^{kl}_{m=N_x,n=-1} \\
  0 & 0 & \ldots & 0 & 0 & \ldots & \ldots & \vdots & \ddots & \vdots \\
  \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
  0 & 0 & \ldots & 0 & 0 & \ldots & \ldots & \vdots & \ddots & \vdots \\
  a^{kl}_{m=-N_x,n=0} & a^{kl}_{m=-N_x,n=1} & \ldots & a^{kl}_{m=-N_x,n=N_y} & 0 & \ldots & 0 & a^{kl}_{m=-N_x,n=-N_y} & \ldots & a^{kl}_{m=-N_x,n=-1} \\
  \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
  a^{kl}_{m=-1,n=0} & a^{kl}_{m=-1,n=1} & \ldots & a^{kl}_{m=-1,n=N_y} & 0 & \ldots & 0 & a^{kl}_{m=-1,n=-N_y} & \ldots & a^{kl}_{m=-1,n=-1}
\end{bmatrix}.$$

Zeroes pad each row so that $M_x$ is the next second-power of $(2N_x-1)$, and $M_z$ is the second-power of $(2N_z-1)$. Thus, the product $A^{kl} \cdot J^l$ can then assessed without explicit construction and storage of $A^{kl}$ via convolution of $c^{kl}$ and $J^l$, i.e.,

$$A^{kl} \cdot J^l = \text{ifft2} \left[ \text{fft2} \left( c^{kl} \right) \ast \text{fft2} \left( J^l \right) \right].$$

In this last equation, $\text{fft2}$ identifies the $M_x$-by-$M_z$ point 2D Fourier transform operator, $\text{ifft2}$ is the corresponding inverse transform, and the operator $\ast$ denotes term-by-
term multiplication. The result of the matrix product $\mathbf{A}^k \cdot \mathbf{J}^t$ appears in the first $N_x$-by-$N_z$ submatrix obtained through 

$\text{ifft2}$.

The entries of $\mathbf{c}^k$ are calculated only once for the entire inversion by successively solving Eqs. (D.4) and (D.8). Then, for each update of the electric current distribution $\mathbf{E}$, the currents contrasts are calculated via Eq. (D.6) and the product $\mathbf{A} \cdot (\Delta \sigma \cdot \mathbf{E}) = \sum_{l=x,y,z} \mathbf{A}^k \cdot \mathbf{J}^t$ is calculated using Eq. (D.9). Subsequently, we calculate the residual $\|\mathbf{E} - \mathbf{A} \cdot (\Delta \sigma \cdot \mathbf{E}) - \mathbf{E}_b\|_L$, and $\mathbf{E}$ is updated through a Bi-Conjugate Gradient Stabilized (biCGstab) method until the residual reaches a prescribed tolerance. For the cases simulated in this chapter, the choice $L = 1$ for the biCGstab stabilization order yielded faster convergence than larger values of $L$.

### D.3 COMPARISON WITH THE ANALYTICAL SOLUTION OF SCATTERING DUE A HOMOGENEOUS DISC

We consider a homogeneous disc-shape scatterer and analyze the numerical error existing between (a) the internal electric fields calculated with the 2D FFT-MoM method described above, and (b) the internal fields calculated analytically with a cylindrical expansion (see Appendix E). The numerical approach discretizes the disc on a grid of 401x401 pixels, i.e., the disc has a radius equal to 200 pixels. The frequency is varied logarithmically from 10 kHz to 1 GHz and the electrical parameters used for this comparison are the following: $\sigma_w = 1$ S/m, $\kappa_w = 70$, $\sigma_{\text{disc}} = 0.01$ S/m, and $\kappa_{\text{disc}} = 20$. The diameter of the disc is only 401 $\mu$m, which makes the analytical value for the internal electric field constant over the entire disc surface. In what follows, the projections of the numerical error for each pixel $i$ are defined as:

$$\text{error}^i = \frac{E^i - E^a}{E^a} ,$$

(D.10)
where $E^i_{x,z}$ are the Cartesian projections of the internal electric field calculated for pixel $i$, and $E^a_{x,z}$ are the projections of the analytical internal electric field calculated close to the disc center. Figure D.1 shows the results of this analysis. For all the tested frequencies, the top panels show that the numerical error within the disc lies within $10^{-2}$ or 1% of the analytical solution. The white disc periphery (zones of maximal error) illustrates the increasing importance of fringing effects for decreasing values of frequency. We employ two norms, the infinity norm $L_{\infty}$ (maximal relative error amplitude) and the $L_1$ norm (mean relative error amplitude) to measure the overall numerical error achieved at each frequency. The bottom panel of Fig. D.1 shows the results obtained by computing the errors over the complete or part of the scatterer body. A disc radius of 200 pixels stands for the entire disc discretized on the 401x401 pixel grid, whereas smaller concentric discs ignore the outmost pixels of the scattering disc where fringing occurs. The $L_1$ norm yields less than 1% error at all frequencies regardless of fringing effects. On the other hand, the $L_{\infty}$ norm achieves a similar accuracy when it is computed over the central 180-pixel disc, but it shows the degradation of the fields homogeneity at the disc edge when it is computed for larger radii.
Figure D.1: Analysis of 2D FFT-MoM numerical error for the internal electric fields within a homogeneous cylinder of 401x401 pixel resolution. Top panels: distribution of the error for both $x$ and $z$ projections at several frequencies. Bottom panel: $L_{\infty}$ and $L_1$ norms of the relative error computed as a function of frequency and over decreasing disc radii within the scatterer.
Appendix E: Cylindrical Mode Expansion of the Electric Fields Scattered by Homogeneous and Isotropic Infinite Cylinder due to TM Plane-Wave Excitation

We calculate the electric field scattered by a homogeneous circular cylinder due to a transverse-magnetic (TM) plane wave excitation perpendicular to the circular cross-section of the cylinder. This is achieved with a cylindrical modal expansion and by subsequently matching boundary conditions at the surface of the cylinder (Balanis, 1989). In so doing, radial coordinates are used to describe the incident electric field according to the geometrical framework described in Fig. 5.1. The radial coordinates include \( \rho \), the radial distance from the center of the scatterer (i.e. the axis of the infinite cylinder), and \( \theta \), the angle formed between the direction of the incident field and the location vector \( \mathbf{r} \). At the radian frequency \( \omega \) and for a homogeneous complex effective conductivity \( \sigma^* \), the wave number \( k_h \) within the homogeneous cylinder is given by

\[
k_h^2 = i\omega \mu_0 \sigma^* .
\]  

(E.1)

The TM plane wave excitation is defined by the \((x, z)\) Cartesian components of the electric field given by Eq. (5.7) or, equivalently, by the \(y\) component (perpendicular to the plane of the scatterer) of the dual magnetic field \( H_y^{pw} \) expanded in cylindrical harmonics as:

\[
H_y^{pw} (\rho, \theta) = H_0 \sum_{n \geq 1} (-i)^n J_n (k_h \rho) \exp (in \theta) ,
\]

(E.2)

where \( J_n \) is the Bessel function of the first kind and order \( n \). In expanded notation, the magnetic field induced at points outside the cylinder can be written as

\[
H_y^{out} (\rho > a, \theta) = H_0 \sum_{n = -\infty}^{\infty} (-i)^n B_n J_n (k_h \rho) \exp (in \theta) .
\]

(E.3)

Inside the cylinder, the harmonic expansion of the induced magnetic field is given by
\[ H_y^{in}(\rho < a, \theta) = H_0 \sum_{n \geq 1} (-i)^n B_n J_n(k_a \rho) \exp(in\theta). \tag{E.4} \]

The coefficients \( B_n \) in the above expressions are calculated by enforcing the continuity of the longitudinal magnetic fields (projections on the \( y \) axis) and the continuity of the tangential electric field at the boundary of the cylinder. The first continuity condition reads as
\[ H_y^{pw}(\rho = a) + H_y^{out}(\rho = a) = H_y^{in}(\rho = a), \tag{E.5} \]
and the second,
\[ E_\theta^{pw}(\rho = a) + E_\theta^{out}(\rho = a) = E_\theta^{in}(\rho = a). \tag{E.6} \]

The tangential and radial electric fields are calculated from the longitudinal magnetic field via the relations:
\[ E_\theta(\rho) = -\frac{i}{\omega \varepsilon} \frac{\partial H_y}{\partial \rho} \quad \text{and} \quad E_\rho(\rho) = \frac{1}{\omega \varepsilon} \frac{\partial H_y}{\partial \theta}. \tag{E.7} \]

By deriving the tangential components of the electric fields from Eqs (E.2), (E.3), (E.4) and (E.7), and by simultaneously solving Eqs. (E.5) and (E.6), one obtains an explicit solution for the coefficients \( B_n \), given by
\[ B_n = \frac{A_n H_n^{(1)}(k_a a) + J_n(k_a a)}{J_n(k_a a)} \tag{E.9} \]

where
\[ A_n = \sqrt{\frac{E_n}{E_n}} J_n(k_a a) J_n'(k_a a) - \sqrt{\frac{E_n}{H_n^{(1)}}} J_n(k_a a) J_n'(k_a a). \tag{E.10} \]

In Eqs. (E.9) and (E.10), \( J_n' \) is the derivative of the Bessel function of the first kind and order \( n \), and \( H_n^{(1)} \) is the Hankel function of the first kind and order \( n \).

Inside the cylinder, the azimuthal and radial components of the electric field are given by

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\[ E_{\theta}^{\text{in}}(\rho, \theta) = i \sqrt{\frac{\mu_0}{\varepsilon_n}} H_0 \left[ B_0 J_1(k_0 \rho) - 2 \sum_{n \geq 1} (-i)^n B_n J_n'(k_0 \rho) \cos(n\theta) \right], \quad \text{(E.11)} \]

and

\[ E_{\rho}^{\text{in}}(\rho, \theta) = -\frac{2i}{\omega \varepsilon_b} \frac{1}{\rho} H_0 \sum_{n \geq 1} \rho (-i)^n B_n J_n'(k_0 \rho) \sin(n\theta), \quad \text{(E.12)} \]

respectively.

The normalized amplitude of the incident plane wave, \( H_0 \), is related to the unit amplitude of the dual electric field given by Eq. (5.7). At the center of the scatterer, \( \rho = 0 \), and Eq. (E.8) reduces to

\[ E_{\phi}^{\text{pw}}(\rho = 0, \theta) = \frac{i}{\omega \varepsilon_b} \lim_{\rho \to 0} \left( \frac{1}{\rho} \frac{\partial H_{\phi}^{\text{pw}}}{\partial \theta} \right) = -\sqrt{\frac{\mu_0}{\varepsilon_b}} H_0 \cos \theta. \quad \text{(E.13)} \]

Given the geometrical description of Fig. 5.1, at the center of the scatterer the unit amplitude of the background field \( E_b \) is oriented opposite to the tangential component \( E_{\phi}^{\text{pw}}(0, \phi) \). Thus,

\[ 1 = -E_{\theta}^{\text{pw}}(\rho = 0, \theta = \phi), \quad \text{(E.14)} \]

and

\[ H_0 = \sqrt{\frac{\varepsilon_b}{\mu_0 \cos \phi}}. \quad \text{(E.15)} \]

Projection of the azimuthal and radial components of Eqs. (E.11) and (E.12), respectively, together with substitution of the plane-wave incidence angle \( \phi \) and the position angle \( \theta \), yield the Cartesian components of the electric field within the homogeneous cylinder, \( E_h \).
Appendix F: Practical Implementation of the Minimization Problem

Numerical experiments indicate that the estimated values of effective electric conductivity and dielectric constant obtained from the minimization of the cost function defined by Eq. (5.12) are not always consistent with the expected asymptotic behavior at low and high frequencies. To circumvent this problem, we first define the electrical field and electric-current residuals as

\[ \Delta \mathbf{E} = \mathbf{E} - \mathbf{E}_h, \text{ and} \]
\[ \Delta \mathbf{J} = \mathbf{\bar{\sigma}}^* \mathbf{E} - \mathbf{\bar{\sigma}}^*_h \mathbf{E}_h, \]

respectively. Moreover, we note that, according to Schwartz’ inequality,

\[ \Psi = \left\| \Delta \mathbf{J} - \mathbf{\bar{\sigma}}^* \Delta \mathbf{E} \right\|_{L^2} \leq \left\| \Delta \mathbf{J} \right\|_{L^2} + \left\| \mathbf{\bar{\sigma}}^* \right\| \times \left\| \Delta \mathbf{E} \right\|_{L^2}. \]  

We now compare the performance of three choices of cost function when inverting the conductivity and dielectric constant of a homogeneous disc-shaped pore map. These cost functions are defined as:

\[ \Psi_1 = \left\| \Delta \mathbf{J} - \mathbf{\bar{\sigma}}^* \Delta \mathbf{E} \right\|_{L^2}, \]
\[ \Psi_2 = \left\| \text{Re} \left( \Delta \mathbf{J} - \mathbf{\bar{\sigma}}^* \Delta \mathbf{E} \right) \right\|_{L^2} + \left\| \text{Im} \left( \Delta \mathbf{J} - \mathbf{\bar{\sigma}}^* \Delta \mathbf{E} \right) \right\|_{L^2}, \text{ and} \]
\[ \Psi_3 = \left\| \Delta \mathbf{J} \right\|_{L^2} + \left| \mathbf{\bar{\sigma}}^* \right| \times \left\| \Delta \mathbf{E} \right\|_{L^2}. \]

To assess the performance of the three cost functions defined above, we consider combinations of three values of conductivity \( \sigma_{\text{disc}} \) (0.001, 0.01 and 0.1 S/m) and three values of dielectric constant \( \kappa_{\text{disc}} \) (20, 200 and 2000) assigned to homogeneous disc-shaped pore maps. We compute the internal electric fields for frequencies ranging from 1 kHz to 1 GHz, and use the three cost functions described by Eqs. (F.4) to (F.6) to invert the effective properties \( \sigma_{\text{eff}} \) and \( \kappa_{\text{eff}} \) starting from the same forward simulation results. In all cases, the brine background consists of 1 S/m
conductivity and a dielectric constant equal to 70. Results from this exercise are shown in Fig. F.1.

When \( \sigma_{\text{disc}} \) is at least equal to 0.1 S/m, both \( \sigma_{\text{eff}} \) and \( \kappa_{\text{eff}} \) are properly estimated with the three cost functions – with slightly better results for the cost function \( \Psi_3 \) compared to \( \Psi_1 \) and \( \Psi_2 \). Incorrect results are obtained when \( \kappa_{\text{disc}} \) is as large as 2000 above 3 MHz – fortunately this case is not realistic in saturated rocks. When \( \sigma_{\text{disc}} \) is lower that 0.1 S/m, \( \Psi_1 \) overestimates \( \kappa_{\text{eff}} \) at low frequencies and systematically yields wrong (even negative) values for \( \sigma_{\text{eff}} \). Cost function \( \Psi_2 \) yields relatively better results, always leads to the right values of \( \kappa_{\text{eff}} \), but the inverted values \( \sigma_{\text{eff}} \) are as inconsistent as those obtained with \( \Psi_1 \). Cost function \( \Psi_3 \) yields the most accurate and stable results in all the cases. As indicated in Fig. F.1, bounds exist beyond which \( \kappa_{\text{eff}} \) and/or \( \sigma_{\text{eff}} \) are not properly inverted with cost function \( \Psi_3 \).

For realistic cases of rock/fluid mixtures, it can be conservatively stated that the dielectric constant is never higher than 50 above 1 MHz. In this case, we expect the minimization algorithm to converge for conductivities above 0.01 S/m and for frequencies as high as 1 GHz. Similarly, we expect the minimization algorithm to converge for conductivities above 0.001 S/m and for frequencies as high as 10 MHz.

In the presence of low-frequency enhancement due to clays or other electrochemical factors, the dielectric constant might increase up to several thousands below 1 MHz. In this case, both dielectric constant and conductivity are correctly inverted for conductivity values as low as 0.01 S/m.
Figure F.1: Inversion results for a 501x501 pixels homogeneous disc with different combinations of effective conductivity $\sigma_{\text{disc}}$ and dielectric constant $\kappa_{\text{disc}}$, with different cost functions. Dash-dotted lines: using cost function $\Psi_1$; dashed lines: $\Psi_2$; plain lines: $\Psi_3$. Dotted lines designate the true values for $\sigma_{\text{disc}}$ and $\kappa_{\text{disc}}$. 
Abbreviations and Nomenclature

1D One-dimensional
2D Two-dimensional
3D Three-dimensional

\( a \) Tortuosity factor in modified Archie’s equations

\( a, b, c \) Geometric parameters [m]

A Evolution matrix in Bloch’s equations

\( A \) Partial NMR porosity (amplitude) linked to a given relaxation time bin [dimensionless]

B Magnetic field density in the spin rotating frame

\( B_0 \) Background magnetic field density exerted by permanent tool magnet

\( B_0 \) Norm of \( B_0 \) [Tesla]

\( \Delta B_0 \) Background magnetic field density in the spin rotating frame

\( \Delta B_0 \) Norm of \( \Delta B_0 \) [Tesla]

\( B_1 \) RF magnetic field density exerted by tool coils

\( B_1 \) Norm of \( B_1 \) [Tesla]

BET Brunauer-Emmett-Teller

biCGstab Bi-conjugate gradient stabilized

c Throat center

C Compaction coefficient of a consolidated cubic-centered periodic grain pack. Ion density in brine [dimensionless] [m^{-3}]

C Pore center. Grain center

CEC Cation exchange capacity
<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
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<tbody>
<tr>
<td>CPMG</td>
<td>Carr-Purcell-Meiboom-Gill</td>
</tr>
<tr>
<td>CRIM</td>
<td>Complex refractive index method</td>
</tr>
<tr>
<td>CT</td>
<td>Computer tomography</td>
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<tr>
<td>D</td>
<td>Electric displacement field</td>
</tr>
<tr>
<td>D</td>
<td>Diffusivity (or diffusion coefficient) $\left[ m^2.s^{-1} \right]$</td>
</tr>
<tr>
<td>DC</td>
<td>Direct-current</td>
</tr>
<tr>
<td>e</td>
<td>Ellipse eccentricity $\left[ \text{dimensionless} \right]$</td>
</tr>
<tr>
<td>E</td>
<td>Electric field</td>
</tr>
<tr>
<td>$E$</td>
<td>Norm of $E$ $\left[ \text{Volts} \right]$</td>
</tr>
<tr>
<td>$E_0$</td>
<td>Electric field unit amplitude $\left[ \text{Volts} \right]$</td>
</tr>
<tr>
<td>EDL</td>
<td>Electrical double-layer</td>
</tr>
<tr>
<td>EM</td>
<td>Electromagnetic</td>
</tr>
<tr>
<td>f</td>
<td>Frequency $\left[ \text{Hertz} \right]$</td>
</tr>
<tr>
<td>FFT</td>
<td>Fast Fourier transform</td>
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<tr>
<td>$F_R$</td>
<td>Resistivity formation factor</td>
</tr>
<tr>
<td>g</td>
<td>Probability of transfer through a membrane of permeability $P$. Green’s function for the electric field</td>
</tr>
<tr>
<td>$\tilde{G}$</td>
<td>Dyadic Green’s tensor for the electric field</td>
</tr>
<tr>
<td>G</td>
<td>Magnetic field gradient</td>
</tr>
<tr>
<td>$G$</td>
<td>Norm of $G$ $\left[ \text{Gauss.m}^{-1} \right]$</td>
</tr>
<tr>
<td>h</td>
<td>Micro-fracture aperture $\left[ \text{m} \right]$</td>
</tr>
<tr>
<td>H</td>
<td>Magnetic field</td>
</tr>
<tr>
<td>$H$</td>
<td>Norm of $H$ $\left[ \text{Amp.m}^{-1} \right]$</td>
</tr>
<tr>
<td>$H_0$</td>
<td>Magnetic field unit amplitude $\left[ \text{Amp.m}^{-1} \right]$</td>
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<tr>
<td>Symbol</td>
<td>Definition</td>
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<td>--------</td>
<td>------------</td>
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<tr>
<td>$I_R$</td>
<td>Resistivity index</td>
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<td>$J$</td>
<td>Current density</td>
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<td>$k$</td>
<td>Wave vector in a homogeneous medium</td>
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<tr>
<td>$k$</td>
<td>Exchange rate through a membrane of permeability $P$. Wave number in a homogeneous medium (norm of $k$)</td>
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<td>Depolarization factor</td>
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<tr>
<td>$L, L'$</td>
<td>Distances of a diffusion path</td>
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<td>$L_1, L_2$</td>
<td>Maximal amplitude norm, quadratic norm</td>
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<tr>
<td>LWD</td>
<td>Logging-while-drilling</td>
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<tr>
<td>$m$</td>
<td>Archie’s cementation (or lithology) exponent</td>
</tr>
<tr>
<td>$M$</td>
<td>Spin-packet magnetization</td>
</tr>
<tr>
<td>$M$</td>
<td>Norm of $M$</td>
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<tr>
<td>$M'$</td>
<td>Spin-packet reduced magnetization</td>
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<tr>
<td>$M_0$</td>
<td>Equilibrium spin-packet magnetization (aligned with $B_0$)</td>
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<td>$M_0$</td>
<td>Norm of $M_0$</td>
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<td>MoM</td>
<td>Method of moments</td>
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<td>MOW</td>
<td>Mixed-oil-wet</td>
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<tr>
<td>MRI</td>
<td>Magnetic resonance imaging</td>
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<tr>
<td>$n$</td>
<td>Archie’s saturation exponent</td>
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<tr>
<td>$n$</td>
<td>Vector of random numbers</td>
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<tr>
<td>$\hat{n}$</td>
<td>Unit vector normal to a boundary</td>
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<tr>
<td>N</td>
<td>Tetrahedron neighboring $\Omega$</td>
</tr>
<tr>
<td>NMR</td>
<td>Nuclear magnetic resonance</td>
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<tr>
<td>O</td>
<td>Geometric center of the NMR volume of investigation</td>
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<tr>
<td>Symbol</td>
<td>Definition</td>
</tr>
<tr>
<td>--------</td>
<td>------------------------------------------------</td>
</tr>
<tr>
<td>OBM</td>
<td>Oil-based mud</td>
</tr>
<tr>
<td>OW</td>
<td>Oil-wet</td>
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<td>( P )</td>
<td>Membrane permeability</td>
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<td>( p_1, p_2 )</td>
<td>Killing probability associated with a surface relaxivity ( \rho_1, \rho_2 )</td>
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<td>p.u.</td>
<td>Porosity units</td>
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<td>( Q )</td>
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<td>( r )</td>
<td>position vector</td>
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<tr>
<td>( r )</td>
<td>Norm of ( r )</td>
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<tr>
<td>( r_0 )</td>
<td>Throat size</td>
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<tr>
<td>( R )</td>
<td>Radius. Electric resistance</td>
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<tr>
<td>( R_0 )</td>
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<td>RF</td>
<td>Radio-frequency</td>
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<td>( S )</td>
<td>Fluid saturation</td>
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<td>( S/V )</td>
<td>Surface-to-volume ratio</td>
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<td>( t )</td>
<td>Time</td>
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<td>( t_{90}, t_{180} )</td>
<td>Duration of a ( \pi/2 ) B1 RF pulse, of a ( \pi ) B1 RF pulse</td>
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<td>( T )</td>
<td>Film thickness. Temperature</td>
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<td>( T_1 )</td>
<td>Longitudinal relaxation time</td>
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<td>( T_2 )</td>
<td>Transversal relaxation time</td>
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<tr>
<td>( TE )</td>
<td>Echo time</td>
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<tr>
<td>( TW )</td>
<td>Wait time</td>
</tr>
<tr>
<td>TM</td>
<td>Transverse magnetic</td>
</tr>
<tr>
<td>WBEM</td>
<td>Wide-band electromagnetic</td>
</tr>
</tbody>
</table>
WBM  Water-based mud
WW  Water-wet
\(\hat{x}, \hat{y}, \hat{z}\)  Orthonormal vectors forming the fixed basis \(\Gamma\)
\(\hat{x}', \hat{y}'\)  Orthonormal vectors forming the rotating frame \(\Sigma\)
X  Reactance. Salinity  \([\Omega] [\text{ppm}]\)
Y  Admittance  \([\text{Siemens}]\)
Z  Impedance  \([\Omega]\)

Symbols and Greek characters
\(\alpha\)  Blob size geometric factor  \([\text{dimensionless}]\)
\(\beta\)  Incremental film thickness geometric factor. Counter-ion surface charge density  \([\text{dimensionless}] [\text{Coulomb.m}^{-2}]\)
\(\gamma\)  Gyromagnetic ratio  \([\text{rad.Gauss}^{-1}.\text{s}^{-1}]\)
\(\delta\)  Double-layer efficiency  \([\text{dimensionless}]\)
\(\delta(...)\)  Dirac function
\(\delta t\)  Infinitesimal random walk step duration  \([\text{s}]\)
\(\delta r\)  Infinitesimal random walk step size increment  \([\text{m}]\)
\(\delta \phi\)  Infinitesimal spin phase shift in the \((x',y')\) rotating frame  \([\text{rad}]\)
\(\Gamma\)  Geometrical basis
\(\Delta...\)  Property vector referenced from the sweet spot for NMR calculations
\(\Delta...\)  Property contrast between background and scattering elements for EM calculations  \([\text{dimensionless}]\)
\(\varepsilon\)  Dielectric permittivity. Boolean  \([\text{Farad.m}^{-1}] [\text{dimensionless}]\)
\(\varepsilon_0\)  Dielectric permittivity of vacuum  \([\text{Farad.m}^{-1}]\)
\( \theta \)  
Polar angle  
[rad]

\( \theta_x, \theta_y \)  
Orientation of a microfracture with respect to the \( x \) axis, to the \( y \) axis  
[rad]

\( \kappa \)  
Dielectric constant  
[dimensionless]

\( \mu_0 \)  
Magnetic permeability of vacuum  
[Newton.Amps\(^{-2}\)]

\( \Pi \)  
Plane defining one face of \( \Omega \)

\( \Pi' \)  
Plane limiting one side of a microfracture

\( \rho \)  
Surface relaxivity. Electric resistivity  
[m.s\(^{-1}\)] [Ω.m]

\( \sigma \)  
Conductivity  
[Siemens.m\(^{-1}\)]

\( \Sigma \)  
Spin rotating frame

\( \tau \)  
Tortuosity. Half echo time. Electric polarization relaxation time  
[dimensionless] [s] [s]

\( \phi \)  
Porosity. Spin phase shift. Angle of incidence of an impinging wave with respect to \( z \) axis  
[dimensionless] [rad] [rad]

\( \omega \)  
Radian frequency  
[rad/s]

\( \Omega \)  
Unit tetrahedron within the Delaunay tessellation

\( \langle ... \rangle \)  
Average over a statistical population

\( \| ... \| \)  
Norm over a vector of data points

\( \int ... \)  
Integral operator

\( * \)  
Term-by-term vector multiplication operator

\( \times \)  
Curl operator. Scalar multiplication

Subscripts

\( b \)  
Background
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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</thead>
<tbody>
<tr>
<td>$B$</td>
<td>Bulk property</td>
</tr>
<tr>
<td>CRIM</td>
<td>Property calculated using the CRIM model</td>
</tr>
<tr>
<td>$D$</td>
<td>Diffusion property</td>
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<tr>
<td>$disc$</td>
<td>Homogeneous disc property</td>
</tr>
<tr>
<td>$eff$</td>
<td>Effective property</td>
</tr>
<tr>
<td>$f$</td>
<td>Fluid type</td>
</tr>
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<td>$h$</td>
<td>Homogenous scatterer property</td>
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<tr>
<td>$host$</td>
<td>Property assigned to the host phase in a mixture</td>
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<tr>
<td>$o$</td>
<td>Oil</td>
</tr>
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<td>$r$</td>
<td>Rock</td>
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<td>$r, \theta$</td>
<td>Polar projections (radial, tangential)</td>
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<tr>
<td>$s$</td>
<td>Pore size</td>
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<tr>
<td>$S$</td>
<td>Surface property</td>
</tr>
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<td>$V$</td>
<td>Velocity-induced property (drift)</td>
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<td>$w$</td>
<td>Water</td>
</tr>
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<td>$x, y, z$</td>
<td>Cartesian projections</td>
</tr>
<tr>
<td>$\Pi'$</td>
<td>Projected on $\Pi'$</td>
</tr>
</tbody>
</table>

**Superscripts**

- $app$ | Apparent
- $f$ | Fluid index
- $i$ | Value of a property at random-walk step $i$
- $s$ | Pore size index
- $*, ', '"$ | Complex property, real part, imaginary part
\begin{tabular}{l l}
$T$ & Matrix transposition \\
\_ & Total property \\
\end{tabular}
Bibliography


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