"Hydrogeophysical characterization of soil using ground penetrating radar"

Lambot, Sébastien

Abstract
The knowledge of the dynamics of soil water is essential in agricultural, hydrological and environmental engineering as it controls plant growth, key hydrological processes, and the contamination of surface and subsurface water. Nearby remote sensing can be used for characterizing non-destructively the hydrogeophysical properties of the subsurface. In that respect, ground penetrating radar (GPR) constitutes a promising high resolution characterization tool. However, notwithstanding considerable research has been devoted to GPR, its use for assessing quantitatively the subsurface properties is constrained by the lack of appropriate GPR systems and signal analysis methods. In this study, a new integrated approach is developed to identify from GPR measurements the soil water content and hydraulic properties governing water transfer in the subsurface. It is based on hydrodynamic and electromagnetic inverse modeling. Research on GPR has focused on GPR design, forward modeling of GPR signal...

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Hydrogeophysical characterization of soil using ground penetrating radar

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NOVEMBRE 2003
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The most incomprehensible thing about the universe is that it is comprehensible.

Albert Einstein
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Contents

1 Introduction 1
  1.1 Research Topic .............................................. 1
  1.2 Project Objectives ......................................... 4
  1.3 Scientific Originality and Innovation ..................... 8

2 A new hydrodynamic inverse modeling procedure 11
  2.1 Introduction ................................................. 12
  2.2 Theory ...................................................... 14
    2.2.1 The direct flow problem ............................... 14
    2.2.2 The inverse problem .................................. 16
  2.3 Methodology ................................................. 22
    2.3.1 Simulation of transient flow experiments ............. 22
    2.3.2 Parameterization ...................................... 24
    2.3.3 Sensitivity analysis, sampling design, and parameter identifiability .. 24
    2.3.4 Infiltration experiment on a laboratory sand ........ 27
  2.4 Results and Discussion .................................... 27
    2.4.1 Uniqueness of the inverse solution and GMCS-NMS performances . 27
    2.4.2 Stability of the inverse solution ...................... 32
    2.4.3 Laboratory case study .................................. 35
  2.5 Summary and Conclusions .................................. 36

3 Hydrodynamic inversion in laboratory conditions 39
  3.1 Introduction ................................................. 40
  3.2 Materials and Methods ..................................... 42
    3.2.1 Hydrodynamic model parameterization ................ 42
    3.2.2 Inversion ................................................ 44
    3.2.3 Laboratory experiments description ................... 44
  3.3 Results and Discussions .................................... 48
    3.3.1 Response surface analysis ............................. 48
    3.3.2 Hydraulic properties ................................... 49
    3.3.3 Water transfer ........................................... 52
  3.4 Summary and Conclusions .................................. 56

4 GPR design and modeling 59
  4.1 Introduction ................................................. 60
  4.2 Ground Penetrating Radar System ......................... 61
    4.2.1 Frequency domain radar ................................ 61
    4.2.2 TEM horn antenna ...................................... 62
  4.3 System Description and Modeling Assumptions ............. 64
    4.3.1 Radar measurements ..................................... 64
    4.3.2 The Fraunhofer approximation .......................... 64
    4.3.3 Antenna equation in the frequency domain ............ 66
    4.3.4 Virtual source point of the TEM horn ............... 68
  4.4 Formulation of Electromagnetic Field Equations .......... 69
    4.4.1 Dielectric properties of materials ................... 69
    4.4.2 Frequency dependence ................................... 70
    4.4.3 Model configuration ..................................... 71
    4.4.4 Frequency domain Maxwell’s equations ............... 72
    4.4.5 Spectral domain Maxwell’s equations ................. 73
## Contents

4.5 Solution for Ground Penetrating Radar .................................. 74  
4.5.1 Fields in a homogeneous medium ......................................... 74  
4.5.2 Source above a layered stack ........................................... 77  
4.5.3 Response of the multilayered medium .................................... 79  
4.6 Inverse Spatial Fourier Transformation ................................. 80  
4.6.1 Transition to polar coordinates ........................................ 80  
4.6.2 Numerical evaluation of the integral ................................... 83  
4.7 Simulations and Measurements ............................................ 83  
4.7.1 Frequency response of the TEM horn .................................. 83  
4.7.2 Reflection on a metal sheet ........................................... 86  
4.7.3 Inverse estimation of the antenna position ............................ 87  
4.7.4 Free space response of the antenna ................................... 88  
4.8 Summary and Conclusions .................................................. 89  

5 Soil dielectric properties from GPR signal inversion ................. 91  
5.1 Introduction ........................................................................ 92  
5.2 Materials and Methods ...................................................... 94  
5.2.1 Model inversion .......................................................... 94  
5.2.2 Experiments description ............................................... 95  
5.3 Results and Discussions .................................................... 96  
5.3.1 Response surface analysis ............................................... 96  
5.3.2 Water content estimation .............................................. 99  
5.3.3 Electric conductivity estimation ....................................... 102  
5.4 Summary and Conclusions ................................................ 102  

6 Accurate modeling of GPR signal ........................................ 105  
6.1 Improved antenna model .................................................... 106  
6.2 Frequency dependence of the electric conductivity ..................... 108  
6.3 Experiment Description .................................................... 108  
6.3.1 Setup ........................................................................ 108  
6.3.2 Measurements and analysis ........................................... 109  
6.4 Results and Discussion .................................................... 110  
6.4.1 Effect of the frequency dependence .................................. 110  
6.4.2 Water content estimation .............................................. 111  
6.4.3 Electric conductivity estimation ....................................... 113  
6.4.4 Sensitivity analysis ...................................................... 115  
6.5 Summary and Conclusions ................................................ 116  

7 Measuring the water retention curve using GPR ....................... 119  
7.1 Model Configuration .......................................................... 120  
7.2 Numerical Experiments ...................................................... 121  
7.3 Outdoor Experiment .......................................................... 123  
7.3.1 Description ................................................................ 123  
7.3.2 Results and discussions ............................................... 124  
7.4 Summary and Conclusions ................................................ 126  

8 Summary, conclusions, and perspectives ............................... 129  
8.1 Hydrodynamic Inversion ..................................................... 129  
8.2 Ground Penetrating Radar and Electromagnetic Inversion ........... 131  
8.3 Further Perspectives ........................................................ 133  

References .............................................................................. 135
Contents

List of publications 145
International Conferences 147
About the author 149
Chapter 1

Introduction

1.1 Research Topic

The importance of an accurate characterization of the shallow subsurface is increasingly recognized in the fields of agricultural and environmental engineering, groundwater hydrology, meteorology, soil physics, and civil and military engineering. In hydrology, for instance, the readiness of a catchment to generate surface runoff during storm rainfall is related to its root zone storage capacity, a variable which can be computed accurately when the soil moisture profile is known. In agriculture, crop growth and the associated evapotranspiration is largely determined by the available amount of water in the root zone, so soil moisture profile information is necessary for irrigation scheduling and crop yield forecasting. Soil water content monitoring is important to maintain an optimal balance between crop yield and groundwater pumping, for flood control, and to maintain ecosystem harmony [Schlesinger et al., 1990]. Among many other applications, for example, the knowledge of the soil water content is also relevant to maintain proper moisture in highway subgrades [Birchak et al., 1974] or to support humanitarian landmine identification [Scheers, 2001; Lambot et al., 2003f].

More particularly, the characterization of the inherent spatial variability of the soil properties in cropped fields is needed to further develop site-specific farming practices that match agricultural inputs with local crop requirements [Stafford, 2000; Zhang et al., 2002]. Soil properties such as soil water content and nutrient status vary considerably across a given field. Ignoring the within field soil variability may result in over- and/or undersupplied areas when crops are fertilized or irrigated. Runoff and leachate from overfertilized areas will contaminate the water resources, while crop yield and quality may be restricted in undersupplied areas. Ignoring the within field variability of soil properties may thereby result in low land use and management efficiencies. Following the new paradigm of modern agriculture, farmers must balance the competing goals of supplying enough inputs to their crop with minimizing inputs in order to avoid adverse environmental effects. This is particularly relevant in countries where fertilizer quotas are already enforced or where water resources are scarce.
Site-specific land management relies on three main elements: information, technology, and decision support. In recent years, advances in global positioning systems, geographical information systems, and variable rate applicators, interfaced with computer control systems, have enabled to develop the technological pillar of precision agriculture. Crop growth models together with soil water balance models and soil nutrient status models are now widely available and enable to calculate the nutrient and water demand in terms of time variable boundary conditions [e.g., Carbone et al., 1996; Basso et al., 2001]. Additionally, various types of physically based distributed models have been developed that are powerful tools for evaluating the impact that different land management strategies exert on hydrological and erosion processes, and on contamination of surface and subsurface water. For the calibration and reliable application of these sophisticated models a large number of input data and model parameters need to be determined, especially the water content and hydraulic properties of soil that control unsaturated flow processes, and the composition of water which determines the nutrient status for the crop, as well as the water quality. Estimates of the soil hydraulic properties are also needed to design efficient and reliable remediation plans.

An important gap in the current knowledge resides in a lack of information related to the spatial variability of the soil properties within a field. Most of the current reference methods for assessing soil properties are too costly or too labour intensive to enable accurate and detailed assessments of the within field variation in practical context. Indeed, most of these methods are destructive and are characterized by a low support volume. Hence intensive sampling and elaborated sample analysis is needed to characterize the within field soil and crop properties. In addition, a time delay exists between sampling and analysis. These constraints make the reference methods inappropriate within a context of site specific land management or precision agriculture. As an example, the lack of suitable characterization techniques have been cited as the most critical factor preventing the wider implementation of precision agriculture [Bouma et al., 1999; Stafford, 2000; Kirchmann and Thorvaldsson, 2000].

To overcome these limitations, remote sensing techniques can be used for delineating field management zones which are spatially homogeneous in terms of soil and crop properties. Soil electric sounding is commonly used as a technique to generate "proxy's" of soil moisture and salinity, supporting site specific management [Lesch et al., 1998; Sudduth et al., 2001]. Soil electric sounding can be performed by classical geo-electric or electromagnetic induction techniques. The electric conductivity depends mainly on the soil water content, the ion composition of the soil water, and the soil type [Rhoades et al., 1976, 1990; Mualem and Friedman, 1991]. However, since these parameters vary independently within a field, their respective correlation with the electric conductivity can not be interpreted easily and is subject to large uncertainties.
1.1. Research Topic

Remote sensing techniques are based on the emission and reception of electromagnetic waves, for which the propagation through a medium is governed by its constitutive electromagnetic properties and their spatial distribution, namely, the dielectric permittivity, electric conductivity, and magnetic permeability. For most earth materials, the magnetic permeability is equal to the one of free space. In contrast, the dielectric permittivity exhibits a monotonic and highly correlated dependence on the water content [Topp et al., 1980; Tabbagh et al., 2000]. This makes this property a valuable surrogate measure of the soil water content. A commonly used and well established method to measure this property in the laboratory and in-situ is time domain reflectometry (TDR) [Dalton et al., 1984; Heimovaara, 1993; Noborio, 2001]. The benefit of this technology stems from the fact that it provides simultaneously and in the same sample volume both the dielectric permittivity and electric conductivity. Its appropriateness in field mapping applications is however limited, since it requires the careful insertion of a probe into the ground, which can be laborious and time-consuming, particularly in dry soils. A sufficient spatial resolution can not be achieved with TDR in a practical context.

For illustrating to what extent the soil properties may vary in space and time, we performed TDR measurements in an agricultural field from the Agricultural Research Center of Gembloux, Belgium [Lambot et al., 2003f]. Both the water content, derived from the dielectric permittivity, and electric conductivity of the top layer (40 cm) were mapped at five different dates. Figures 1.1 and 1.2 show the spatial distribution of, respectively, the water content and electric conductivity for two different dates (May 2 - May 22, 2001). TDR measurements were performed with a spatial resolution of 5 meters, resulting in 400 measurements, which necessitated one day of measurements for each date. The maps were obtained using kriging, based on the corresponding observed semivariograms [Isaaks and Srivastava, 1989]. We can observe that the water content varies considerably at the field scale (120 m × 120 m), and also during a short period of time. For instance, on May 2, the water content varies in space from about 0.26 to 0.38 m$^3$m$^{-3}$. Similar results are obtained for the electric conductivity. It is worth noting that in this field the electric conductivity is weakly correlated to the water content. This outlines the limitation of electric sounding techniques for assessing soil water content. The shape of the semivariograms indicates that the structure of the variability can be completely different from one date to another. The correlation sill distance varies from about 40 m till more than 120 m. The observed nugget effect is mainly to be attributed to the local variability (< 5 m), and to a lesser extent, to TDR measurement errors. This example emphasizes the need to command a fast remote sensing technique for characterizing locally the subsurface properties, and more specifically, the water content.

Ground penetrating radar (GPR) [Annan, 2002; Davis and Annan, 2002],
Chapter 1. Introduction

Figure 1.1. Spatial distribution of the soil water content ($\theta$) within an agricultural field (Agricultural Research Center of Gembloux, Belgium) at two different dates, namely, May 2, 2001 (top), and May 22, 2001 (bottom), and corresponding semivariograms. Measurements were performed using time domain reflectometry (TDR).

Based on the same basic principles as TDR, seems to be the most appropriate tool to perform such a characterization, as it does not require contact with the soil. Electromagnetic waves are emitted and received by means of antennae. Nevertheless, notwithstanding considerable research and applications have been devoted to GPR since the 1960s, the use of GPR for assessing quantitatively the shallow subsurface dielectric properties is presently still limited. For practical applications, the current state of technology still needs new developments.

1.2 Project Objectives

The principal objective of this research project is to develop and evaluate a new integrated GPR based remote sensing method for characterizing the within field variability of soil moisture, soil salinity and soil hydraulic properties, and this within a context of site specific agricultural and environmental management.
1.2. Project Objectives

Figure 1.2. Spatial distribution of the soil electric conductivity ($\sigma$) within an agricultural field (Agricultural Research Center of Gembloux, Belgium) at two different dates, namely, May 2, 2001 (top), and May 22, 2001 (bottom), and corresponding semivariograms. Measurements were performed using time domain reflectometry (TDR).

Figure 1.3 represents the proposed GPR information processing flow chart on which this research is founded. It aims at optimizing the quantity of information that can be remotely acquired from GPR. The depth dependent soil electromagnetic properties are derived from the GPR signal by inverting an electromagnetic model. Then, a soil specific relation (Petrophysical model I) allows directly estimating the soil water content profile. The dynamics of water in the soil can then be monitored, and using an hydrodynamic inverse modeling procedure, the soil hydraulic properties can be estimated. Finally, the use of an appropriate relation (Petrophysical model II) provides an assessment of the electric conductivity of the soil solution.

In this framework, the special scientific issues outlining this thesis are:

1. To demonstrate through the development and validation of an hydrodynamic inverse modeling procedure that the soil hydraulic properties are effectively obtainable from only soil moisture measurements under natural field boundary conditions. This issue is first dealt with in this thesis, since it justifies the need of an accurate remote sensing technique for measuring the soil water content. In Chapter 2, we develop and validate
Chapter 1. Introduction

Figure 1.3. GPR information processing flow chart.
1.2. Project Objectives

1. Theoretically a new hydrodynamic inverse modeling procedure. Also the theoretical basis of inverse modeling is introduced. In particular, the optimization issue is examined since it may be problematic in both hydrodynamic and electromagnetic inverse problems. In Chapter 3, the overall method is validated for physical experiments under laboratory conditions.

2. To design and model an appropriate radar system which presents a high degree of mobility for enabling real time mapping, and which allows further for an accurate and efficient electromagnetic inversion. The proposed radar system and its advantages compared to the traditionally used systems are presented in Chapter 4. Particular attention has been paid to propose a low cost system, and simultaneously, a computationally efficient signal analysis method in order to promote its application. A first version of a new radar-antenna model is presented, which allows for a better understanding of the fundamental electromagnetic wave propagation phenomena within the antenna. Then, the full solution of the Maxwell equations is specifically derived for describing electromagnetic wave propagation in the subsurface.

3. To inverse the electromagnetic model for estimating the soil electromagnetic properties, and to validate the overall integrated remote sensing approach in conditions with an increasing complexity. In Chapter 5, the well-posedness of the electromagnetic inverse problem is examined theoretically and for physical experiments in the case of a one-layered soil. For responding to the encountered issues in Chapter 5, Chapter 6 introduces some improvements in the radar and subsurface model, and validates the method in the case of a two-layered soil. Finally, Chapter 7 investigates theoretically and for physical experiments the estimation of a continuously variable dielectric profile. This last chapter makes a link with the hydraulic properties of soil.

Petrophysical models are now widely available [Topp et al., 1980; Tabbagh et al., 2000; Rhoades et al., 1990; Mualem and Friedman, 1991; Malicki and Walczak, 1999; Amente et al., 2000], but their validation is beyond the scope of this research. We aim mainly at providing new fundamental concepts, based on the flow chart presented in Figure 1.3, that still have to be improved, validated, and integrated in future research. Accuracy issues in GPR sensing and accuracy requirements in practical contexts are briefly introduced in Chapter 8.
1.3 Scientific Originality and Innovation

The originality of the presented study builds on three scientific innovations:

1. Currently, numerous hydrodynamic inverse modeling procedures exist and are powerful tools for identifying in an effective way the soil hydraulic properties [Hopmans et al., 2002]. However, most of these methods are either only applicable in laboratory conditions under specific boundary conditions, or necessitate many hydraulic variables as input. Moreover, the well-posedness of the inverse problem is not always demonstrated, and the inversion procedures suffer usually from a lack of robustness regarding the optimization algorithm. An innovative aspect of this research is that it proposes and validates a new inverse modeling procedure that is promising for in-situ characterization using remote sensing technology.

2. Although GPR has proven to be a reference technique for non-destructive mapping of soil properties [Du and Rummel, 1994; Weiler et al., 1998; al Hagrey and Müller, 2000; Huisman et al., 2001; Annan, 2002], only few applications exist in precision agricultural and environmental management. Current radars and signal analysis methods require several measurements for the characterization of a single soil profile, and information is only obtained for the top soil horizons [Huisman et al., 2001]. Generally, only the dielectric constant is estimated. Moreover, the actual used GPR technology considers surface contact antennae, limiting the application of this technology for real time mapping of dielectric spectra in-situ. Finally, to the best of our knowledge, no method exists today which provides, with a single measurement, simultaneously and quantitatively the depth dependent dielectric constant and electric conductivity of the soil. A very innovative aspect of this research project is that this should be possible with the proposed methodology, thereby integrating the radar system optimization with detailed modeling and inversion of the radar signal for real soils. Applications of such an approach would also be very valuable in other fields of applied geophysics such as humanitarian landmine detection [Scheers, 2001].

3. Relating the soil electric conductivity with agronomic variables is a commonly used approach in precision agriculture using remote sensing electromagnetic induction techniques [Lesch et al., 1998; Sudduth et al., 2001]. Yet, limitations of the method arise from the fact that the electric conductivity of the soil depends heavily and simultaneously on different soil properties such as water content, ion concentration of the soil solution, and soil type [Rhoades et al., 1976]. The innovative value
in the research project arises from the fact that both the dielectric constant and electric conductivity of the soil are measured at the same scale and with the same remote sensing technique (GPR). Using soil specific petrophysical relations, the effect of the water content on the soil electric conductivity can be eliminated and an estimate of the soil solution electric conductivity can be obtained. This will result in a significantly better correlation between agronomic and environmental variables and the characterized soil solution electric conductivity, which is a surrogate for soil nutrient status [Heimovaara et al., 1995; Nissen et al., 1998; Wraith and Das, 1998; Das et al., 1999; De Neve et al., 2000].
Chapter 2

A new inverse modeling procedure to characterize the unsaturated soil hydraulic properties from soil moisture time series

Abstract  We present a new inverse modeling procedure to characterize the hydraulic properties of partially saturated soils from soil moisture measurements during a natural transient flow experiment. The inversion of the governing one-dimensional Richards equation is carried out using the Global Multilevel Coordinate Search optimization algorithm in sequential combination with the local Nelder-Mead Simplex algorithm (GMCS-NMS). We introduce this optimization method in the area of unsaturated zone hydrology since it is adapted for solving accurately and efficiently complex nonlinear problems. Several numerical experiments have been conducted to evaluate the proposed inversion method using synthetic error-free and error-contaminated data for different textured soils. Inversion of the simulated error-free data and examination of the related response surfaces demonstrated the uniqueness of the inverse solution and the suitability of the GMCS-NMS strategy when identifying four key parameters of the hydraulic functions described by the Mualem-van Genuchten model. Inversion of the error-contaminated data proved further the good stability of the inverse solution that is consistent with the needs required by real experiments.

Chapter 2. A new hydrodynamic inverse modeling procedure

2.1 Introduction

Fate and transport models of pollutants in subsurface unsaturated porous media are now becoming readily available tools to design and evaluate management strategies for preserving the soil and water quality. Nonetheless, the effectiveness with which these modeling tools in environmental management can be adopted relies heavily on the quality with which unsaturated flow parameters can be identified.

Quite a lot of progress has been made in the characterization of the hydraulic properties of partially saturated soils using inverse modeling methods [Leij and van Genuchten, 1999]. With these methods, experimental data from a dynamic flow experiment are combined with a validated flow model and an appropriate optimization algorithm to estimate the soil hydrodynamic parameters. The inversion is generally based on the optimization of an objective function which represents disparities between the real response of the soil system and the simulated response with the given model subject to a trial parameter set. Inversion methods for estimating the flow properties of partially saturated soils were already introduced in the early 80s [e.g., Zachmann et al., 1982; Dane and Hruska, 1983; Hornung, 1983], when efficient numerical solutions of the nonlinear flow governing equation became available. For instance, the one-step outflow method, first introduced by Gardner [1956], was evaluated using numerical inversion methods by Kool et al. [1985]. Experiments from alternative outflow designs were further treated by more efficient computational methods by Eching and Hopmans [1993], van Dam et al. [1994], and Durner et al. [1999]. Reviews on the use of inversion methods for characterizing unsaturated flow parameters are given in particular by Hopmans and Simunek [1999] and Durner et al. [1999].

Compared to classical direct laboratory methods [e.g., see Klute and Dirksen, 1986], the principal advantages of the flow inversion procedures are that they require lesser experimental efforts and result in effective flow parameter estimates. Classical laboratory methods are often time consuming because they need to reach several stages of steady state conditions. Moreover, their utility for predicting subsurface flow is questionable [Mishra and Parker, 1989]. Flow inversion procedures, as far as they are concerned, allow much more flexibility in the experimental design and yield model parameters that maximize the ability of the model to reproduce the transient flow event. In the particular case of partially saturated flow models, the inversion may yield simultaneous effective estimates of both the soil water retention function $\theta(h)$ and the unsaturated hydraulic conductivity function $K(\theta)$.

The major limitation on the use of inversion techniques for estimating partially saturated flow parameters is related to the nonuniqueness and instability of the inverse solution. Nonuniqueness leads to a range of parameter sets, each
yielding an optimal value for the objective function, i.e., the objective function is not characterized by a single well defined global optimum. Instability is related to the fact that small errors in the observed state variables may result in large changes in the optimized parameters. To be stable, the solution must depend continuously on the measured state variables, and in particular on their associated errors [Carrera and Neuman, 1986b]. Nonuniqueness and instability will depend very much on the considered soil response, and thus on the experimental design. Assuming that the used model adequately describes the soil system and that the parameters are identifiable, i.e., one and only one parameter set leads to a given model response, a well-posed inverse problem requires that the transient flow experiment yields enough information from the soil system.

For one-step outflow experiments, Kool et al. [1985] showed that uniqueness problems could be minimized if the experiment is designed such that a wide range in water content is covered. The one-step outflow method was further improved first by van Dam et al. [1990] with the multistep outflow method, which was later dealt with by, e.g., van Dam et al. [1994], Zurnühl [1996], and Hollenbeck and Jensen [1998a] who studied different variants of the method and investigated the identifiability of the Mualem-van Genuchten parameters [Mualem, 1976; van Genuchten, 1980]. Uniqueness and stability for evaporation experiments were analyzed in particular by Wendroth et al. [1993], Tamari et al. [1993], and Romano and Santini [1999]. Inverse estimation from in-situ infiltration experiments was investigated early by Dane and Hruska [1983] and recently by Inoue et al. [2000] and Zou et al. [2001].

In addition to a proper design, a successful inversion method also needs an efficient and robust inversion algorithm. Earlier studies emphasized the difficulty to estimate simultaneously more than two hydraulic parameters [e.g., Kool and Parker, 1988; Toorman et al., 1992; Eching and Hopmans, 1993]. The optimization problem is complicated by the topographical complexity of the objective function exhibiting many local minima [Russo et al., 1991; Durner et al., 1999; Jacques et al., 1999; Si and Kachanoski, 2000]. When gradient-based local optimization algorithms such as the traditional Levenberg-Marquardt method [Marquardt, 1963] are used, local minima may constitute traps which cause the inverse solution to be very sensitive to initial parameter guesses. Global optimization approaches are less susceptible to the presence of these local solutions. Takeshita and Kohno [1999] presented a global method that uses a Genetic algorithm [Michalewicz, 1996] to estimate the saturated hydraulic conductivity $K_s$ and parameters $\alpha$ and $n$ of the van Genuchten retention model. Pan and Wu [1999] coupled the heuristic Simulated Annealing [Ingber, 1996] algorithm with a fast local Downhill Simplex algorithm to estimate five parameters of the Mualem-van Genuchten equations. Abbaspour et al. [1997, 1999] presented the sequential uncertainty domain parameter fit-
Chapter 2. A new hydrodynamic inverse modeling procedure

ting (SUFI) method to estimate four hydraulic parameters simultaneously. Yet, more research is needed to improve the well-posedness of the inverse problems, the robustness of the inversion methods, as well as their applicability for the subsurface hydrodynamic characterization.

The objective of this study is to describe and evaluate a new inverse modeling procedure for estimating the unsaturated soil hydraulic properties. The classical least squares criterion is chosen to define the objective function, and the formulated optimization problem is solved by the Global Multilevel Coordinate Search algorithm (GMCS) [Huyer and Neumaier, 1999] that we have combined sequentially with the local Nelder-Mead Simplex algorithm (NMS) [Lagarias et al., 1998]. This method is well suited to get over the complex topography of nonlinear objective functions containing many local minima and can also handle discontinuities. The forward problem is solved by numerically solving the Richards equation and assuming soil hydraulic properties to be described by the coupled Mualem-van Genuchten model. Only observed time series of soil moisture from a transient infiltration-redistribution experiment are used as input. Preference is given to the use of moisture content data in the objective function, since the measurement technology is now available to monitor this state variable in-situ with a high temporal resolution. The present analysis situates therefore in the context of including soil moisture monitoring programs in effective parameter identification procedures. In this study, the methodology is first validated theoretically on simulated error-free and error-contaminated data for a range of different textured soil types. The method is further tested using data collected from a column scale flow experiment.

2.2 Theory

2.2.1 The direct flow problem

The governing flow model relates the parameters characterizing the subsurface hydraulic properties to the response of the system that defines the input in the inversion algorithm. One-dimensional vertical transient water flow in homogeneous isotropic rigid porous media is described by the Richards equation, expressed here in terms of pressure head [Jury et al., 1996]:

\[ C(h) \frac{\partial h}{\partial t} = \frac{\partial}{\partial z} \left[ K(\theta) \left( \frac{\partial h}{\partial z} - 1 \right) \right] \]  

(2.1)

where \( h \) is the time and depth dependent pressure head (L), \( C(h) = \partial \theta(h) / \partial h \) is the differential water capacity (L\(^{-1}\)) with \( \theta(h) \) being the water retention curve and \( \theta \) being the volumetric moisture content (L\(^3\)L\(^{-3}\)), \( K(\theta) \) is the hydraulic conductivity (LT\(^{-1}\)), \( t \) is the time (T), and \( z \) is the depth taken positive.
2.2. Theory

downward \((L)\). The relations \(\theta(h)\) and \(K(\theta)\) are the characteristic constitutive functions which describe the soil hydraulic properties. For the case of infiltration under variable flux conditions, (2.1) is solved, subject to the following initial and boundary conditions:

\[
\begin{align*}
    h(z) &= h(L) + z - L & 0 \leq z \leq L & t = 0 \\
    q(t) &= K(\theta) \left( \frac{\partial h}{\partial z} - 1 \right) & z = 0 & t > 0 \\
    \begin{cases}
        q(t) = 0 & \text{if } h(t) < 0 \\
        h(t) = 0 & \text{otherwise}
    \end{cases} & z = L & t > 0
\end{align*}
\]

which prescribe at the upper boundary the downward infiltration rate \(q(t)\), and at the lower boundary a lysimeter boundary condition, with \(L\) the soil column length. \((L)\).

The nonhysteretic unimodal Mualem-van Genuchten model (MVG) is used in this study to describe the soil hydraulic properties \([\text{Mualem}, 1976; \text{van Genuchten}, 1980]\). The water retention curve is given by:

\[
\theta(h) = \theta_r + (\theta_s - \theta_r) \left[ 1 + |\alpha h|^n \right]^{-m}
\]  

(2.3)

where \(\theta_r\) and \(\theta_s\) are, respectively, the residual and saturated water content \((L^3L^{-3})\), \(\alpha\) \((L^{-1})\) and \(n\) (nondimensional) are curve shape parameters which are, respectively, inversely related to the air entry value and the width of the pore size distribution, and \(m\) (nondimensional) is restricted by the Mualem condition \(m = 1 - 1/n\) with \(n > 1\). The hydraulic conductivity relationship is given by:

\[
K(\theta) = K_s S_e^\lambda \left[ 1 - \left( 1 - S_e^{-m} \right)^{-m} \right]^2
\]

(2.4)

where \(K_s\) is the saturated hydraulic conductivity \((LT^{-1})\), \(S_e = (\theta - \theta_r)/(\theta_s - \theta_r)\) is the effective saturation (nondimensional), and \(\lambda\) is a factor that accounts for the pore connectivity or pore tortuosity (nondimensional). A high value of \(\lambda\) corresponds to a low pore connectivity or a high pore tortuosity.

The MVG model has been found capable of generating a reasonable class of analytical curves approximating observations of \(\theta(h)\) and \(K(\theta)\) from various laboratory and field experiments. However, \(\text{Fuentes et al. [1992]}\) pointed out that MVG should be used with care in clayey soil conditions. The total number of unknown hydraulic parameters in the MVG model is six, i.e., \(\theta_r\), \(\theta_s\), \(\alpha\) and \(n\) for the water retention curve, plus \(K_s\) and \(\lambda\) for the unsaturated hydraulic conductivity. \(\theta_s\) has a clear physical significance and can easily be obtained by direct measurements. \(\theta_r\) is usually defined as the residual water content corresponding to a value of \(h \to -\infty\). Generally, this parameter is regarded as an empirical parameter and can be fixed either to a value which...
yields the best fit to the experimental water retention data [Kool et al., 1985], or to the value of zero [Nimmo, 1991; Fuentes et al., 1992]. If $\lambda$ is to be interpreted in terms of pore connectivity and pore tortuosity, it must be greater than zero so that $Se^{\lambda}$ varies between zero and one. A negative value of $\lambda$ implies that the connectivity increases with decreasing water contents, which is physically incoherent. However, Mualem [1976] among many others obtained negative as well as positive values for $\lambda$, throwing doubt that the MVG model can be entirely interpreted in a physical way. Furthermore, for small negative values of $\lambda$, $K(\theta)$ can increase with desaturation, which is physically unrealistic. Therefore, in this case it is necessary to consider the condition $\partial K(\theta)/\partial \theta > 0$ which leads to the following constraint on $\lambda$:

$$\lambda > -2 \left( 1 - Se^{\frac{1}{m}} \right)^{m-1} Se^{1 \over m} \over 1 - \left( 1 - Se^{1 \over m} \right)^m$$

(2.5)

2.2.2 The inverse problem

Objective function. Soil hydraulic parameter identification by inverse modeling is a nonlinear optimization problem which consists in finding the parameter vector $b = [\theta_r, \theta_s, \alpha, n, K_s, \lambda]^T$ so that an objective function $\phi(b)$ is minimized. In the particular case where no prior information on the parameters is taken into account and assuming observation errors to be normally distributed, independent, and homoscedastic, the maximum likelihood theory reduces to the classical least squares problem [Carrera and Neuman, 1986a]. Considering only water content data to describe the response of the soil system, the objective function is thus formulated as follows:

$$\phi(b) = (\theta^* - \theta)^T (\theta^* - \theta) = e^T e$$

(2.6)

where $b$ is the model parameter vector (size $p \times 1$), $\theta^* = \theta^*(z_j, t_i)$ and $\theta = \theta(z_j, t_i, b)$ are the vectors (size $n \times 1$) containing, respectively, the observed and simulated water content data relative to depths $z_j$ and times $t_i$, $e = \theta^* - \theta$ is the vector of residuals, and $n$ is the total number of observations.

Global Multilevel Coordinate Search - Nelder-Mead Simplex method. The minimization of equation (2.6) is carried out using the Global Multilevel Coordinate Search (GMCS) algorithm [Huyer and Neumaier, 1999] combined sequentially with the classical Nelder-Mead Simplex algorithm (NMS) [Lagarias et al., 1998]. Since, to the best of our knowledge, GMCS has never been used before in the area of unsaturated zone hydrology, we briefly describe hereafter the main concepts behind the algorithm.
2.2. Theory

The GMCS method belongs to a category of increasingly popular global optimization algorithms that are designed to get over the complex topography and multi-modality of the multidimensional nonlinear objective functions without requiring excessive computing resources. The GMCS algorithm is an intermediate between purely heuristic methods, i.e., methods that find the global minimum only with a high probability like, e.g., Simulated Annealing or Genetic algorithms, and stochastic methods that guarantee to find the global minimum with a required accuracy. In contrast to many stochastic methods that operate only at the global level and are therefore quite slow, GMCS contains local enhancements that lead to quick convergence once the global part of the algorithm has found a point in the basin of attraction of the global minimum. Moreover, GMCS does not need to calculate derivatives of the objective function, causing it to be very insensitive to possible discontinuity of the objective function. Huyer and Neumaier [1999] have shown that GMCS has excellent theoretical convergence properties if the objective function is continuous in the neighborhood of the global minimum, and that it is strongly competitive with other existing algorithms in the case of problems with reasonable finite bound constraints.

More precisely, the GMCS algorithm solves the bound constrained optimization problem

\[
\min f(x) \quad x \in [u, v] 
\]

(2.7)

where \( u \) and \( v \) are \( n \)-dimensional vectors defining the search space box

\[
B[u, v] \subset \{ x \in \mathbb{R}^n \mid u_i \leq x_i \leq v_i, \ i = 1, \ldots, n \} 
\]

(2.8)

GMCS tries to find the global minimum by splitting successively the search space \( B[u, v] \) into smaller boxes. Each generated box \( B[x, y] \) is completely defined by a base point \( x \) whose function value is known, generally a vertex, and an opposite point \( y \). As a measure of the number of times a box has been split, a level \( s \in \{0, 1, \ldots, s_{\max}\} \) is assigned to each box. Boxes with level \( s_{\max} \) are considered too small for further splitting. Every time a box of level \( s \) is split, its level is set to zero, and its descendants get level \( s + 1 \) or \( s + 2 \) according to splitting rules. The partitioning procedure is not uniform but boxes where low function values are expected to be found are partitioned more frequently. In each step, boxes are split only along a single coordinate. Whenever a box is split along the coordinate \( i \) for the first time, and particularly in case of the root box \( B[u, v] \), this is done at \( L_i = 3 \) user defined values \( x_i^l \) \((l = 1, \ldots, L_i)\),

\[
x_i^1 = \frac{5x_i + y_i}{6} \quad x_i^2 = \frac{x_i + y_i}{2} \quad x_i^3 = \frac{x_i + 5y_i}{6} 
\]

(2.9)
and, in this particular case, at $L_i - 1$ values $z^l_i$ calculated as follows:

$$z^l_i = x^{l-1}_i + q^k \left( x^l_i - x^{l-1}_i \right) \quad l = 2, \ldots, L_i$$

(2.10)

where $q = (\sqrt{5} - 1)/2$ is the golden section ratio, and $k = 1$ or 2 is chosen such that the part with the smaller function value gets the larger fraction of the interval. These five points $(x^1_i, x^2_i, x^3_i, z^2_i, z^3_i)$ plus the two boundary points $(x_i$ and $y_i$) partition the initial interval into six subintervals. If the box has already been split along the coordinate $i$, the interval is partitioned at the golden section split and at

$$z_i = x_i + \frac{2}{3} \left( \zeta(x_i, y_i) - x_i \right)$$

(2.11)

where $\zeta(x_i, y_i)$ is a function that enables to handle correctly large or unbounded intervals. If the interval $[x_i, y_i]$ is not too large, $\zeta(x_i, y_i)$ reduces to $y_i$. When a box of level $s$ is split, boxes with the smaller fraction of the golden section split get level $s + 2$ and all other boxes get level $s + 1$.

The algorithm starts with an initialization procedure producing an initial set of boxes. The root box $B[u, v]$ is subsequently split along all its coordinates $i$ following the above-described interval splitting procedure. The objective function $f$ is first evaluated at an initial point $x^*$. Then, for $i = 1, \ldots, n$, $f$ is evaluated at $L_i - 1$ points $x^l_i$ in $[u, v]$ that agree with $x^*$ in all coordinates $k \neq i$. When the box has been partitioned along one coordinate, the point with the smallest function value is renamed $x^*$ before repeating the procedure with the next coordinate.

After the initialization procedure, the algorithm proceeds by a series of sweeps through the levels. A sweep consists in scanning the list of boxes with level $s \neq 0$ and defining a record list containing for each level $s$ the box with the lowest function value. These boxes are then split or not according to splitting rules. After each split, the record list is updated. The splitting rules distinguish two cases. If

$$s > 2n \left( \min n_j + 1 \right)$$

(2.12)

where $n_j$ is the number of times coordinate $j$ has been split in the history of the box, the box is always split, and the splitting index is a coordinate $i$ with $n_i = \min n_j$. This means that, although the box has already reached a rather high level, there is at least one coordinate along which the box has not yet been split very often, namely, coordinate $i$. This split is therefore mainly made to reduce the size of a large interval. If condition (2.12) is not satisfied, the box may be split along a coordinate where the maximal gain in function value is expected according to a local separable quadratic model obtained by fitting
2.2. Theory

$n + 1$ function values. This quadratic model is a reasonably simple local approximation of $f$. Nevertheless, if the expected gain is not large enough, the box is not split at all, but its level is increased by one. This box may then possibly satisfy to condition (2.12) and be split later.

At the end of each sweep, local searches are carried out. All base points $x$ of boxes of level $s_{\text{max}}$ that have been collected in the sweep are stored in a list. Then, in order to know if the points $x$ are likely to belong or not to the basin of attraction of an already known minimum, the monotonicity properties of $f$ are examined between each point $x$ and all the points $w$ that constitute already known minima of the objective function. For the points $x$ that do not appear to belong to such basins of attraction, a local search is performed. The resulting function values are put in the list containing the points $w$, from which the global minimum will be extracted at the end of the optimization.

The local search algorithm used consists essentially in building a local quadratic model by triple searches, then defining a promising search direction by minimizing the quadratic model on a suitable box, and finally making a line search along this direction. The local search stops according to local optimization rules (not presented here) and if a specified limit ($\beta_{\text{max}}$) on function calls has been exceeded. GMCS balances thus global and local search capabilities at different levels: this is the multilevel coordinate search approach.

The convergence of GMCS algorithm toward the global minimum $x_g$ will be ensured if the objective function is continuous in the neighborhood of the global minimum, if there exists an $\varepsilon > 0$ such that $f(w) > f(x_g) + \varepsilon$ for any local minimum $w$, and if the local search algorithm reaches a local minimum after a finite number of steps. Indeed, in this case, it can be demonstrated that there exist $s_{\text{cr}}$ and $N_{\text{sw}}$ such that, for any $s_{\text{max}} \geq s_{\text{cr}}$, GMCS will find the global minimum with a given accuracy after at most $N_{\text{sw}}$ sweeps. This means that, provided that $s_{\text{max}}$ is large enough, the solution of the optimization problem (2.7) will certainly be reached after a limited number of function evaluations. This follows from the fact that the set of points sampled by the algorithm forms a dense subset of the search space when $s_{\text{max}} \to \infty$. Hence, in our study, we used as stopping criterion for the GMCS optimization task the maximum number of iterations, namely, $\alpha_{\text{max}}$. An additional maximum number of function evaluations, $\beta_{\text{max}}$, has also to be defined for limiting each local search. Neither $\alpha_{\text{max}}$ nor $\beta_{\text{max}}$ are known a priori for a specific optimization problem. These criteria should be stringent enough such that they do not waste too many function values after the global minimum has been reached, but they should also be loose enough to ensure convergence. To get over this issue, we adopted the following strategy. Since local optimizations are performed many times, a too large $\beta_{\text{max}}$ is likely to increase considerably the total number of function calls. Therefore, $\beta_{\text{max}}$ was held to a relatively reasonable value. However, it is possible that, using this limit, the global minimum $x_g$ found
Chapter 2. A new hydrodynamic inverse modeling procedure

by GMCS is not quite optimal. Thus, we combined sequentially to GMCS an additional local search algorithm (NMS) to improve the solution. The NMS algorithm was chosen because it is a nonlinear fast local search method that does not need to calculate an explicit formulation of the objective function Jacobian. NMS starts from the GMCS solution and stops when iterations do not improve significantly the solution. This strategy improves the efficiency of the overall optimization task since GMCS needs only to find an approximate solution. Several trials on our specific optimization problem led us to set $\alpha_{\text{max}} = 150n^2$, $\beta_{\text{max}} = 75$, and $s_{\text{max}} = 5n + 10$.

**Linear quantification of parameter uncertainty.** An important aspect of inverse parameter identification is the quantification of the estimation errors. For linear optimization problems, assuming no model errors, the uncertainty of the parameter estimates is statistically derived from the objective function in the neighborhood of the global minimum. Uncertainty is related to the curvature of the objective function at the optimum. However, for nonlinear fitting models, knowledge of the true distributions of the optimized parameters is required. These distributions can be obtained using the Monte Carlo method, whereby many realizations of optimized parameter sets are generated from model fitting of data corrupted with measurement errors [Clausnitzer et al., 1998]. Because this demands high computing resources, we approximated parameter confidence intervals using linear regression analysis for our nonlinear problem.

Accordingly, parameter uncertainty is determined on the basis of the parameter variance-covariance matrix $C$ [Kool and Parker, 1988]:

$$C = \frac{e^T e}{n - p} H^{-1}$$  \hspace{1cm} (2.13)

where $H$ is the Hessian matrix ($size \ p \times \ p$) whose elements $H_{i,j}$ are defined as follows:

$$H_{i,j} = \frac{\partial^2 \phi(b)}{\partial b_i \partial b_j}$$  \hspace{1cm} (2.14)

Approximate confidence intervals of the estimated parameters are then given by:

$$b_i - t_{1-\alpha/2}^{n-p} \sqrt{C_{i,i}} \leq b_i \leq b_i + t_{1-\alpha/2}^{n-p} \sqrt{C_{i,i}}$$  \hspace{1cm} (2.15)

where $t_{1-\alpha/2}$ is the value of the Student distribution with $(n - p)$ degrees of freedom and confidence level $(1 - \alpha)$. In our analyses, the 95% confidence interval, i.e., $\alpha = 0.05$, is used to quantify the uncertainty in the parameter estimates. Assuming that the estimated parameter vector $b$ is the global minimum of the objective function, (2.15) is expected to yield reasonable approximations of the confidence interval [Donaldson and Schnabel, 1987].
2.2. Theory

Note that when the estimated parameters are correlated, the consideration of only the diagonal terms of $C$ may lead to an overestimation of the actual variability of the parameters, and thus of the confidence intervals [Carrera and Neuman, 1986a]. The elements $A_{i,j}$ of the parameter correlation matrix $A$ (size $p \times p$) are defined as:

$$A_{i,j} = \frac{C_{i,j}}{\sqrt{C_{i,i}C_{j,j}}}$$  \hspace{1cm} (2.16)

High correlation coefficients between estimated parameters could also lead to nonuniqueness problems.

**Model sensitivity with respect to parameters.** Sensitivity analysis prior to the parameter identification is important because it provides valuable insights to optimize the experimental design and to determine to what extent the parameters can be identified. Generally, the larger the sensitivity coefficient of a model parameter is, the higher is the likelihood for the parameter to be identified. Therefore, preference must be given to measurements that are the most sensitive to changes in the unknown parameters. Let’s note however that even though high sensitivity is a necessary condition for successful parameter estimation, it is not sufficient since, as stated before, strong parameter correlations may make the inverse problem ill-posed.

Parameter sensitivity coefficients characterize the behavior of the objective function at a particular point in the parameter space. In this study, sensitivity is only analyzed in the vicinity of the true parameter values. Elements $S_{i,j}$ of the sensitivity matrix $S$ (size $n \times p$) are computed as follows:

$$S_{i,j} = b_j J_{i,j}$$  \hspace{1cm} (2.17)

where $J$ is the Jacobian matrix (size $n \times p$) whose elements $J_{i,j}$ are defined as the partial derivatives $\partial e_i / \partial b_j$. The elements of $J$ are obtained by forward difference approximation with $\partial b_j = 0.01 \times b_j$. Elements $S_{i,j}$ represent the change of the measurement variable $\theta$ relative to a change of 1% of the parameter $b_j$, normalized by $b_j$ so that a comparison of sensitivities between different parameters can be made independently of their magnitudes. The matrix $S$ gives the distribution of sensitivities both in time and space. In order to compare the different parameter sensitivities, it is useful to define an average value of the sensitivity corresponding to each parameter as:

$$\zeta_j = \frac{1}{n} \sum_{i=1}^{n} S_{i,j}$$  \hspace{1cm} (2.18)
2.3 Methodology

2.3.1 Simulation of transient flow experiments

For analyzing the parameter identifiability properties of the proposed inversion method, i.e., uniqueness and stability, numerical transient flow experiments were generated for five different textured soils, considering three different levels of errors in the data, resulting in 15 different scenarios. The hydrodynamic data for the different soil textural classes were obtained from the European database of soil hydraulic properties HYPRES [Wösten et al., 1999]. Hydrodynamic properties are given in Table 2.1 and the related water retention curves are illustrated in Figure 2.1. Inversions were performed on error-free and error-contaminated data, which allows us to elucidate, respectively, the uniqueness and the stability of the inversion procedure. This numerical approach has the benefit of dealing with experiments for which the true hydraulic properties defining the porous media of interest are known and for which the response is perfectly described by the flow model considered.

Water content data sets, characterizing the soil system response, were generated numerically by solving the differential equation (2.1) given the specific initial and boundary conditions (2.2a), (2.2b), and (2.2c), and the relations \( \theta(h) \) (equation (2.3)) and \( K(\theta) \) (equation (2.4)). In this study, we implemented the numerical solution of the WAVE model as described by Vanloosber et al. [1996]. In this solution, the differential equation (2.1) is approximated by finite differences with an implicit discretization scheme and with an explicit linearization of the conductivity and differential moisture capacity. In order to reduce discretization errors that invariably arise in numerical approximations, WAVE uses the iterating Newton-Raphson technique [e.g., Carnahan et al., 1969] based on a mass conservative user defined convergence criterion. A water mass balance equation is developed for each compartment. A fully implicit scheme is used to advance the solution in time with automatically varying time steps. The spatial flow domain was discretized into 30 equidistant linear elements representing each 1 cm of the 30 cm length flow domain.

One-dimensional infiltration-redistribution experiment in a homogeneous 30 cm vertical soil column was simulated. The initial condition was taken as the equilibrium pressure head profile with \( h = -300 \) cm at the bottom of the soil column. The bottom boundary condition was a free draining lysimeter condition allowing free outflow when saturation occurs at the bottom. As long as the bottom of the soil column is not saturated (negative pressure), the bottom boundary reduces to a zero flux Neuman-type condition. When the pressure head exceeds zero, water drains out of the column and the pressure head is fixed at a zero pressure head Dirichlet condition. At the upper boundary, we consider a zero flux from time \( t_0 \) to time \( t_1 \), a downward constant flux
Table 2.1. Mualem-van Genuchten parameters corresponding to the five major soil textural classes of HYPRES database and to the laboratory sand.

<table>
<thead>
<tr>
<th>Texture</th>
<th>$\theta_r$ (m$^3$m$^{-3}$)</th>
<th>$\theta_s$ (m$^3$m$^{-3}$)</th>
<th>$\alpha$ (cm$^{-1}$)</th>
<th>$n$ (-)</th>
<th>$K_s$ (cm min$^{-1}$)</th>
<th>$\lambda$ (-)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coarse</td>
<td>0.025</td>
<td>0.403</td>
<td>0.0383</td>
<td>1.3774</td>
<td>4.17e-2</td>
<td>1.2500</td>
</tr>
<tr>
<td>Medium</td>
<td>0.010</td>
<td>0.439</td>
<td>0.0314</td>
<td>1.1804</td>
<td>8.38e-3</td>
<td>-2.3421</td>
</tr>
<tr>
<td>Medium fine</td>
<td>0.010</td>
<td>0.430</td>
<td>0.0083</td>
<td>1.2539</td>
<td>1.58e-3</td>
<td>-0.5884</td>
</tr>
<tr>
<td>Fine</td>
<td>0.010</td>
<td>0.520</td>
<td>0.0367</td>
<td>1.1012</td>
<td>1.72e-2</td>
<td>-1.9772</td>
</tr>
<tr>
<td>Very fine</td>
<td>0.010</td>
<td>0.614</td>
<td>0.0265</td>
<td>1.1033</td>
<td>1.04e-2</td>
<td>2.5000</td>
</tr>
<tr>
<td>Laboratory sand</td>
<td>0.000</td>
<td>0.357</td>
<td>0.0459</td>
<td>4.5100</td>
<td>6.79e-1</td>
<td>0.5000</td>
</tr>
</tbody>
</table>

*Read 4.17e-2 as 4.17 × 10$^{-2}$.*

Figure 2.1. Water retention curves for the five soils from HYPRES and for the laboratory sand. Square markers represent measured data for the sand.
from time $t_1$ to $t_2$, and again a zero flux enabling water redistribution from $t_2$ to the end of the experiment, when the hydraulic equilibrium has almost been reached. Following the idea of Wildenschild et al. [2001], the downward constant flux has been fixed specifically for every soil textural classes to a value varying approximately from 0.5% to 50% of $K_s$, in order to investigate different relative flow rates additionally to the different soil types. It is worth to mention here that the above-described initial and boundary conditions are in accordance with real-world conditions.

2.3.2 Parameterization

In this study, we optimized four key parameters ($\alpha$, $n$, $K_s$ and $\lambda$) of the Mualem-van Genuchten model, fixing $\theta_r$ and $\theta_s$. The exponent $\lambda$ is generally fixed at a value of 0.5. However, the fit to the data is improved if this parameter is optimized as well [Wildenschild et al., 2001]. This is also in agreement with Russo [1988] and van Dam et al. [1994] who also considered the optimization of $\lambda$ to improve the prediction of the $K(\theta)$ function. $\theta_s$ was fixed because this parameter can be directly measured from the experiment itself, or inferred from bulk density measurements. Following Fuentes et al. [1992] and van Dam et al. [1994], we forced $\theta_r$ to be zero, to be in accordance with its physical definition. This constraint does not invalidate the previously described parametric models [Russo, 1988] and is in particular discussed by Nimmo [1991]. Moreover, $\theta_r$ needs measurements at very low pressure heads to make the inversion sensitive to this parameter. This condition is not satisfied in our experimental scheme being designed to be easily applicable, both in the laboratory and in-situ, under natural initial and boundary conditions.

2.3.3 Sensitivity analysis, sampling design, and parameter identifiability

For gaining more information from the transient flow experiment and for analyzing parameter identifiability, a sensitivity analysis of the simulated water content time series to the four key parameters to be optimized was carried out. Sensitivities were calculated with (2.17) by perturbing independently each parameter around its true value (1%). Distributions with space and time of the absolute sensitivities are illustrated in Figure 2.2 for the medium fine textured soil. The shape of these graphs is practically similar for the five considered experiments. Slight differences arise from the nonlinear structure of the Richards equation that makes the sensitivity coefficients dependent on both the model parameter values and the experimental conditions.

Sensitivity analysis allowed to identify optimal moisture sampling locations. We observe that the sensitivities for all parameters are the highest at the
2.3. Methodology

Figure 2.2. Distribution in time and space of the absolute sensitivity of water content to the 1% change of parameters $\alpha$, $n$, $K_s$ and $\lambda$ (Medium Fine textured soil).

bottom of the soil profile. In addition, $K_s$ and $\lambda$ present high values in the upper part of the profile in contrast to the parameters $\alpha$ and $n$. This suggests considering sampling points both at the upper part and the lower part of the soil profile. To a lesser extent, other results (not presented here) suggest adding an additional sampling point close to the middle of the soil profile. Therefore, we will consider three sampling points whose positions are, respectively, 5, 15 and 25 cm. The analysis of the temporal dynamics of the sensitivities shows that the highest sensitivities are found approximately when the second time derivative of the water content changes sign (see Figures 2.2 and 2.3). Although we do not use and take advantage of this particularity, this observation may lead to the suggestion of using this second time derivative to weight the different data in the objective function, following the idea of Vrugt et al. [2001].

If the parameters are identifiable, i.e., if the columns of the Jacobian are linearly independent, then the estimation accuracy depends on the magnitude of the sensitivity coefficients at the sampling points. Considering the space-time averaged sensitivity coefficients $\zeta_k$ for the different parameters, as calculated with (2.18) and reported in Table 2.2, we observe that $\alpha$ and $n$ will be more accurately estimated than $K_s$ and $\lambda$ following the order $n > \alpha > K_s > \lambda$. 
Figure 2.3. Comparison of measured (markers) and inversely predicted (lines) water content time series related to the three considered levels of error (case I, case II, and case III) corresponding to the Medium Fine textured soil, and to the laboratory experiment on the sand.

Table 2.2. Space-time averaged sensitivity coefficients $\zeta_k$ (nondimensional) related to the parameters $\alpha$, $n$, $K_s$, and $\lambda$ for the five transient flow experiments.

<table>
<thead>
<tr>
<th></th>
<th>$\zeta_\alpha$</th>
<th>$\zeta_n$</th>
<th>$\zeta_{K_s}$</th>
<th>$\zeta_\lambda$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coarse</td>
<td>5.01e-2</td>
<td>4.93e-1</td>
<td>1.61e-2</td>
<td>9.94e-3</td>
</tr>
<tr>
<td>Medium</td>
<td>4.61e-2</td>
<td>7.64e-1</td>
<td>7.44e-3</td>
<td>5.46e-3</td>
</tr>
<tr>
<td>Medium fine</td>
<td>5.89e-2</td>
<td>4.18e-1</td>
<td>9.32e-3</td>
<td>7.02e-4</td>
</tr>
<tr>
<td>Fine</td>
<td>3.59e-2</td>
<td>1.08e-0</td>
<td>7.18e-3</td>
<td>2.11e-3</td>
</tr>
<tr>
<td>Very fine</td>
<td>4.31e-2</td>
<td>1.15e-0</td>
<td>8.86e-3</td>
<td>2.58e-3</td>
</tr>
</tbody>
</table>
2.3.4 Infiltration experiment on a laboratory sand

In order to get further insight into the proposed inverse method, an actual infiltration experiment was conducted on a laboratory column (30 cm high, 15.3 cm diameter) filled with a homogeneous sand. The hydraulic parameters of this sand were determined using direct laboratory methods [e.g., see Klute and Dirksen, 1986] and are reported in Table 2.1 (see also Figure 2.1). A suction plate apparatus was used to determine the water retention curve whereas $K_s$ was measured directly on the sand column. Only parameter $\lambda$ was fixed to the commonly used value of 0.5. Intentionally, a structured soil was not considered in this study as processes like preferential flow are not taken into account by the WAVE model.

Soil moisture was monitored by means of Time Domain Reflectometry (TDR) probes installed horizontally at the three aforementioned depths (5, 15, and 25 cm). They consisted of three stainless steel rods (9.3 cm length and 0.5 cm diameter) with a 2.5 cm rod spacing. Water content measurements were carried out automatically with a Tektronix 1502C metallic TDR cable tester and a SDMX50-CR10X-RS232 system (Campbell Scientific Inc.). Gravimetric measurements of water content led us to use the equation of Ledieu et al. [1986] to estimate the volumetric water content from the dielectric permittivity.

Initial condition was taken as the equilibrium pressure head profile generated by an imposed pressure head of $h = -15$ cm at $z = 30$ cm. This suction was imposed in order to cover at least a range of moisture > 0.10 m$^3$m$^{-3}$ during the infiltration experiment. The bottom boundary condition was also determined by this imposed pressure head whereas the upper boundary condition consisted in a variable downward water flow. Water was uniformly applied on the surface through an electromagnetic pulse pump feeding 45 needles distributed evenly above the soil surface.

2.4 Results and Discussion

2.4.1 Uniqueness of the inverse solution and GMCS-NMS performances

Response surfaces analysis. Uniqueness of the inverse solution was first investigated using response surfaces of the objective function which partially reveal the presence of a well-defined solution, the occurrence of local minima and also qualitatively the parameter sensitivities and correlations. Response surfaces are two-dimensional contour plots representing the objective function as a function of two parameters, while all the other parameters are held constant at their true value. In our study, they represent therefore only cross sections of the full four-dimensional parameter space.
The inversion took place in a sufficiently large parameter space \((0.005 < \alpha < 0.05 \text{ cm}^{-1}; 1.05 < n < 2; 5 \times 10^{-4} < K_s < 1 \times 10^{-1} \text{ cm min}^{-1}; -3 < \lambda < 3)\) such that it contains simultaneously all the parameter vectors corresponding to each of the five different considered textured soils. Figure 2.4 shows the response surfaces of the logarithm of the objective function for the six different parameter planes \(\alpha - n, \alpha - K_s, \alpha - \lambda, n - K_s, n - \lambda\) and \(K_s - \lambda\), illustrated here for the coarse textured soil experiment. The range of each parameter has been divided into 100 discrete values resulting in 10000 objective function calculations for each contour plot. As also observed by Abbaspour et al. [1999], a too low resolution has an effect to give the misleading impression, as artifact of the plotting software (here MATLAB, version 5.3 [The MathWorks, 1999]), that local minima are present whereas they actually do not exist. Response surfaces for the four other textured soils feature mostly the same concave shapes and particularities as shown in Figure 2.4. Each surface shows a well-defined global minimum corresponding to the true parameter values. This illustrates partially the uniqueness of the solution for the given experimental design. The discontinuities delimiting areas where \(\log \phi = 0\) (blank areas) are due to either non-convergence of the forward numerical solution, or to parameter sets which do not satisfy to condition (2.5). For these cases, the objective function value is forced to be equal to 1, representing intentionally a quite high value compared to the overall objective function. This strategy enables faster convergence of the optimization task since unrealistic parameter regions are then explored less frequently. In our case, non-convergence problems arise in particular when a ponding appears too fast at the upper part of the soil profile, e.g., as a result of too small \(K_s\) values.

The structure of the response surfaces is very consistent with values of the sensitivity coefficients presented above. The banana shape contour plot in the \(\alpha - n\) space suggests an important negative correlation between these parameters, which is not advantageous for their estimation. Considering the absolute values of both parameters and the gradient pattern of the objective function we suggest, thanks to equation (2.17), that the flow model may be more sensitive to \(n\) than to \(\alpha\). Indeed, at the same time, the absolute gradient of the objective function is greater following the \(n\) direction and the absolute value of \(n\) is greater than those of \(\alpha\). Let’s note however that the Jacobian in equation (2.17) is not directly related to the gradient of the objective function. The \(\alpha - K_s\) and \(\alpha - \lambda\) response surfaces exhibit a slight elliptical minimum, suggesting a weak positive correlation between \(\alpha\) and \(K_s\) and a weak negative correlation between \(\alpha\) and \(\lambda\). The minima of \(n - K_s\) and \(n - \lambda\) response surfaces are, respectively, almost parallel to the \(K_s\) and \(\lambda\) direction, suggesting these two parameter pairs to be uncorrelated. Concerning \(K_s - \lambda\) response surface, it appears that the related parameters are positively correlated, but nothing can be deduced as regards to their sensitivity.
2.4 Results and Discussion

Figure 2.4. Response surfaces of the objective function logarithm $\log_{10}(\phi(b))$ in the $\alpha - n$, $\alpha - K_s$, $\alpha - \lambda$, $n - K_s$, $n - \lambda$, and $K_s - \lambda$ slicing parameter planes. A star represents the true parameter values.
No local minima were observed in the response surfaces (Figure 2.4), which is very advantageous for the optimization process. However, as it will be discussed later, their presence was identified in the full dimensional parameter space using the local NMS algorithm alone. The presence of these local minima imposes the use of a global search approach in the optimization procedure. It is worth noting, as also observed by Abbaspour et al. [1999], that sometimes a parameter becomes sensitive only within a particular zone of the parameter space. For instance, we can see on Figure 2.4, $\alpha - \lambda$ response surface, that $\lambda$ is only really sensitive for $\alpha > 0.025$. This emphasizes even more the need to use a global approach for the optimization and suggests that sensitivity analyses should be made in the entire parameter space to be more accurate and more representative. This is a consequence of the nonlinearity of the Richards equation that results in unequal sensitivity over the entire space of hydraulic parameters.

**Inverse identification from error-free observation data.** The GMCS-NMS inversion from error-free data (case I) led, for the five considered textured soils experiments, exactly to the true parameter values which is illustrated in Table 2.3. This illustrates the suitability of the given algorithm combination to deal with such objective functions and demonstrates its excellent convergence properties and accuracy. It further shows that time series of water content from a transient flow experiment may contain sufficient information to estimate the four selected hydraulic flow parameters in a unique way.

Although the correlation among some parameters is high (not shown), the 95% confidence intervals are quite small, indicating that all parameters are well determined. The relative magnitudes of the correlation coefficients are in agreement with the observed patterns of the response surfaces, except for the couple $K_s - \lambda$. This latter discrepancy may be explained by the existence of indirect correlations, i.e., correlations not shown in the $K_s - \lambda$ plane, which overwhelm the direct correlations.

**GMCS-NMS compared to other optimization methods.** Huyer and Neumaier [1999] have already shown that GMCS is strongly competitive with other existing algorithms in the case of problems with reasonable finite bound constraints. In order to situate the accuracy and effectiveness of the sequential GMCS-NMS strategy for the special case of identifying unsaturated flow properties, we compared the performances of GMCS-NMS, in terms of the number of objective function calls and convergence toward the global minimum, with the performances of GMCS alone, NMS alone, a Genetic algorithm (GA) alone, and GA also sequentially combined with NMS (GA-NMS). We used the GA implemented in Matlab by Houk et al. [1995], parameterized with its
Table 2.3. Inversely estimated parameters and related statistics for the 15 hypothetical cases and the laboratory experiment.

<table>
<thead>
<tr>
<th>Scenario</th>
<th>Estimated parameters ± 95% confidence interval</th>
<th>Statistics</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\alpha$ (cm$^{-1}$)</td>
<td>$n$ (-)</td>
</tr>
<tr>
<td>Actual</td>
<td>0.0383</td>
<td>1.3774</td>
</tr>
<tr>
<td>Case I</td>
<td>0.0383 ± 1.95e-4</td>
<td>1.3774 ± 7.51e-4</td>
</tr>
<tr>
<td>Case II</td>
<td>0.0408 ± 2.73e-3</td>
<td>1.3687 ± 9.52e-3</td>
</tr>
<tr>
<td>Case III</td>
<td>0.0382 ± 4.91e-3</td>
<td>1.3517 ± 1.73e-2</td>
</tr>
<tr>
<td>Medium Actual</td>
<td>0.0314</td>
<td>1.1804</td>
</tr>
<tr>
<td>Case I</td>
<td>0.0314 ± 1.44e-4</td>
<td>1.1804 ± 3.34e-4</td>
</tr>
<tr>
<td>Case II</td>
<td>0.0211 ± 4.45e-3</td>
<td>1.2142 ± 2.13e-2</td>
</tr>
<tr>
<td>Case III</td>
<td>0.0138 ± 6.69e-4</td>
<td>1.2420 ± 7.27e-3</td>
</tr>
<tr>
<td>Medium fine Actual</td>
<td>0.0083</td>
<td>1.2539</td>
</tr>
<tr>
<td>Case I</td>
<td>0.0083 ± 8.48e-6</td>
<td>1.2539 ± 1.85e-4</td>
</tr>
<tr>
<td>Case II</td>
<td>0.0094 ± 6.64e-4</td>
<td>1.2335 ± 1.20e-2</td>
</tr>
<tr>
<td>Case III</td>
<td>0.0057 ± 3.51e-4</td>
<td>1.3022 ± 1.71e-2</td>
</tr>
<tr>
<td>Fine Actual</td>
<td>0.0367</td>
<td>1.1012</td>
</tr>
<tr>
<td>Case I</td>
<td>0.0367 ± 1.12e-4</td>
<td>1.1012 ± 1.17e-4</td>
</tr>
<tr>
<td>Case II</td>
<td>0.0377 ± 1.01e-2</td>
<td>1.1001 ± 1.01e-2</td>
</tr>
<tr>
<td>Case III</td>
<td>0.0302 ± 6.43e-3</td>
<td>1.0984 ± 8.39e-3</td>
</tr>
<tr>
<td>Very fine Actual</td>
<td>0.0265</td>
<td>1.1033</td>
</tr>
<tr>
<td>Case I</td>
<td>0.0265 ± 6.28e-5</td>
<td>1.1033 ± 1.02e-4</td>
</tr>
<tr>
<td>Case II</td>
<td>0.0270 ± 4.62e-3</td>
<td>1.1025 ± 7.29e-3</td>
</tr>
<tr>
<td>Case III</td>
<td>0.0197 ± 6.85e-4</td>
<td>1.1068 ± 1.66e-3</td>
</tr>
<tr>
<td>Laboratory sand Direct</td>
<td>0.0459</td>
<td>4.5100</td>
</tr>
<tr>
<td>Inverse</td>
<td>0.0278 ± 1.00e-4</td>
<td>7.0169 ± 8.10e-2</td>
</tr>
</tbody>
</table>
default values. NMS requires an initial guess for the parameter vector. As no prior information on the hydraulic parameters is assumed, we trivially chose the middle of the parameter space, i.e., \((u + v)/2\).

Results are presented in Table 2.4. As mentioned previously, GMCS-NMS converged exactly to the global minimum for each optimization, after 2500 to 3100 iterations. For four soils, GMCS alone found exactly the true solution, whereas for the medium fine textured soil the basic GMCS search found only the solution approximately, in the basin of attraction of the global minimum. This solution was further improved by the additional local NMS search which eventually converged exactly to the true parameter vector. This reveals the accuracy of GMCS alone, but also the importance of combining GMCS and NMS. NMS alone converged quickly in each case, but each time in a local minimum. Although GA alone presents, coincidentally, approximately the same number of function calls than GMCS, it never converged to the solution. Its combination with NMS showed further that for one case (coarse), it did not find the basin of attraction of the global minimum. For the four other cases, GA-NMS found only the solution approximately and always with a greater number of function calls than GMCS-NMS. Notwithstanding the fact that other parameterizations of GA may be more competitive, they will never be as accurate as GMCS, because, as explained before, GA are only purely heuristic methods.

2.4.2 Stability of the inverse solution

For verifying the continuous dependence between the response of the system and the estimated parameter values, i.e., the solution stability, we added errors to the observation data to solve the inverse problem and see if the identified parameters converge to the same values when the observation errors tend to zero. A discontinuous dependence may appear for instance when a local minimum in the objective function becomes progressively more pronounced with vary-

<table>
<thead>
<tr>
<th>Experiment</th>
<th>GMCS-NMS</th>
<th>GMCS</th>
<th>NMS</th>
<th>GA</th>
<th>GA-NMS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coarse</td>
<td>2550 C</td>
<td>2400 C</td>
<td>113 NC</td>
<td>2434 NC</td>
<td>2570 NC</td>
</tr>
<tr>
<td>Medium</td>
<td>2550 C</td>
<td>2400 C</td>
<td>144 NC</td>
<td>2352 NC</td>
<td>3027 CA</td>
</tr>
<tr>
<td>Medium fine</td>
<td>3070 C</td>
<td>2400 NC</td>
<td>157 NC</td>
<td>2419 NC</td>
<td>3220 CA</td>
</tr>
<tr>
<td>Fine</td>
<td>2539 C</td>
<td>2400 C</td>
<td>173 NC</td>
<td>2394 NC</td>
<td>2656 CA</td>
</tr>
<tr>
<td>Very fine</td>
<td>2553 C</td>
<td>2400 C</td>
<td>177 NC</td>
<td>2386 NC</td>
<td>2680 CA</td>
</tr>
</tbody>
</table>

*a*C, optimization converges towards the global minimum;  
*b*NC, optimization does not converge towards the global minimum;  
*c*CA, optimization converges approximately towards the global minimum.
2.4. Results and Discussion

ing the soil response. In this case, this original local minimum may become suddenly the global one.

In practice, soil moisture measurements are corrupted with random and instrumental errors that depend on the measurement technique used. We consider that dielectric measurement techniques like TDR are available to monitor moisture content continuously in the soil. According to Heimovaara and Bouten [1990], the precision of volumetric moisture content measurements using TDR, in terms of reproducibility, is characterized by a standard deviation varying from $5 \times 10^{-4}$ m$^3$m$^{-3}$ for sandy soils to $25 \times 10^{-4}$ m$^3$m$^{-3}$ for clayey soils. For analyzing the stability of the inverse solution, we considered two levels of error. First, we assumed the random errors of the water content measurements to be normally distributed with mean equal to zero and standard deviation equal to $25 \times 10^{-4}$ m$^3$m$^{-3}$ (case II). This case considers the infiltration model to be correct and the TDR calibration to be soil specific. Subsequently, in order to represent a case of uncertainty, in an indirect way, in the mathematical model and/or a reasonable TDR calibration error with a systematic bias, we added to the data, additionally to the random error, a systematic error as suggested by Romano and Santini [1999]. We assumed therefore a normal distributed error with a mean of $0.01$ m$^3$m$^{-3}$ (the systematic bias) and a standard deviation of $25 \times 10^{-4}$ m$^3$m$^{-3}$ as random component (case III). In these two cases, initial and boundary conditions were not directly subject to errors. The two error corrupted data sets are illustrated in Figure 2.3, case II and case III.

In order to compare soil hydraulic properties estimated from the error-contaminated data with the actual ones, we used the root mean square error (RMSE) criterion as a measure of prediction accuracy. The RMSE related to the soil water retention characteristics is defined as

$$RMSE_\theta = \sqrt{\frac{1}{n} \sum_{i=1}^{n} [\theta^*(h_i) - \theta(h_i)]^2}$$

(2.19)

and the RMSE related to the hydraulic conductivity characteristics is defined as

$$RMSE_{\log(k)} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} [\log(K^*(\theta_i)) - \log(K(\theta_i))]^2}$$

(2.20)

where $\theta^*(h)$ and $K^*(\theta)$ refer to the estimated hydraulic properties, $\theta(h)$ and $K(\theta)$ to the actual ones, and $n = 1000$ is the number of points between residual and saturated water content for which the hydraulic functions were evaluated.

Close analysis of the objective functions for these 10 cases (not presented here) reveals that, compared to error-free data inversion, the global minimum
and shape of the objective functions only shifted slightly. This was also observed by Pan and Wu [1999] and Si and Kachanoski [2000]. Objective function values are only higher and minimum regions a little flatter leading to an increase of the confidence regions around the global minimum. This suggests that the structure of the problem is not really affected when data are error corrupted. This is also confirmed from the optimization results presented in Table 2.3. In general, in accordance with their relative sensitivity, estimated parameters are close to their true value. Only parameter $\alpha$ for the medium textured soil, case III, is less well determined. As already stated, this could be attributed to its high correlation with other parameters, and in particular with $n$.

Statistics of the estimated model parameters for these 10 considered optimization scenarios are also reported in Table 2.3. As expected, we can observe that parameter confidence intervals increase with the combined effect of the error and the diminution of the Hessian in the neighborhood of the minimum. For all cases, confidence intervals stay to reasonable values for all parameters. The root mean square error statistics are always small indicating that the shape of the retention and hydraulic curves are estimated accurately. This is illustrated in Figure 2.5, representing the actual and estimated hydraulic properties for the medium fine textured soil, case III. This case represents one of the most critical ones in terms of hydraulic properties prediction ($RMSE_\theta = 6.80 \times 10^{-3}$, $RMSE_{\log(K)} = 2.03 \times 10^{-1}$) and nevertheless shows that the hydraulic curves are relatively well estimated. This means that the inverse problem such as posed here is quite stable, i.e., the solution depends continuously, in the mathematical sense of the term, on the error on the state variables. It should be noted that the errors in $K_s$ estimations are always less than one order of magnitude, which is the error level that one could expect with standard laboratory $K_s$ measuring techniques. Provided that the model describes adequately the soil hydraulic properties, this suggests that the proposed inversion method is promising to procure a physical value for $K_s$. The correlation between measured and fitted water content data (not shown here) decreases logically with increasing error level on the parameters, but remains for all scenarios relatively close to 1 ($r^2 > 0.9825$). This illustrates the excellent agreement between measured and predicted time series, as shown in Figure 2.3, for the medium fine textured soil.

We have also examined the parameter correlation coefficients (results not shown). The different combinations of the four parameters have different degrees of correlation. The optimized parameters $\alpha$, $n$ and $K_s$ were found for most scenarios to be locally strongly correlated in nearly all cases ($r^2 > 0.9$). Yet, practically all these parameters were estimated correctly with reasonable confidence intervals (Table 2.3). In contrast, correlation coefficients related to the tortuosity parameter $\lambda$ are generally the lowest ones. This could be attributed to the lowest and differently structured sensitivity of this parameter in
2.4. Results and Discussion

Figure 2.5. Comparison of actual (line) and inversely estimated (dots) soil water retention curve and hydraulic conductivity function corresponding to the Medium Fine textured soil, case III.

Comparison with the others.

2.4.3 Laboratory case study

For the identification of the laboratory column hydraulic properties, $\theta_r$ was fixed to zero, as stated above, and $\theta_s$ was fixed to its column-scale TDR measured value of 0.337 m$^3$m$^{-3}$. The solution of a first inversion swept out of the predefined parameter interval which we subsequently increased. The maximal value of $n$ was extended to 7, and $K_s$ was searched in the range $[10^{-2}, 10^2]$ cm min$^{-1}$.

The inversion results showed very good agreements ($r^2 = 0.9963$) between the simulated moisture time series and the measured ones (Figure 2.3, laboratory sand). This indicates that the hydrodynamic model used to simulate the water flow in this homogeneous sand is quite appropriate. Some differences appear due possibly to a hysteresis effect during the drainage phase which was not taken into account in the encoded flow model. Even small variations in water content, e.g., at $z_2$ between times $t = 100$ min and $t = 150$ min, are remarkably well described.

Considering discrepancies between directly measured and inversely estimated hydraulic functions (Table 2.3), we observe poorer results ($RMSE_{\theta} = 5.73 \times 10^{-2}$ and $RMSE_{\log(K)} = 3.63 \times 10^{-0}$). All parameters are relatively different. For instance, the inversely estimated value of $K_s$ is one order of magnitude greater than the directly measured value. These differences can be explained as follows. First of all, the scales at which the hydraulic properties were determined are different. For the direct determination of the water retention parameters, only samples of about 50 cm$^3$ were used whereas for the infiltration experiment, the size of the sample is about 5.5 dm$^3$. Even $\theta_s$ was different: 0.357 m$^3$m$^{-3}$ for the small sample, and 0.337 m$^3$m$^{-3}$ for the sand.
column. An another reason may be the difference between the real system and the modeled one. Indeed, it is conceivable that the distribution of the sand density in the column, and therefore of the hydraulic properties, is not quite homogeneous. This hypothesis is supported by the fact that the measured volumetric water content at time $t = 0$ and depth $z_1$ (see Figure 2.3), where the density is probably lower, is lower than the simulated one. Air entrapment may also constitute a source of error. All these error sources cannot be attributed to the inversion procedure and are inherent to modeling any environmental system.

2.5 Summary and Conclusions

Estimating unsaturated soil hydraulic properties using inverse modeling methods is interesting because it allows a high flexibility in the experimental design and because it provides effective hydraulic parameters. Drawbacks related to this technique are related to nonuniqueness and instability problems. Further, the presence of many local minima in the objective function complicates the use of inversion techniques. To circumvent these questions, sufficient information from the physical system response need to be considered in the objective function definition and a powerful inversion technique is required.

This study was conducted to evaluate an inversion method that allows the identification of subsurface hydraulic properties from only continuously measured soil moisture times series during a one-dimensional infiltration-redistribution experiment. Inversion of the governing flow equation is performed using the advanced Global Multilevel Coordinate Search algorithm (GMCS) [Huyer and Neumaier, 1999] combined sequentially with the classical Nelder-Mead Simplex algorithm (NMS) [Lagarias et al., 1998]. We have introduced this optimization method in the area of unsaturated zone hydrology since it is suited for solving accurately and efficiently complex nonlinear problems. Besides its global search capabilities, GMCS-NMS needs neither initial guesses on the parameters (only parameter ranges) nor an evaluation of the functional derivatives of the objective function. This makes it very stable and robust to deal with discontinuous nonlinear multimodal inverse problems as encountered in the unsaturated flow domain. The combination GMCS-NMS allows for a faster convergence toward the solution. Moreover, the procedure being intermediate between purely heuristic optimization methods and stochastic methods has the particularity to be very accurate.

Numerical experiments were designed to evaluate the proposed inversion method to identify four hydrodynamic parameters, i.e., $\alpha$, $n$, $K_s$, and $\lambda$ of the Mualem-van Genuchten model. Analysis of the flow model sensitivity to these hydraulic parameters has provided valuable information for locating optimally
the moisture measurement depths. Examination of the slicing hyper planes from the four-dimensional objective functions related to five different textured soils suggested that the inversion problem as posed has a unique solution. Inversion of the corresponding error-free data sets confirmed these observations and yielded exactly the true parameter values, notwithstanding the presence of local minima and discontinuities in the objective functions. The stability of the solution was further investigated by inverting data sets corrupted with different plausible levels of moisture measurement error. It was shown that the considered levels of error have little influence on the prediction of the unsaturated hydraulic properties. This indicated that the inversion procedure as designed is well-posed and contains sufficient information to enable unique and reliable estimation of the soil hydraulic parameters. Note that some limitations have been observed due seemingly to high correlation between some parameter pairs.

Inversion of real data is more challenging than inversion from numerically generated data. In this case, measurement errors are lumped with modeling error and are often hard to quantify. Nevertheless, our laboratory case study on a homogeneous sand column performed relatively well. The response of the system was modeled efficiently. Only differences between directly measured hydraulic properties and estimated ones where observed. They were attributed mainly to the scale of characterization, and also to a lesser extent, to hysteresis effects and variability within the soil column.

The advantageous aspects of the proposed flow inversion method compared to most existing methods, besides its demonstrated well-posedness properties, are: (i) the required boundary conditions are appropriate for setting up both laboratory and in-situ experiments, and furthermore, are compatible with real-world conditions, (ii) only readily obtainable moisture time series with high temporal resolution are required as model input, (iii) the GMCS-NMS approach is at the same time relatively accurate, efficient, and can handle complex objective functions.

Provided that the flow models describe adequately the hydrodynamic behavior of soils, we can therefore conclude that the proposed inversion method is promising for estimating the effective subsurface unsaturated hydraulic properties. Moreover, adapted parameterizations of GMCS-NMS would allow one to solve problems with a higher number of parameters, and thus, to consider more complex phenomena in the direct flow model.
Chapter 3

Laboratory evaluation of the hydrodynamic inverse modeling procedure

Abstract  The inverse modeling method of Lambot et al. [2002] for estimating the hydraulic properties of partially saturated soils, which was numerically validated, is further tested on laboratory scale transient flow experiments. The method uses the Global Multilevel Coordinate Search algorithm combined sequentially with the local Nelder-Mead Simplex algorithm to inverse the one-dimensional Richards equation using soil moisture time series measured at three different depths during natural infiltration. Flow experiments were conducted on a homogeneous artificial sand column and three undisturbed soil columns collected from agricultural fields. Three models describing the unsaturated soil hydraulic properties were used and compared: the model of Mualem-van Genuchten, the model of Assouline, and the decoupled van Genuchten-Brooks and Corey combination. The performances of all three models were similar, except Assouline’s model which provided poorer results in two cases. The inversion method provided relatively good estimates for the water retention curves, and also for the saturated conductivity when the moisture range explored was not too small. Water content time series were very well reproduced for the artificial soil and a sandy loam soil, but for two silt loam soils larger errors were observed. The prediction of the water transfer behavior in the soil columns was poor when flow properties were estimated using directly determined hydraulic properties. The main limiting factor for applying the inversion method, particularly for non sandy soils, was the characterization of the initial conditions in terms of the pressure head profile.

Chapter 3. Hydrodynamic inversion in laboratory conditions

3.1 Introduction

The development of appropriate methods for the determination of the unsaturated flow properties of soils remains a challenging task for the soil science community and is needed for the many agricultural and environmental engineering applications involving water and solute flow modeling. During the last few years, identification of the unsaturated flow properties from transient flow experiments by means of inverse modeling procedures has gained a lot of interest [Hopmans et al., 2002].

A critical step in the identification process by means of inverse modeling is the optimization of an objective function which expresses, in terms of the parameter values, the difference between the measured and simulated soil response. The inherent topographical complexity of the nonlinear multidimensional objective functions encountered when estimating flow properties from transient flow experiments limits the classical gradient based local search optimization algorithms to converge to the optimal solution [Si and Kachanoski, 2000; Abbaspour et al., 2001; Vrugt and Bouten, 2002; Vrugt et al., 2003]. To overcome this, more efficient and reliable global search optimization algorithms have been proposed. For instance, Abbaspour et al. [1997] presented the Sequential Uncertainty domain parameter FItting method (SUFI), and demonstrated for different problems of increasing complexity its stability and good convergence properties. Takeshita and Kohno [1999] investigated Genetic algorithms to estimate simultaneously the saturated hydraulic conductivity and parameters $\alpha$ and $n$ of the van Genuchten water retention model. Vrugt et al. [2001] combined a Genetic algorithm with a local simplex optimization algorithm to infer simultaneously hydraulic and root water uptake parameters. More recently, Lambot et al. [2002] took advantage of both heuristic and stochastic global optimization methods with the Global Multilevel Coordinate Search algorithm [Huyer and Neumaier, 1999] to identify hydraulic parameters during natural infiltration events. Vrugt et al. [2003] used the Shuffled Complex Evolution Metropolis algorithm to investigate identifiability in different parametric models.

In addition to the convergence properties of the optimization algorithm, the identifiability, uniqueness, and stability conditions in the inverse problem must be satisfied, i.e., the inverse problem must be well-posed [Carrera and Neuman, 1986b; Hopmans et al., 2002]. The model parameters will be identifiable if one and only one parameter set leads to a given system response. The solution will be unique if a system response leads to one and only one optimized parameter set, i.e., the objective function contains only one well defined global optimum. A lack of sensitivity of the system response to certain parameters, as well as high parameter correlations, may cause nonuniqueness. The solution will be stable if it depends continuously on the measured system
response so that it is not very sensitive to measurement and modeling errors, i.e., small measurement and modeling errors do not result in large changes of the optimized parameters. The well-posedness of an inverse problem depends on the boundary conditions of the specific flow experiment, on the considered system response (measured data), and on the forward model and its parameterization. Intensive efforts have been devoted to their definition [Wendroth et al., 1993; van Dam et al., 1994; Gribb, 1996; Simunek and van Genuchten, 1996; Durner et al., 1999; Romano and Santini, 1999]. For instance, Kool et al. [1985] showed that the uniqueness likelihood could be improved if the experiment is designed in such a way that a wide range of soil moisture is covered. Identifiability, uniqueness and stability may also be improved, for a given transient flow experiment, if additional measurements of one or more response variables are considered [Eching and Hopmans, 1993; Vrugt et al., 2002]. For example, Zou et al. [2001] used a two parts constructed objective function which included both pressure head time series and water content data. By this way, they improved significantly the uniqueness of the solution. More recently, Ritter et al. [2003] used the inversion method of Lambot et al. [2002] to investigate a wide range of alternatives with different combinations of variables and measurement depths for infiltration experiments. Finally, identifiability, uniqueness and stability may be improved by the inclusion of prior information in the inversion, either as initial guess or parameter space constrains in the optimization process, or by adding a regularization term in the objective function itself [Carrera and Neuman, 1986a; Si and Kachanoski, 2000].

The quality of the inversion is further subject to the appropriateness of the predictive forward model to describe the system of concern [Hollenbeck and Jensen, 1998b; Vrugt et al., 2003]. It may be expected that numerically validated inversion methods, i.e., methods which have shown to converge to unique and stable parameter solutions in numerical experiments, may fail if model errors are too large. This may become particularly important when applying inverse modeling to real world data where flow may be influenced by a series of processes which are not included or well conceived within the governing flow model such as hysteresis, preferential flow, air entrapment, and spatio-temporal variability of the flow properties. Generally, different models and parameterizations for the hydraulic properties are tested [Romano and Santini, 1999; Vrugt et al., 2003]. Finally, given that measurements at different scales are generally exploited, it may be expected that the identified properties by inverse procedures in heterogeneous media differ from the properties identified from conventional methods [Veh et al., 1985].

All this shows that the different characteristics of an inversion procedure need to be carefully assessed before using the inversion procedure as an operational tool in soil water flow modeling.

In this chapter we evaluate in laboratory conditions the inverse model-
Chapter 3. Hydrodynamic inversion in laboratory conditions

ing procedure proposed by Lambot et al. [2002] for estimating the subsurface unsaturated hydraulic properties from transient flow experiments. The inversion method uses the Global Multilevel Coordinate Search algorithm [Huyer and Neumaier, 1999] combined sequentially with the local Nelder-Mead Simplex algorithm [Lagarias et al., 1998] (GMCS-NMS) to inverse the one-dimensional Richards equation from soil moisture time series during transient infiltration. This procedure was previously numerically validated for different hypothetical soils. Uniqueness and stability of the inverse problem were found to be entirely satisfied as far as the forward model is appropriate, and the measurement errors on the system state variables, i.e., the measured time series of soil moisture, are acceptable. In the present study, the method is further evaluated in laboratory conditions on four different soils: an artificial homogeneous sand and three undisturbed soils representing agricultural soils of central Belgium. In this way, the stability properties of the inverse problem are further investigated for real measurement errors and different model conceptualization errors. In order to get some insight into the importance of the forward model, three different models describing the unsaturated soil hydraulic properties were used and compared.

The strength of the considered inversion method compared to other existing methods is that, additionally to its demonstrated well-posedness properties and the robust optimization algorithm used, soil hydraulic properties are assessed from only soil moisture time series gathered during a natural infiltration process. This thereby leads to highly representative hydraulic parameters and rises the possibility to use purely non-destructive soil moisture sensors such as ground penetrating radar (GPR) to enable field scale hydraulic characterization with a high spatial resolution.

3.2 Materials and Methods

3.2.1 Hydrodynamic model parameterization

For investigating the impact of the forward model on the inverse modeling results, without increasing the number of parameters, we used three different models to describe the unsaturated hydraulic properties: (i) the commonly used nonhysteretic unimodal Mualem-van Genuchten model (MVG) [Mualem, 1976; van Genuchten, 1980], (ii) the recently developed model of Assouline [2001] (ASS), and (iii) the van Genuchten relation subject to Burdine’s condition \( m = 1 - 2/n \) with \( n > 2 \) for the water retention curve combined with the Brooks and Corey relation for the hydraulic conductivity function (VBC), as recommended by Fuentes et al. [1992]. Romano and Santini [1999] concluded that in some cases unsaturated hydraulic conductivity functions with parameters independent of the soil water retention functions are needed for accurate
3.2. Materials and Methods

MVG model is described in Section 2.2.1 (page 14). Assouline et al. [1998] derived a conceptually based expression for the water retention curve:

$$\theta(h) = \theta_r + (\theta_s - \theta_r) \left(1 - \exp\left[-\xi \left(\frac{1}{|h|} - \frac{1}{|h_r|}\right)^\mu\right]\right)$$

(3.1)

where $\xi (L^\mu)$ and $\mu (-)$ are fitting parameters, and $h_r$ is the pressure head ($L$) corresponding to the residual water content. The pressure head $h$ is bounded as $0 \leq |h| \leq |h_r|$. It can be assumed that $h_r \to -\infty$. This model hypothesizes that the soil structure results from a uniform random fragmentation process which determines in this way the particle size distribution from which the pore size distribution is derived using a power function. The fragmentation likelihood of a soil particle is supposed to be proportional to its size. Good agreement between this model and measured soil data have been observed for a wide range of soil textures from sand to clay, demonstrating at the same time its flexibility and suitability for both high and low water contents [Assouline et al., 1998]. Applying the Mualem statistical approach, Assouline [2001] has recently proposed an expression for the hydraulic conductivity function by using the first two moments of the aforementioned ASS water retention model:

$$K(Se) = K_s Se^{\lambda} \left[\frac{\xi^\frac{1}{\mu} \gamma\left(\frac{1}{\mu}, \xi \alpha\right) - \frac{1}{|h|} e^{-\xi \alpha} + \frac{1}{|h_r|}}{\xi^\frac{2}{\mu} \Gamma\left(\frac{1}{\mu}\right) + \frac{1}{|h_r|}}\right]^\eta$$

(3.2)

where $\gamma(\beta, \nu)$ and $\Gamma(\nu)$ are, respectively, the incomplete and complete Gamma functions, $\alpha = \left(|h|^{-1} - |h_r|^{-1}\right)^\mu$, and $\eta$, as defined hereafter, is a parameter depending on the water retention function. This model is less restrictive than the MVG model concerning the pore configuration. Indeed, it assumes that the length of the constitutive capillary elements is not necessarily proportional to their diameter. The power value $\eta$ depending on the soil structure and texture, which both define the water retention function, Assouline [2001] proposed to relate $\eta$ to the mean $r_G$ and the variance $\sigma^2$ of the water retention function:

$$r_G = \xi^\frac{1}{\mu} \Gamma\left(1 + \frac{1}{\mu}\right) + \frac{1}{|h_r|}$$

(3.3)

$$\sigma^2 = \xi^\frac{2}{\mu} \left[\Gamma\left(1 + \frac{2}{\mu}\right) - \Gamma^2\left(1 + \frac{1}{\mu}\right)\right]$$

(3.4)

The model was calibrated on a large variety of soils and a strong correlation between $\eta$ and these water retention function characteristics was found using the adjusted equation:

$$\eta = 1.18 \left(\frac{\sigma}{r_G}\right)^{-0.61}$$

(3.5)
The VBC hydraulic conductivity function, which is not derived from the water retention curve, gives:

\[ K(\theta) = K_s \theta^{-\eta} \]  

(3.6)

where the exponent \( \eta \) is a curve shape parameter (\( - \)).

In this study, for the three considered models, following Nimmo [1991] and Fuentes et al. [1992], we assume that \( h_r \to -\infty \) and that \( \theta_r \to 0 \).

### 3.2.2 Inversion

The saturated water content \( \theta_s \) was determined using a direct method. Therefore, the size of the parameter vector \( b \) to be identified reduces to four for the three considered models: \( b = [\alpha, n, K_s, \lambda]^T \) for MVG, \( b = [\xi, \mu, K_s, \lambda]^T \) for ASS, and \( b = [\alpha, n, K_s, \eta]^T \) for VBC. The objective function is defined by equation (2.6) and is minimized using the GMCS-NMS approach, as described in Section 2.2.2. Since, as shown in the following, dealing with real data does not increase necessarily the complexity of the objective function topography compared to synthetic error free data, we use the same algorithm parameterization as used in Lambot et al. [2002]. In this way, the convergence toward the global minimum is ensured. Consequently, optimization issues will not be further questioned in this study.

All inversions were performed in the same large parameter space bounded as \([0.001 < \alpha < 0.500 \text{ cm}^{-1}; 1.01 < n < 8; 1 \times 10^{-3} < K_s < 1 \times 10^2 \text{ cm min}^{-1}; 0 < \lambda < 10] \) for MVG and, accordingly, as \([2.40 < \xi < 1.65 \times 10^8 \text{ cm}^\mu; 1 \times 10^{-3} < K_s < 1 \times 10^2 \text{ cm min}^{-1}; 0 < \lambda < 10] \) for ASS and as \([0.001 < \alpha < 0.500 \text{ cm}^{-1}; 2.01 < n < 8; 1 \times 10^{-3} < K_s < 1 \times 10^2 \text{ cm min}^{-1}; 2.9 < \eta < 530] \) for VBC. The ASS and VBC parameter spaces were determined from the MVG one by fitting, respectively, ASS and VBC models on MVG model for a wide range of MVG parameter combinations situated in the MVG parameter space. The MVG parameter space was inferred from the range of MVG parameters typically retrieved in soil hydrodynamic data bases.

### 3.2.3 Laboratory experiments description

Laboratory infiltration experiments were conducted on a homogeneous disturbed sand column and three undisturbed soil columns consisting of a sandy loam soil and two similar silt loam soils, according to the USDA textural classification. The soil columns were 30 cm high and 15.3 cm diameter. The artificial homogeneous sand was set up to respond at best to the considered water transfer model. The undisturbed soil samples were collected from experimental agricultural fields of the Agronomic Research Center of Gembloux.
in Belgium and represent high quality arable soils. The three columns originate from the illuvial Bt-horizon (40-70 cm). Intentionally, high clay content soils were not considered in this study, as it is likely that shrinking and swelling processes would affect both the infiltration experiments and the water content monitoring. The physical characteristics of the four samples, as well as the saturated water content $\theta_s$, are listed in Table 3.1. The saturated water content was measured directly using time domain reflectometry (TDR) after saturating progressively the soil columns.

The directly estimated hydraulic parameters are given for the three considered hydraulic models (Direct MVG, Direct ASS, and Direct VBC) in Table 3.2. Hydraulic parameters were determined using direct conventional laboratory methods (e.g., see Klute and Dirksen [1986]) on 100 cm$^3$ samples using a sand-box apparatus (suction range 0-100 cm) and a pressure cell (suction range 200-13000 cm) to determine the drying water retention curve, and a constant head apparatus to determine the saturated conductivity $K_s$. For the undisturbed soils, the hydraulic properties pertain to samples taken about 30 cm apart from the soil columns. Parameter $\lambda$ was fixed to the commonly used value of 0.5 [Mualem, 1976].

During the infiltration experiments, soil water content was monitored continuously by means of TDR probes installed horizontally at the three specified depths (5, 15, and 25 cm). TDR measurements were carried out with a Tektronix 1502C metallic TDR cable tester and the different channels corresponding to the different probes were multiplexed automatically with a SDMX50 multiplexer system (Campbell Scientific Inc.). A total of 12 TDR probes were used in this study. They were constructed in the laboratory and they consisted of three stainless steel rods (9.3 cm long and 0.5 cm diameter) with a 2.5 cm rod spacing. The Tektronix was connected to a computer with an RS232 interface to acquire numerically the TDR signal. The soil dielectric constant was derived from the TDR signal using the WinTDR98 program developed by the Soil Physics Group at Utah State University [Or et al., 1998]. After experimental verification of its validity for the considered soils, we used Topp’s model [Topp et al., 1980] to relate the soil dielectric constant to the soil volumetric

<table>
<thead>
<tr>
<th>Soil</th>
<th>Sand (%)</th>
<th>Silt (%)</th>
<th>Clay (%)</th>
<th>OM (%)</th>
<th>Bulk density (g cm$^{-3}$)</th>
<th>$\theta_s$ (m$^3$m$^{-3}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sand</td>
<td>100.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.00</td>
<td>1.56</td>
<td>0.337</td>
</tr>
<tr>
<td>Sandy loam</td>
<td>76.5</td>
<td>12.2</td>
<td>11.3</td>
<td>0.45</td>
<td>1.57</td>
<td>0.361</td>
</tr>
<tr>
<td>Silt loam 1</td>
<td>4.0</td>
<td>77.1</td>
<td>18.9</td>
<td>0.80</td>
<td>1.55</td>
<td>0.392</td>
</tr>
<tr>
<td>Silt loam 2</td>
<td>4.3</td>
<td>74.3</td>
<td>21.4</td>
<td>0.65</td>
<td>1.54</td>
<td>0.372</td>
</tr>
</tbody>
</table>

*OM: organic matter.
Additionally to TDR probes, three tensiometers were inserted horizontally at the same depths in order to characterize the initial conditions in terms of the pressure head profile. The tensiometers were made of 2.5 cm long, 0.6 cm outside diameter, 1-bar porous cups. Tension was measured with a SMS5000 (SDEC) hand-held pressure sensing device. Initial conditions were imposed so that a relatively wide range of water content was covered during the infiltration experiments. For the artificial sandy soil, an initial pressure head profile in hydrostatic equilibrium was readily established by imposing a suction of 15 cm at the bottom of the soil column. For the other three soils, higher initial pressure head profiles were required. Hence, soil columns were led to a higher suction by producing in the soil a drying downward air stream. After waiting several weeks for hydrostatic equilibrium, the pressure head was subsequently measured at the three measurement depths and the whole pressure head profile was inferred using linear interpolation and extrapolation. In contrast to the silt loam 1 soil, the initial pressure head profile of the silt loam 2 soil was led to a suction exceeding the capacity of the tensiometers in order to explore a wider water content range. Consequently, we estimated its initial pressure head profile from the water content measurements using its directly determined water retention curve. It is worth noting that hydrostatic equilibrium was not reached in this case since water fluxes were too slow at this suction.

The seepage face bottom boundary condition was ensured by a two layered 2.5 cm drainage package of coarse sand and fine gravel situated just under the 30 cm high soil column. The upper boundary condition consisted in a downward constant water flow. Water was uniformly applied on the surface through an irrigation system consisting of a microtube peristaltic pump (MCP V5.16, Ismatec) feeding 21 microtubes distributed evenly above the soil surface. The flow rate for each column was adjusted following preliminary infiltration experiments so as to avoid surface ponding and to minimize air entrapment [Wildenschild et al., 2001]. Infiltration rate equaled \(4.70 \times 10^{-1}\), \(2.61 \times 10^{-2}\), \(5.60 \times 10^{-3}\), and \(6.01 \times 10^{-3}\) cm min\(^{-1}\) for the sand, the sandy loam, the silt loam 1, and the silt loam 2 soil, respectively.

For the four infiltration experiments, six modeling scenarios were considered. Three scenarios refer to the hydraulic parameters determined using the direct methods for the three hydraulic models (Direct MVG, Direct ASS, and Direct VBC), and three scenarios refer to the inversely estimated parameters from the observed soil moisture time series (Inverse MVG, Inverse ASS, and Inverse VBC).

The root mean square error statistic was used to quantify the difference between observed and modeled data for both the water retention curves and the water content time series, respectively, \(RMSE_{\theta(h)}\) and \(RMSE_{\theta(z,t)}\).
### Table 3.2. Hydraulic Parameters of the Four Considered Soils Estimated from Direct Measurements (Direct) and Hydrodynamic Inverse Modeling (Inverse) for the three hydraulic models

<table>
<thead>
<tr>
<th>Scenario</th>
<th>α / ξ</th>
<th>n / μ</th>
<th>K_s (cm min^-1)</th>
<th>λ / η</th>
<th>RMSE_{θ(h)} (m^3 m^-3)</th>
<th>RMSE_{θ(z,t)} (m^3 m^-3)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Sand</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Direct MVG</td>
<td>4.40e-2</td>
<td>4.76</td>
<td>6.79e-1</td>
<td>0.50</td>
<td>1.51e-2</td>
<td>9.50e-2</td>
</tr>
<tr>
<td>Direct ASS</td>
<td>1.64e4</td>
<td>3.17</td>
<td>6.79e-1</td>
<td>0.50</td>
<td>1.22e-2</td>
<td>9.50e-2</td>
</tr>
<tr>
<td>Direct VBC</td>
<td>4.71e-2</td>
<td>5.34</td>
<td>6.79e-1</td>
<td></td>
<td>1.43e-2</td>
<td>-</td>
</tr>
<tr>
<td>Inverse MVG</td>
<td>2.82e±2±5.26e-5</td>
<td>7.32±2±5.26e-2</td>
<td>5.36e0±6.21e-1</td>
<td>1.59±2±5.20e-1</td>
<td>8.65e-2</td>
<td>2.18e-3</td>
</tr>
<tr>
<td>Inverse ASS</td>
<td>1.48e±2±1.27e0</td>
<td>4.71±2±1.06e-2</td>
<td>6.69±0±1.10e-1</td>
<td>1.27±2±4.39e-1</td>
<td>8.97e-2</td>
<td>3.44e-3</td>
</tr>
<tr>
<td>Inverse VBC</td>
<td>2.90e-2±6.46e-5</td>
<td>7.67±2±5.08e-2</td>
<td>5.25e0±6.19e-1</td>
<td>4.31±2±5.13e-1</td>
<td>8.73e-2</td>
<td>2.23e-3</td>
</tr>
<tr>
<td><strong>Sandy loam</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Direct MVG</td>
<td>3.15e-1</td>
<td>1.42</td>
<td>3.48e-2</td>
<td>0.50</td>
<td>8.89e-3</td>
<td>1.11e-1</td>
</tr>
<tr>
<td>Direct ASS</td>
<td>3.01e0</td>
<td>0.52</td>
<td>3.48e-2</td>
<td>0.50</td>
<td>9.15e-3</td>
<td>5.26e-2</td>
</tr>
<tr>
<td>Direct VBC</td>
<td>4.58e-1</td>
<td>2.38</td>
<td>3.48e-2</td>
<td></td>
<td>8.57e-3</td>
<td>-</td>
</tr>
<tr>
<td>Inverse MVG</td>
<td>1.42e±1±1.81e-2</td>
<td>1.50±2±1.35e-2</td>
<td>2.59e0±4.66e0</td>
<td>2.97±2±2.92e-1</td>
<td>2.06e-2</td>
<td>6.29e-3</td>
</tr>
<tr>
<td>Inverse ASS</td>
<td>4.24e±1±1.02e0</td>
<td>0.57±4±1.44e-3</td>
<td>7.20e0±1.00e0</td>
<td>6.70±2±0.34e-1</td>
<td>1.77e-2</td>
<td>6.30e-3</td>
</tr>
<tr>
<td>Inverse VBC</td>
<td>1.85e-1±5.14e-3</td>
<td>2.46±3±3.90e-3</td>
<td>3.84e0±4.52e-1</td>
<td>9.21±2±1.68e-1</td>
<td>2.16e-2</td>
<td>6.31e-3</td>
</tr>
<tr>
<td><strong>Silt loam 1</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Direct MVG</td>
<td>1.65e-2</td>
<td>1.13</td>
<td>2.05e-1</td>
<td>0.50</td>
<td>1.64e-2</td>
<td>3.35e-2</td>
</tr>
<tr>
<td>Direct ASS</td>
<td>7.07e0</td>
<td>0.25</td>
<td>2.05e-1</td>
<td>0.50</td>
<td>1.91e-2</td>
<td>3.58e-2</td>
</tr>
<tr>
<td>Direct VBC</td>
<td>2.46e-2</td>
<td>2.12</td>
<td>2.05e-1</td>
<td></td>
<td>1.41e-2</td>
<td>-</td>
</tr>
<tr>
<td>Inverse MVG</td>
<td>3.04e±2±1.63e-3</td>
<td>1.15±2±3.71e-3</td>
<td>3.61e3±2.01e3</td>
<td>45.0±2±3.38e0</td>
<td>3.27e-2</td>
<td>6.05e-3</td>
</tr>
<tr>
<td>Inverse ASS</td>
<td>2.81e±2±1.01e0</td>
<td>0.13±4±1.64e-3</td>
<td>1.12e3±5.55e2</td>
<td>74.8±2±3.24e0</td>
<td>4.03e-2</td>
<td>4.95e-3</td>
</tr>
<tr>
<td>Inverse VBC</td>
<td>4.34e-2±1.16e-3</td>
<td>2.13±2±1.27e-3</td>
<td>3.70e3±2.69e3</td>
<td>83.2±2±5.35e0</td>
<td>2.81e-2</td>
<td>5.73e-3</td>
</tr>
<tr>
<td><strong>Silt loam 2</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Direct MVG</td>
<td>1.25e-2</td>
<td>1.17</td>
<td>7.22e-2</td>
<td>0.50</td>
<td>2.74e-2</td>
<td>2.76e-2</td>
</tr>
<tr>
<td>Direct ASS</td>
<td>9.00e0</td>
<td>0.31</td>
<td>7.22e-2</td>
<td>0.50</td>
<td>2.95e-2</td>
<td>3.85e-2</td>
</tr>
<tr>
<td>Direct VBC</td>
<td>1.92e-2</td>
<td>2.16</td>
<td>7.22e-2</td>
<td></td>
<td>2.46e-2</td>
<td>-</td>
</tr>
<tr>
<td>Inverse MVG</td>
<td>5.90e-2±4.72e-4</td>
<td>1.26±2±8.16e-3</td>
<td>6.39e±2±1.26e-2</td>
<td>4.82±2±4.64e-4</td>
<td>3.23e-2</td>
<td>1.48e-2</td>
</tr>
<tr>
<td>Inverse ASS</td>
<td>1.77e-2±1.01e0</td>
<td>1.46±2±1.78e-3</td>
<td>4.30e-3±6.30e-4</td>
<td>9.15±2±4.25e-1</td>
<td>8.70e-2</td>
<td>1.43e-2</td>
</tr>
<tr>
<td>Inverse VBC</td>
<td>7.01e-2±2.58e-4</td>
<td>2.25±2±3.62e-3</td>
<td>3.91e-3±1.32e-4</td>
<td>14.5±2±1.22e-1</td>
<td>3.29e-2</td>
<td>1.56e-2</td>
</tr>
</tbody>
</table>

*Read 6.79e-1 as 6.79 × 10^{-1}.*
RMSE_{\theta(h)} was defined as

$$RMSE_{\theta(h)} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} [\theta^*(h_i) - \theta(h_i)]^2}$$ (3.7)

where $\theta^*(h_i)$ and $\theta(h_i)$ denote, respectively, the modeled and measured water content at pressure head $h_i$, and $n$ is the number of points between residual and saturated water content for which the function was evaluated. Similarly, $RMSE_{\theta(z,t)}$ was defined as

$$RMSE_{\theta(z,t)} = \sqrt{\frac{1}{nmn} \sum_{i=1}^{n} \sum_{j=1}^{m} [\theta^*(z_i, t_j) - \theta(z_i, t_j)]^2}$$ (3.8)

where $\theta^*(z_i, t_j)$ and $\theta(z_i, t_j)$ denote, respectively, the modeled and measured water content at depth $z_i$ and time $t_j$, $n = 3$ is the number of observation depths, and $m$ is the number of observation times.

### 3.3 Results and Discussions

#### 3.3.1 Response surface analysis

For the MVG model, Lambot et al. [2002] analyzed the inverse problem and performed a thorough objective function topography analysis using response surfaces for both synthetic error-free and error-contaminated data. They observed that, compared to error-free data, the global minimum and shape of the objective functions for error-contaminated data only shifted slightly. This was also observed by Pan and Wu [1999] and Si and Kachanoski [2000]. Objective function values were only higher and minimum regions a little flatter leading to an increase of the confidence regions around the global minimum. This indicated that the complexity of the optimization problem is not really affected when data are error corrupted.

We performed such a response surface analysis for the real inversion experiments dealt with in this study. Figure 3.1 represents two of the response surfaces pertaining to the silt loam 1 soil, for which, as shown hereafter, the model error is relatively large. We can observe topographies similar to the ones reported in Lambot et al. [2002]. The minimum regions are just much more flatter, leading to larger confidence intervals on the estimated parameters. A high negative correlation between $\alpha$ and $n$ is observed, whereas no correlation between $n$ and $\lambda$ is visible. It appears however that $\lambda$ is very much less sensitive than $n$, which should result in a less accurate estimation of this parameter. Yet, the optimization problem is apparently no more complex than for
error-free data and the same GMCS-NMS parameterization as used in Lambot et al. [2002] can then be used to find the global minimum of the objective functions. The maximum number of iteration for GMCS was fixed to 2400, and the maximum splitting level to 30.

### 3.3.2 Hydraulic properties

Parameter values obtained for the six scenarios are presented in Table 3.2. First, the three models fitted to the directly measured water retention data (not presented) are in close agreement each other. For clarity, just MVG is presented in Figure 3.2. The $RMSE_{\theta(h)}$ values are slightly higher for ASS model, except for the sand. This observation was not expected considering the results of Assouline et al. [1998] who observed for twelve soils, ranging from sand to clay, that ASS model leads generally to an improvement of the goodness of fit compared to MVG model as a result of its increased flexibility. This disagreement may be either specific to the soils investigated in our study, or may originate from the fact that we fixed $|h_r|$ to infinity and $\theta_r$ to zero (see equations (2.3) and (3.1)), reducing by this way the flexibility of the models. In every cases, Burdine’s condition ($m = 1 - 2/n$) for the van Genuchten model provided better results than Mualem’s condition ($m = 1 - 1/n$).

The inverse identification of the water retention curves agrees well with the directly determined curves, except for ASS model in the case of the two silt loam soils (see Figure 3.2). Also, relatively large $RMSE_{\theta(h)}$ values are obtained for the sand. This stems from the step-function shape which is typical for sandy soils. A small error on $\alpha$, parameter which determines the air entry suction and then the position of the rapid decrease in water content, results therefore in large errors on the water content. Both the MVG and VBC
Chapter 3. Hydrodynamic inversion in laboratory conditions

Figure 3.2. Water retention curves of the four considered soils estimated from direct measurements (Direct) and hydrodynamic inverse modeling (Inverse) for the three considered hydraulic models. Square markers represent the initial conditions for the three measurements depths.

models perform in a similar way, with slightly better results for MVG in the case of the sand, sandy loam, and silt loam 2 soils. Note that the model generally fit the initial condition points well (see square markers in Figure 3.2). Yet, these points are unexpectedly not on the directly determined curves, except for the silt loam 2 soil for which it was imposed. This explains mainly the difference between the directly and inversely estimated curves, and is to be attributed mainly to the different characterization scales and measurement methods used. Initial conditions were determined from TDR measurements (characterization scale of about 250 cm$^3$) for the water content and from tensiometer measurements (characterization scale of some cm$^3$) for the pressure head. The directly measured water retention curves pertain to samples of 100 cm$^3$ with the water content measured by the gravimetric method, and the pressure head imposed by the sand-box and the pressure cell apparatus. Finally, inversely predicted water retention curves characterize the entire soil column, i.e., about $5.5 \times 10^3$ cm$^3$. For anisotropic and heterogeneous porous media as
3.3. Results and Discussions

inherently encountered in the environment, effective soil physical properties depend on the measurement scale (e.g., see Yeh et al. [1985] and Khaleel et al. [2002]).

An additional source of error may be the fact that we considered TDR measurements to return point values of volumetric water content. Yet, TDR has spatially distributed measurement sensitivities, averaging the property of interest over some sample volume. The adopted TDR configuration was however designed to minimize this effect (see Ferré et al. [2002]).

Finally, the hysteretic behavior of the hydraulic properties may exert also influence on the estimations. Actually, drying curves were considered for the direct measurements since they correspond to the initial conditions. But during the infiltration experiments, the soil wets and the hydraulic properties deviate progressively from the drying curve to the wetting curve. Nevertheless, we can observe that the inversely estimated curves are not necessarily on the left side of the direct drying curves (see Figure 3.2), as it would be expected for wetting curves. That suggests that the effects of the characterization method is more important than the hysteresis effect.

Uncertainty in the parameter estimates was assessed by the 95% confidence intervals using linear regression analysis [Kool and Parker, 1988]. Generally, VBC model leads to smaller confidence intervals on the parameters, especially regarding the saturated conductivity $K_s$. For the sand and particularly for the silt loam 2 soil (MVG scenario), inversely predicted $K_s$ values agree well with the direct measurements: the differences are inferior to one order of magnitude. This kind of error on the saturated conductivity is commonly observed for direct measurements [Schaap and Leij, 2000]. Bruckler et al. [2002] also observed such discrepancies, and even larger, in the estimated hydraulic conductivities using inversion of infiltration data. For the sandy loam and the silt loam 1 soils, $K_s$ values are largely overestimated (two and four orders of magnitude higher, respectively). We attribute these unrealistic values to the fact that the experiments were limited to unsaturated flow conditions. In particular, for the silt loam 1 soil, a relatively small soil moisture range (about 5%) was explored during the infiltration experiment. In this case, the sensitivity of the soil response to the saturated conductivity is smaller, leading to larger uncertainties in the inverse estimation. Moreover, the large values obtained for parameter $\lambda$ compensate partly for the effect of a high saturated conductivity on the hydraulic conductivity. Preferential flow processes are expected to play a negligible role in the $K_s$ overestimations since unsaturated flow conditions were forced. Decoupling the hydraulic conductivity function from the water retention curve with the VBC model did not improve the estimation of the hydraulic properties, although confidence intervals are generally smaller.

Table 3.3 shows the parameter correlation coefficients pertaining to the three models. High correlations exist between some parameter pairs. Specif-
ically, $\alpha$ and $n$ for the MVG parameterization show the highest negative correlations, which is clearly illustrated in Figure 3.1. These parameters are less correlated using VBC. The corresponding parameters ($\xi$ and $\mu$) in ASS are also highly correlated. $K_s$ and $\lambda$ (and $K_s$ and $\eta$) show the highest positive correlations, particularly for ASS model. Though high correlation among parameters does not inhibit convergence to the global minimum of the objective function [Durner et al., 1999], it may lead to larger uncertainties. For instance, the strong interdependency between $K_s$ and $\lambda$ may account for the unrealistic values obtained for these parameters. Other parameter pairs are not very correlated.

### 3.3.3 Water transfer

Observed and fitted water content time series are presented in Figure 3.3. The simulated curves represent the best fit that the given hydrodynamic model can make since the estimated parameters correspond theoretically to the global minimum of the objective function. For the sand and sandy loam soils, results are very good, but for both silt loam soils, results are visibly less satisfactory. All three models lead to similar results (see RMSE values in Table 3.2). For the sandy soil, ASS model was less flexible, which is revealed in the parameter correlation matrix. The correlation between $\alpha$ and $n$ is equal to $-0.2868$ for MVG model, whereas the correlation between $\eta$ and $\mu$ is less conducive and equal to $0.9985$ for ASS model (see Table 3.3). For the silt loam 1 soil, in contrast, ASS parameters are not very much correlated compared to MVG model and the ASS derived time series are better reproduced. Using the decoupled VBC model did not lead to better results.

Since the inverse problem dealt with in this study is theoretically well-posed, the observed discrepancies between the measured and modeled water content time series are to be attributed to measurement and conceptual model errors. The main source of measurement errors is the linear interpolation and extrapolation of the pressure head values to obtain the entire initial pressure head profile. When hydrostatic equilibrium is not reached due to a high suction level, as occurring for the silt loam 2 experiment, the inferred vertical pressure head profile is subject to a high uncertainty. In the same way, unbalanced horizontal variations are also expected to exist and then, the relatively point suction values returned by the tensiometers may not be representative for a specified depth.

For the artificial homogeneous sand, the hydrodynamic model reproduces very well the soil response, as expected. Hysteresis and air entrapment processes are therefore not very important. Also, the TDR point measurement approximation seems to be valid. Errors stem only from the random noise on the TDR measurements. Then, for the undisturbed sandy loam, the observed
### Table 3.3. Parameter Correlation Coefficients for Mualem-van Genuchten’s Model (MVG), Assouline’s Model (ASS), and van Genuchten-Brooks and Corey’s Model (VBC).

<table>
<thead>
<tr>
<th>Scenario</th>
<th>$\alpha / \xi - n / \mu$</th>
<th>$\alpha / \xi - K_s$</th>
<th>$\alpha / \xi - \lambda / \eta$</th>
<th>$n / \mu - K_s$</th>
<th>$n / \mu - \lambda / \eta$</th>
<th>$K_s - \lambda / \eta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sand</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MVG</td>
<td>-0.2868</td>
<td>-0.4177</td>
<td>-0.3644</td>
<td>0.4002</td>
<td>0.4289</td>
<td>0.9619</td>
</tr>
<tr>
<td>ASS</td>
<td>0.9985</td>
<td>-0.2293</td>
<td>-0.5031</td>
<td>-0.2524</td>
<td>-0.5212</td>
<td>0.9050</td>
</tr>
<tr>
<td>VBC</td>
<td>-0.5489</td>
<td>-0.4983</td>
<td>-0.4498</td>
<td>0.4013</td>
<td>0.4019</td>
<td>0.9586</td>
</tr>
<tr>
<td>Sandy loam</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MVG</td>
<td>-0.9971</td>
<td>0.6466</td>
<td>-0.4915</td>
<td>-0.6457</td>
<td>0.4852</td>
<td>0.3393</td>
</tr>
<tr>
<td>ASS</td>
<td>0.9627</td>
<td>-0.1663</td>
<td>-0.1421</td>
<td>-0.1537</td>
<td>-0.1734</td>
<td>0.9780</td>
</tr>
<tr>
<td>VBC</td>
<td>0.9232</td>
<td>0.5475</td>
<td>-0.4336</td>
<td>0.5433</td>
<td>-0.5017</td>
<td>-0.9664</td>
</tr>
<tr>
<td>Silt loam 1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MVG</td>
<td>-0.9422</td>
<td>-0.2353</td>
<td>-0.5145</td>
<td>0.2947</td>
<td>0.5113</td>
<td>0.9136</td>
</tr>
<tr>
<td>ASS</td>
<td>0.8422</td>
<td>-0.1794</td>
<td>-0.2239</td>
<td>-0.1005</td>
<td>-0.2663</td>
<td>0.9512</td>
</tr>
<tr>
<td>VBC</td>
<td>-0.7529</td>
<td>0.1824</td>
<td>-0.0752</td>
<td>-0.0370</td>
<td>0.1257</td>
<td>0.9506</td>
</tr>
<tr>
<td>Silt loam 2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MVG</td>
<td>-0.9610</td>
<td>0.6044</td>
<td>-0.0277</td>
<td>-0.5257</td>
<td>0.0475</td>
<td>0.7258</td>
</tr>
<tr>
<td>ASS</td>
<td>0.8118</td>
<td>0.1992</td>
<td>0.2494</td>
<td>0.3331</td>
<td>0.2304</td>
<td>0.9221</td>
</tr>
<tr>
<td>VBC</td>
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<td>-0.8918</td>
<td>-0.4941</td>
<td>0.8613</td>
<td>0.1049</td>
<td>0.2602</td>
</tr>
</tbody>
</table>
errors are likely to stem mainly from the fact that it is not perfectly homogeneous, as assumed in the adopted forward model. Accordingly, the error increases mostly with depth and time since water has then crossed more heterogeneities. In contrast to the sand and sandy loam soils, we observed in both silt loam soil columns the presence of some macropores originating from roted roots and earthworm galleries. Although preferential flow is prevented by the imposed unsaturated conditions, the air filled macropores may influence water transfer and also to some extent TDR measurements. Local variations of the hydraulic properties are also expected to be inherently present.

Additional complications were reported by Schultze et al. [1999] who cautioned that transient flow experiments might include air-phase effects that should be incorporated by two-phase flow modeling instead of describing water flow by the traditional Richards equation only.

Figure 3.4 represents the water content time series predicted from the directly determined hydraulic properties. The prediction errors are very important: the $RMSE_{\theta(z,t)}$ values are more than one order of magnitude higher than for inverse modeling simulations. Small errors on the hydraulic proper-
ties produce therefore large errors on the system response. This is a corollary of a well-posed inverse problem for which the solution must be stable, i.e., errors on the system response must lead to small errors on the estimated parameters. Nevertheless, it is worth emphasizing that for both simulations and measurements, the time at which the soil system responds to the hydraulic perturbation is consistent. That means that the average water velocity in the soil is quite well modeled.

An important part of the discrepancies originates from the initial conditions, since there is a difference of water content for the same directly measured initial pressure heads. As stated before, this stems from the different measurement methods and from the different operating characterization scales. Since characterizing the initial conditions using pressure head measurements is not so appropriate, particularly when a wide range of water content must be explored in non sandy soils, initial conditions should be rather defined in terms of soil water content profile measured by the same method as for the water content time series, i.e., at the same measurement scale. But given that the numerical solution of the forward model (2.1) requires pressure head values as
initial conditions, this would introduce in the inversion problem an additional degree of freedom that may lead to non-uniqueness. Therefore, in this case, it is likely that additional information would be required. This additional information can be additional measurement depths for soil water content or a-priori information on the parameters.

3.4 Summary and Conclusions

The inverse modeling procedure used in this study presents many advantages among the numerous inverse methods that have been developed to estimate soil hydraulic properties: (i) the required boundary conditions are well in accordance with natural flow conditions, making possible the application of the method in field conditions, (ii) apart from the initial conditions, only soil water content time series are required as model input, (iii) this procedure theoretically leads to a unique and stable solution, and (iv) a powerful optimization procedure, namely, the Global Multilevel Coordinate Search algorithm [Huyer and Neumaier, 1999] in combination with the local Nelder-Mead Simplex algorithm [Lagarias et al., 1998], is used to find the solution accurately and efficiently. To capture the soil parameters in the wetting direction makes the method further attractive compared to most existing methods [Young et al., 2002]. Moreover, the duration of the experiment is significantly shorter under infiltration than under evaporation conditions.

Laboratory infiltration experiments were conducted on four different soil columns, including an artificial homogeneous sand and three undisturbed agricultural soils (a sandy loam and two silt loam soils). Although ASS model uses less restrictive assumptions concerning the pore configuration than MVG model, and although the uncoupled VBC is less restrictive concerning the hydraulic conductivity function, all three models produced similar results. The water retention curves estimated by inverse modeling agreed quite well with those obtained by direct measurements. Results pertaining to the flow simulations showed very good results for the homogeneous sand and the undisturbed sandy loam, but prediction was significantly different compared to the measurements for the two silt loam soils. The observed differences were believed to stem mainly from the different methods and scales of characterization (1.0 × 10^2 cm^3 for direct measurements and about 5.5 × 10^3 cm^3 for the inversion procedure), and to some extent from conceptual limitations in the forward transport model which does not consider hysteresis, air entrapment, preferential flow, and the heterogeneities inherent to agricultural soils. The inversely estimated saturated conductivity was well estimated for the homogeneous sand and the silt loam 2 soil, but was largely overestimated when the explored moisture range was small. Water transfer prediction based on the directly measured
hydraulic properties led in every case to very large errors.

Though encouraging results were obtained, an important limitation of the applicability of the presented method for non sandy agricultural soils was the characterization of the initial conditions in terms of the pressure head profile, especially when high suctions must be imposed. To mitigate to this, we propose investigating in future ways to use water content profiles as initialization in the inverse procedure. In such cases, the inverse modeling approach would then be applicable in conjunction with non destructive soil water content measurement methods like ground penetrating radar. The method would then be full of interest to map the soil hydraulic properties at the field scale.
Chapter 4

GPR design and modeling for identifying the shallow subsurface dielectric properties

Abstract A ground penetrating radar system for identifying the shallow subsurface dielectric properties is proposed. It consists in a stepped frequency continuous wave (SFCW) radar combined with a dielectric filled TEM horn antenna to be used off-ground in monostatic mode and operating in the ultrawide band 0.8-4 GHz. This radar configuration is of practical interest since it responds to subsurface mapping requirements and allows for more efficient and realistic forward modeling of the system. Then, forward modeling of the radar-antenna-subsurface system is developed using linear system response functions and the exact solution of the three-dimensional Maxwell equations for wave propagating in a horizontally multilayered medium representing the shallow subsurface. Finally, the model is validated under simple laboratory conditions. This model is destined to be inverted to estimate the shallow subsurface dielectric properties (see Chapter 5), and is further improved in Chapter 6 to account for more advanced electromagnetic phenomena.

4.1 Introduction

Ground penetrating radar (GPR) has proven to be a promising tool for subsurface characterization in the field of environmental and agricultural engineering since the dielectric properties governing GPR wave propagation are strongly correlated to the water content and the soil salinity [Chanzy et al., 1996; Al Hagrey and Müller, 2000; Huismann et al., 2001]. However, for practical applications, the current state of technology still needs improvements. This is not only true for GPR systems, but for signal analysis methods as well. Actually, no method exists today to provide simultaneously and quantitatively the depth dependent dielectric constant and electric conductivity of the subsurface with GPR. As a result, research has focused here on the design and modeling of a radar system being appropriate for both measurements and advanced signal analysis, i.e., inversion of a three-dimensional electromagnetic model. Also, particular attention is paid to propose a low cost system, and simultaneously, a computationally efficient signal analysis method in order to promote its application.

Forward modeling of GPR electromagnetic wave propagation in conductive dielectric media is necessary for understanding complex electromagnetic phenomena and for defining and solving the inverse problem to identify the subsurface dielectric properties. The theoretical basis for GPR wave propagation is found in Maxwell’s equations. Electromagnetic wave simulation methods with application to GPR include ray theory techniques [Cai and Mechan, 1995], pseudospectral methods [Zeng et al., 1995], integral equation methods [Michalski and Mosig, 1997], and finite difference time domain (FDTD) solutions of Maxwell’s equations [Greenfield and Wu, 1991].

In this chapter, a GPR system specifically designed for the characterization of the shallow subsurface by inverse modeling is presented, and its laboratory implementation and modeling approach is described. A first version of a new antenna model based on linear systems in series and parallel is proposed. It permits to understand the basic electromagnetic wave phenomena occurring within the antenna. This basic antenna model is further improved in Chapter 6 to account for additional electromagnetic phenomena. Then, the theory is developed for the full solution of Maxwell’s equations for waves propagating in horizontally layered media representing the shallow subsurface. Numerous authors have derived Green’s functions for layered media [Arbel and Felsen, 1963; Tai, 1994; Michalski and Mosig, 1997; Peterson et al., 1998]. The Green functions represent the electromagnetic field radiated by a unit strength point source. Following the approaches of Michalski [1998], Slob [2000], van der Kruk [2001], and Slob and Fokkema [2002], we compute the Green function of a three-dimensional medium composed of an arbitrary number of horizontal homogeneous layers with different dielectric properties. The Maxwell system
of equations is first solved in the frequency domain and two-dimensional spatial Fourier domain (spectral domain) for a source and a receiver located above \( N \) horizontal reflectors. This leads to the definition of a global reflection coefficient which enables to compute more efficiently the solution back to the spatial domain. For an infinite homogeneous medium, Green’s functions in the spatial domain can be computed analytically. The situation is much more complex in a layered medium where the Green functions must take into account all the transmissions, reflections and refractions that occur at the different interfaces. It leads to Sommerfeld type integrals that must be evaluated numerically.

The multilayered medium Green’s function is related to the radar signal by means of the antenna equation in the frequency domain. After characterizing the antenna equation, the overall forward model is tested under simple laboratory conditions.

4.2 Ground Penetrating Radar System

4.2.1 Frequency domain radar

GPR systems are divided into two major categories: the time domain systems, also called pulse radars, and the frequency domain systems. The principle of a time domain radar is to send a short pulse with a given pulse repetition frequency into the ground and then pick up the backscattered signal as a function of time. In contrast, frequency radar systems send a frequency modulated wave either with a linear sweep (frequency modulated continuous wave, FMCW), or with a stepped sweep (stepped frequency continuous wave, SF CW), over the frequency range of interest. For a long time, pulse radars dominated in subsurface characterization mainly because of the complexity of frequency domain systems making the technology relatively expensive [Daniels, 1996]. However, during the last few years, electronic components became less expensive resulting in more interests in the frequency domain systems, since they possess several advantages over time domain technology:

1. The major value stems from the potential for controlling an ultrawide band (UWB). A large bandwidth is needed for a better depth resolution and to obtain more information from the subsurface. Commercially available GPR systems generally have a bandwidth limited to less than 1 GHz.

2. For stepped frequency radars, the dispersive properties of the UWB antennae are not too essential because proper calibration techniques can take them into account. This results in more flexibility in the choice of the antenna type and design.
3. The signal-to-noise ratio of frequency domain radars is better than for time domain systems, since the mean radiated power is much higher and each sampled frequency is an independent measurement.

4. Concerning modeling issues, working in the frequency domain allows for an easier and faster solution of Maxwell’s equations in the forward model. Temporal inverse Fourier transforms are not to be evaluated and the antenna modeling does not require the evaluation of convolution integrals, which is valuable when performing inverse modeling.

For all these reasons, we decided to use an SFCW radar for the purpose of developing an integrated tool for the real-time characterization of the shallow subsurface.

### 4.2.2 TEM horn antenna

The antenna constitutes an important part of a radar system because its performance depends strongly on the antenna characteristics. The antenna must satisfy several requirements which depend on its application. But in general, the antenna should transmit electromagnetic waves with small internal ringing and radiate energy in a narrow beam to avoid undesirable reflections from surrounding objects.

Commonly used antennae have a low directivity (e.g., dipoles) and require consequently to be used in contact with the soil. Traveling wave transverse electric and magnetic (TEM) horn antennae have a high directivity, which enables off-ground measurements. The focused beaming of the TEM horn yields further high resolution and results in a better delineation of the subsurface structures. It is therefore particularly appropriate for real-time characterization. A TEM horn antenna consists in a pair of triangular conductors forming a V structure guiding essentially a TEM mode between its antenna plates. Let’s note that the directivity of the antenna increases at high frequencies. The basic TEM horn antenna has large physical dimensions in order to ensure a traveling wave mode. To guarantee a high degree of mobility, the dimensions and weight of the antenna can be limited. To reduce the physical size of the antenna, without reducing the bandwidth too much, the antenna is generally filled with a dielectric. The dielectric may also reduce the sensitivity to external electromagnetic fields.

For all these reasons, we combined a SFCW radar with a dielectric filled TEM horn antenna. To model accurately and in an effective way the radar-antenna-subsurface system, we operate in monostatic mode, i.e., the same antenna plays the role of emitter and receiver. As shown in next sections, this results in important simplifications:
1. Since the antenna can be used off-ground, measurements can be done with the subsurface situated in the far-field of the antenna. As a result, the antenna can simply be modeled by a single source and receiver point. This approximation is not valid for commonly used ground based antenna systems.

2. The received signal in this configuration has mainly propagated in the axial vertical direction. Then, the stochastic horizontal variability of the dielectric properties inherently encountered in environmental systems is expected to play a negligible role. The ground can then be modeled accurately by means of a horizontally multilayered configuration. For this configuration, closed form analytical expressions can be derived for the solution of the system of Maxwell’s equations. Time consuming numerical solutions, such as the Finite Difference Time Domain (FDTD) technique [Taflove, 1995], are not required.

3. The monostatic mode allows for faster Sommerfeld integral evaluation in Maxwell’s equation solution since the oscillating Bessel functions vanish and the integrals converge significantly more rapidly [Michalski, 1998].

4. In this mode, there is no coupling (direct air wave) between the antennae. In a bistatic mode of operation, direct signal is the main source of clutter.

5. The propagation distance of the received signal is smaller, and therefore, a deeper depth can be reached.

6. From a practical point of view, the monostatic mode allows for a higher mobility and helps to reduce the price of the radar system as only one antenna is needed.

An important characteristic of an antenna-radar system is the operating frequency. The operating frequency is a trade-off between range resolution and penetration depth. At frequencies below 1 GHz, attenuation losses in the ground are small [Daniels, 1996] and considerable penetration depth can be achieved. Higher frequencies allow for a higher spatial resolution, but suffer from a lower penetration depth. For instance, Ulriksen [1982] observed a relation between GPR amplitude power reflection coefficients and water content. He showed, under laboratory conditions, that information about the vertical distribution of water content can be obtained by using multiple-frequency radar antennae where the high frequency signals sample the shallowest layers, whereas the lower frequency signals sample the deeper layers. In this study, we operate in the UWB 0.8–4GHz, which should be appropriate to set up laboratory experiments.
Chapter 4. GPR design and modeling

4.3 System Description and Modeling Assumptions

4.3.1 Radar measurements

An UWB SFCW monostatic GPR was implemented using a ZVRE (Rohde & Schwarz) vector network analyzer (VNA) with an excellent dynamic range (> 130 dB). In this Chapter, a dielectric filled TEM horn antenna was used as emitter-receiver (in Chapter 6 we test the performances of a different antenna with no dielectric). The whole radar system is represented at Figure 4.1. The TEM horn antenna was developed by Scheers [2001] for landmine detection purposes, and was therefore specifically designed for the off-ground characterization of the shallow subsurface. The lower cut-off frequency of the antenna is 0.8 GHz. The antenna plates were etched on a printed circuit board and terminated by a 50 Ohm load. The antenna plates were replaced by a set of 41 wires to force the current to be radial. In order to reduce the antenna ringing and the influence of external signals from the upper half space, sidewalls were covered with absorbing material. The relatively small 3 dB beam width of the antenna, 32 degrees in the H-plane and 65 degrees in the E-plane, and the small dimensions (12 cm length and 12 cm × 6 cm aperture area) makes it suitable for using off-ground. Details about the characteristics and properties of this antenna are fully described by Scheers [2001].

The antenna was connected to the reflection port of the VNA via a SMA type 50 Ohm impedance coaxial cable. The VNA was calibrated at the connection between the antenna feed point and the cable using a 50 Ohm OSM (Open, Short, Match) series of a high precision standard calibration kit (ZVZ21-N). Thus establishing a reference plane to which the frequency dependent complex ratio $S_{11}$ between the returned signal and the emitted signal is measured. Parameter $S_{11}$ was measured sequentially at 1601 stepped operating frequencies over the range 0.8 - 4 GHz with a frequency step of 2 MHz and an averaging factor of 10 to improve the signal-to-noise ratio. The UWB SFCW system has a transmit power of $-10$ dBm. Laboratory experiments were carried out at the Royal Military Academy of Bruxelles (Belgium).

4.3.2 The Fraunhofer approximation

Calculation of the total field radiated by a current distribution on an antenna surface is an old problem with an extensive literature [Bouwkamp, 1954]. The space surrounding an antenna is subdivided into three regions: (i) the reactive near-field region, (ii) the radiating near-field region (Fresnel region), and (iii) the far-field region (Fraunhofer region). These regions are so designated to identify the field structure in each. Usually, the Fraunhofer region is the one of most practical interest since approximations to simplify the formulation of the
4.3. System Description and Modeling Assumptions

The Fraunhofer region is defined as Balanis, 1997] "that region of the field of an antenna where the angular field distribution is essentially independent of the distance from the antenna". When considering a current distribution on an antenna surface, the Fresnel zone phenomenon is characterized by the alternate addition and cancellation of fields originating from the source distribution (interferences). In contrast, e.g., as shown by Hansen and Bailin [1959], the effect of these interferences become negligible in the far-field region, and the source distribution can be approximated by an equivalent point source. Also, the axial field intensity is inversely proportional to the distance from the origin of the source to the observation, or reflection, point.

The far-field region extends to infinity and its inner boundary is commonly taken to be the radial distance from the antenna aperture as

\[ R_F = \frac{2D^2}{\lambda} \] (4.1)

where \( D \) is the largest dimension of the radiator, and \( \lambda \) is the wavelength. For an aperture antenna the maximum dimension \( D \) is taken to be its diagonal. The aperture of the TEM horn antenna used in this study is rectangular and has dimension 12 cm \( \times \) 6 cm. Therefore, the largest dimension of the radiator is \( D = 13.4 \) cm, and since the maximum operating frequency is 4 GHz, the smallest radial distance of the far-field region to be considered is found to be \( R_F = 48 \) cm. For a maximum frequency of 2 GHz, \( R_F = 24 \) cm. To make the Fraunhofer approximation of the point source valid, the antenna aperture should be situated at least at \( R_F \) from the soil surface. Let’s note that (4.1) gives only a theoretical and approximate indication and must be verified by experiments.
4.3.3 Antenna equation in the frequency domain

A common way of describing antennae in the frequency domain is by means of their frequency response. The antenna and the multilayered medium being time-invariant linear systems, and assuming the antenna to be a point source and receiver, we propose to model them using the block diagram illustrated in Figure 4.2 (this model is enhanced in Chapter 6 to account for phenomena which are more important and brought to the fore with another tested antenna). Accordingly, $S_{11}(\omega)$ measured by the vector network analyzer can be related to the frequency response on the multilayered medium $G_{xx}^\uparrow(\omega)$ in the frequency domain as

$$S_{11}(\omega) = \frac{Y(\omega)}{X(\omega)} = H_i(\omega) + H_t(\omega)G_{xx}^\uparrow(\omega)H_r(\omega)$$ (4.2)

where $H_i(\omega)$, $H_t(\omega)$, and $H_r(\omega)$ are, respectively, the return loss, transmitting, and receiving complex frequency response functions of the antenna that have to be determined, with $\omega$ being the angular frequency ($s^{-1}$). The return loss is actually the internal antenna reflections at the measurement level, which are independent of the picked up signal. The transmitting and receiving transfer functions describe the antenna gain and time delay. This relationship is referred to as the antenna equation in the frequency domain. In the time domain, the scalar products in (4.2) correspond to time convolution integrals. Defining $H(\omega) = H_t(\omega)H_r(\omega)$, (4.2) can be written as

$$S_{11}(\omega) = H_i(\omega) + H(\omega)G_{xx}^\uparrow(\omega)$$ (4.3)

Due to the variations of impedance between the antenna feed point and the antenna aperture, multiple wave reflections occur within the antenna. The part of the ringing that is independent of the backscattered electromagnetic field $G_{xx}^\uparrow(\omega)$ creates a background, the return loss $H_i(\omega)$, which masks the response of the ground or target. In order to remove this constant background, we subtract it from the measured signal $S_{11}(\omega)$ as

$$S_{11}^{(s)}(\omega) = S_{11}(\omega) - H_i(\omega) = H(\omega)G_{xx}^\uparrow(\omega)$$ (4.4)

where $H_i(\omega)$ can be measured by performing $S_{11}(\omega)$ measurements in free space for which $G_{xx}^\uparrow(\omega) = 0$ (the incident field is not measured). Figure 4.3 illustrates the effect of this transformation for measurements performed at different heights above a metal sheet ($1.20 \text{ m} \times 0.90 \text{ m}$) with the antenna aperture elevation ranging from $0.21 \text{ m}$ till $0.46 \text{ m}$. For convenience, measured frequency domain data are presented here in the time domain using the inverse fast Fourier transform

$$s_{11}^{(s)}(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp(j\omega t) S_{11}^{(s)}(\omega) d\omega$$ (4.5)
4.3. System Description and Modeling Assumptions

Figure 4.2. Block diagram representing the VNA-antenna-multilayered medium system modeled as linear systems in series and parallel.

Figure 4.3. Radar measurements transformed in the time domain with the antenna being at different heights $h$ above a metal sheet. Variable $s_{11}$ represents in the time domain the filtered signal using equation (4.4).
Chapter 4. GPR design and modeling

The wave reflection arising from the metal sheet appears more clearly when $S_{11}(\omega)$ is filtered using equation (4.4). Most of the multiple reflections in the antenna vanish. The signal which is observed at the time interval between 0 and 0.5 ns is the reflection from the feed point. Reflection from the aperture takes place at the time interval between 1 and 1.5 ns. The slight ripples on the signal are caused by the inverse Fourier transform since only the frequency signal between 0.8 and 4 GHz is measured.

4.3.4 Virtual source point of the TEM horn

For determining the frequency response $H(\omega)$ of the antenna, we need a model to compute $G_{xx}(\omega)$, but we first have to locate its virtual source point. In the far-field region of the antenna, the virtual source point represents the origin of the radiated field from which the $1/R$ spherical divergence is initiated, $R$ being the path distance from the observation point to the source point. For a monostatic antenna configuration, the localization of the virtual source point can be done experimentally by performing measurements at different heights above a perfect electric conductor (PEC), e.g., a metal sheet.

Let $h$ be the distance between the antenna aperture and the PEC. Then, for different values of $h$ in the far-field, the measured backscattered signal decreases inverse linearly with

$$\frac{1}{R} = \frac{1}{2(h + d)}$$

(4.6)

where $d$ is unknown and defined as the distance between the virtual source point and the antenna aperture.

To quantify the magnitude of the backscattered field from the metal sheet, we use the peak-to-peak value ($PtP$) as defined by Foster [1995] and used by Scheers [2001] for similar purposes. The peak-to-peak value is the difference between the maximum and minimum magnitude of the measured signal expressed in the time domain, as illustrated in Figure 4.4.

At the source point, $PtP$ tends to infinity and then, the inverse of $PtP$ tends to zero. The source point can therefore be determined by linear extrapolation of the measured $1/PtP$ values as a function of $2h$, as illustrated in Figure 4.4. We performed measurements at six different heights of the antenna above the metal sheet and found the root of the fitted linear curve at $2h = -8.6$ cm. So, the virtual source point is located at a distance $|d| = 4.3$ cm from the antenna aperture towards the antenna feed point. This result is in accordance with the findings of Scheers [2001] who characterized the same antenna in bistatic mode on boresight in free space conditions ($|d| = 4.0$ cm). Let’s note finally that the observed linear dependence between $1/PtP$ and $2h$ in Figure 4.4 agrees very well with the determined far-field region (see Section 4.3.2).
4.4 Formulation of Electromagnetic Field Equations

4.4.1 Dielectric properties of materials

The electric conductivity describes currents from free charge flow in response to an imposed electric field $E$ (Vm$^{-1}$). For relatively low frequency alternating electric fields, the response time of charges is negligible and current varies in phase with $E$. With increasing frequency the response time rises and results in an out of phase current. Therefore, the electric conductivity $\sigma$ can be represented by the complex quantity

$$ \sigma = \sigma' + j\sigma'' $$

and the related volume density of electric current, $J_c$ (Am$^{-2}$), is expressed by the differential form of Ohm’s law as

$$ J_c = \sigma E $$

The dielectric permittivity describes currents resulting from bound charge displacement and characterizes material polarizability. With increasing frequency the bound charges become too slow to follow the fast alternating electric field and a relaxation phenomenon appears resulting in a out of phase polarization component. Hence the dielectric permittivity $\varepsilon$ is also described by a complex quantity

$$ \varepsilon = \varepsilon' - j\varepsilon'' $$

and the electric displacement flux density, $J_d$, expressed in the frequency domain, is equal to

$$ J_d = \varepsilon j\omega E $$

The total current density $J$ is therefore equal to

$$ J = J_c + J_d = \left((\varepsilon' + \frac{\sigma''}{\omega}) - j(\varepsilon'' + \frac{\sigma'}{\omega})\right) j\omega E $$
Equation (4.11) shows that both $\sigma'$ and $\varepsilon''$ produce a current that varies in phase with the electric field, whereas $\sigma''$ and $\varepsilon'$ produce a current out of phase with the electric field. In other words, the imaginary part of the dielectric permittivity acts as a conductivity and the imaginary part of the conductivity acts as a permittivity. Therefore, it is of practical value to introduce the notion of effective dielectric permittivity ($\varepsilon_e$) since only the in phase and the out of phase component of the total current can be measured experimentally. This reduces equation (4.11) to

$$J = \varepsilon_e j \omega E$$  \hspace{1cm} (4.12)

with

$$\varepsilon_e = (\varepsilon' + \frac{\sigma''}{\omega}) - j(\varepsilon'' + \frac{\sigma'}{\omega})$$  \hspace{1cm} (4.13)

The effective dielectric permittivity $\varepsilon_e$ accounts for the material conductive properties through its imaginary component. $\sigma'$ represents conduction losses due to migration of unbounded charges (direct current conductivity), and $\varepsilon''$ represents relaxation losses during the polarization/depolarization process. In Maxwell’s equations, the macroscopic parameters $\varepsilon$ and $\sigma$ always occur in the combination $\sigma + j \omega \varepsilon$. Splitting up the two parameters in their real and imaginary components, this combination can be rewritten as

$$\sigma + j \omega \varepsilon = (\sigma' + \omega \varepsilon'') + j(\sigma'' + \omega \varepsilon') = j \omega \varepsilon_e$$  \hspace{1cm} (4.14)

### 4.4.2 Frequency dependence

It is well known that in the operating frequency range of GPR, soil materials can exhibit significant dispersive properties, i.e., the complex effective dielectric permittivity of the soil is function of frequency [Hipp, 1974; Hallikainen et al., 1985; Heimovaara et al., 1996; Teixeira et al., 1998]. At these frequencies, dispersion arises mainly from relaxation mechanisms due to the presence of water bound to mineral surfaces (bound water and double layer polarization effects), and interactions between ions and solid (Maxwell-Wagner effect) [Hilhorst, 1998; West et al., 2003]. For instance, the high dielectric losses in clayey soils have been attributed mainly to relaxation due to bound water effects [Sarrenketo, 1998].

To have a realistic model of propagation of electromagnetic waves in the lossy subsurface, it is therefore necessary to account for these effects. Among many other models, for instance, the frequency dependence is usually described with the empirical extended Debye relaxation equation [Debye, 1929], which involves a single relaxation phenomenon:

$$\varepsilon_e(f) = \varepsilon_{e,\infty} + \frac{\varepsilon_{e,0} - \varepsilon_{e,\infty}}{1 + j \frac{f}{f_c}}$$  \hspace{1cm} (4.15)
where \( f \) is the frequency, \( f_r \) is the relaxation frequency of the material, \( \varepsilon_{e,0} \) is the static permittivity, and \( \varepsilon_{e,\infty} \) is the permittivity at infinite frequency. Let’s note that in reality, the complex permittivity of most subsurface materials contains more than one relaxation mechanism due to the presence of water, granular mixtures, etc. A volumetric mixing model that sums two or more dielectric spectra with different Debye parameters may describe dielectric dispersion of soils more realistically than Debye equation [e.g., see Dobson et al., 1985; Heimovaara et al., 1994].

Over the frequency range of GPR, the real part of the effective dielectric permittivity does not appear to be strongly frequency dependent and may be neglected [Davis and Annan, 1977; Zhou et al., 2001]. For instance, [Weerts et al., 2001; Huisman et al., 2002] observed that for TDR, taking into account the frequency dependence of the dielectric permittivity did not greatly improve the fit between measured and modeled waveforms and that a frequency independent apparent permittivity adequately describes the TDR measurements made in a sandy soil. As a first approximation, we consider also in this study frequency independent apparent parameters. The effect of the frequency dependence is investigated in Chapter 6 to improve the subsurface model.

### 4.4.3 Model configuration

We specifically consider a planar stratified conductive system consisting of \( N \) horizontal layers separated by \( N - 1 \) planar interfaces parallel to the \( x, y \)-plane of a right-handed Cartesian coordinate system, as illustrated in Figure 4.5. Throughout this chapter, vectors and matrices are denoted by boldface letters. The three orthogonal base vectors \( \hat{x}, \hat{y}, \) and \( \hat{z} \) form the origin \( S \) of the coordinate system, where the \( z \)-axis is taken positive downward.

The electric parameters pertaining to the \( n \)th layer, which is bounded by interfaces \( z_{n-1} \) and \( z_n \), are distinguished by subscript \( n \) \((n = 1, 2, \ldots, N)\). The medium of the \( n \)th layer is homogeneous and characterized by the magnetic permeability \( \mu_n \) (H m\(^{-1}\)), the electric permittivity \( \varepsilon_n \) (F m\(^{-1}\)), and the electric conductivity \( \sigma_n \) (S m\(^{-1}\)). The layered medium is excited by electric and magnetic point sources located at \( S = (0,0,0) \). The derivation is carried out in steps, first the basic equations are transformed to the horizontal wave number domain. Then in this domain the electromagnetic field is decomposed into the two fundamental modes, after which a solution is found for sources in a homogeneous domain. Then these solutions are used to construct the solution for a stack of piecewise homogeneous horizontal layers.
Chapter 4. GPR design and modeling

4.4.4 Frequency domain Maxwell’s equations

The propagation of electromagnetic fields is governed by Maxwell’s equations. For homogeneous isotropic lossy materials, the vector Maxwell equations expressed here in their differential form in the frequency domain are

\[-\nabla \times \mathbf{H} + (\sigma + j\omega\varepsilon)\mathbf{E} = -\mathbf{J}^e \tag{4.16}\]
\[\nabla \times \mathbf{E} + j\omega\mu\mathbf{H} = -\mathbf{K} \tag{4.17}\]

where \(\mathbf{H} = \mathbf{H}(x, y, z, \omega)\) is the magnetic field spectral density (A m\(^{-1}\) Hz\(^{-1}\)), \(\mathbf{E} = \mathbf{E}(x, y, z, \omega)\) is the electric field spectral density (V m\(^{-1}\) Hz\(^{-1}\)), \(\mathbf{J}^e = \mathbf{J}^e(x, y, z, \omega)\) is the spectral density of the material electric current volume source density (A m\(^{-2}\) Hz\(^{-1}\)), \(\mathbf{K} = \mathbf{K}(x, y, z, \omega)\) is the spectral density of the material magnetic current volume source density (V m\(^{-2}\) Hz\(^{-1}\)), and \(\omega\) is the angular frequency (Hz). Throughout this chapter we assume time harmonic fields with an \(\exp(j\omega t)\) dependence.

Since we assume electric and magnetic point sources located at the origin of the Cartesian coordinate system, their mathematical representation in the frequency domain is given by

\[\langle \mathbf{J}^e, \mathbf{K} \rangle (x, y, z, \omega) = \langle \mathbf{J}^e, \mathbf{K} \rangle (\omega)\delta(x, y, z) \tag{4.18}\]

where \(\mathbf{J}^e(\omega)\) and \(\mathbf{K}(\omega)\) denote, respectively, electric and magnetic specific currents, and the three-dimensional spatial Dirac delta function \(\delta(x, y, z)\) represents the volume density function defining the position of the sources.
In Cartesian coordinates, the system (4.16)-(4.17) of the electromagnetic field Maxwell equations is given by

\begin{align}
-(\partial_y H_z - \partial_z H_y) + (\sigma + j\omega \varepsilon) E_x &= -J_x^e \\
-(\partial_z H_x - \partial_x H_z) + (\sigma + j\omega \varepsilon) E_y &= -J_y^e \\
-(\partial_x H_y - \partial_y H_x) + (\sigma + j\omega \varepsilon) E_z &= -J_z^e \\
\partial_y E_z - \partial_z E_y + j\omega \mu H_x &= -K_x \\
\partial_z E_x - \partial_x E_z + j\omega \mu H_y &= -K_y \\
\partial_x E_y - \partial_y E_x + j\omega \mu H_z &= -K_z
\end{align}

where the short-hand notation, \( \partial_x = \frac{\partial}{\partial x} \), is employed for partial derivatives.

From Maxwell’s equations, the following boundary conditions are found

\begin{align}
\mathbf{n} \times \mathbf{E} & \quad \text{continuous} \quad (4.21a) \\
\mathbf{n} \times \mathbf{H} & \quad \text{continuous} \quad (4.21b) \\
\mathbf{n} \cdot [ (\sigma + j\omega \varepsilon) \mathbf{E} ] & \quad \text{continuous} \quad (4.21c) \\
\mathbf{n} \cdot (\mu \mathbf{H}) & \quad \text{continuous} \quad (4.21d)
\end{align}

These conditions allow the continuous exchange of electromagnetic energy across an interface with unit normal \( \mathbf{n} \).

### 4.4.5 Spectral domain Maxwell’s equations

In a horizontally layered medium, the interfaces are parallel to the \( x, y \)-plane, which implies that the dielectric properties are independent of the directions of \( \hat{x} \) and \( \hat{y} \). To take advantage of this configuration and facilitate the solution derivation, the two-dimensional Fourier transformation of all fields with respect to the transverse coordinates \( x \) and \( y \) is applied [Peterson et al., 1998; van der Kruk, 2001]. The horizontal Fourier transformation acting on a scalar function \( f(x, y) \) in terms of the transformation parameters \( k_x \) and \( k_y \) is defined as

\[
\tilde{f}(k_T) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \exp(jk_T \cdot \mathbf{x}_T) f(\mathbf{x}_T) \, dx \, dy \quad (4.22)
\]

where the tangential vectors, \( k_T = \{k_x, k_y\} \) and \( \mathbf{x}_T = \{x, y\}^T \) are introduced.

With the introduction of the horizontal vector partial derivative, \( \partial_T = \{\partial_x, \partial_y\} \), and applying the rule that \( \partial_T \rightarrow -j k_T \), the application of the transformation leads to the following Maxwell equations in the transform domain

\begin{align}
jk_y \hat{H}_z + \partial_z \hat{H}_y + (\sigma + j\omega \varepsilon) \hat{E}_x &= -\hat{J}_x^e \\
-\partial_z \hat{H}_x - jk_x \hat{H}_z + (\sigma + j\omega \varepsilon) \hat{E}_y &= -\hat{J}_y^e \\
jk_x \hat{H}_y - jk_y \hat{H}_x + (\sigma + j\omega \varepsilon) \hat{E}_z &= -\hat{J}_z^e
\end{align}
\[ -jk_y \tilde{E}_z - \partial_z \tilde{E}_y + j\omega \mu \tilde{H}_x = -\tilde{K}_x \] (4.24a)
\[ \partial_z \tilde{E}_x + jk_x \tilde{E}_z + j\omega \mu \tilde{H}_y = -\tilde{K}_y \] (4.24b)
\[ -jk_x \tilde{E}_y + jk_y \tilde{E}_x + j\omega \mu \tilde{H}_z = -\tilde{K}_z \] (4.24c)

with sources
\[ (\tilde{J}^e, \tilde{K}) (k_x, k_y, z, \omega) = (J^e, K) (\omega) \delta(z) \] (4.25)

The transformation from the spectral domain back to the spatial domain is carried out by employing the two-dimensional Fourier inverse transformation defined as
\[ f(\mathbf{x}_T) = \left( \frac{1}{2\pi} \right)^2 \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \exp(-j\mathbf{k}_T \cdot \mathbf{x}_T) \tilde{f}(\mathbf{k}_T) \, dk_x \, dk_y \] (4.26)

### 4.5 Solution for Ground Penetrating Radar

#### 4.5.1 Fields in a homogeneous medium

Assuming no magnetic sources \((K = 0)\), first equations (4.23a)-(4.24c) can be written in vector forms
\[ -\partial_z \mathbf{\hat{z}} \times \tilde{\mathbf{H}} + jk_T \times \tilde{\mathbf{H}} + \eta \tilde{\mathbf{E}} = -\tilde{\mathbf{J}}^e \] (4.27a)
\[ \partial_z \mathbf{\hat{z}} \times \tilde{\mathbf{E}} - jk_T \times \tilde{\mathbf{E}} + \zeta \tilde{\mathbf{H}} = 0 \] (4.27b)

which can be separated as
\[ \eta \tilde{E}_z = -\tilde{J}_z^e - jk_T \times \tilde{\mathbf{H}} \] (4.28a)
\[ \zeta \tilde{H}_x = jk_T \times \tilde{\mathbf{E}} \] (4.28b)
\[ \eta \tilde{E}_T = -\tilde{J}_T^e + \partial_z \mathbf{\hat{z}} \times \tilde{\mathbf{H}} - jk_T \times \hat{\mathbf{z}} \tilde{H}_z \] (4.28c)
\[ \zeta \tilde{H}_T = -\partial_z \mathbf{\hat{z}} \times \tilde{\mathbf{E}}_T + jk_T \times \hat{\mathbf{z}} \tilde{E}_z \] (4.28d)

with the quantities \(\eta\) and \(\zeta\) defined as
\[ \eta = \sigma + j\omega \varepsilon \] (4.29)
\[ \zeta = j\omega \mu \] (4.30)

The total electromagnetic field is a vector field. From the structure of the Maxwell equations it is apparent that an electromagnetic field in a homogeneous (sub)-region can be decomposed into in transverse electric (TE) and transverse magnetic (TM) modes of excitation. The TE mode is a configuration of the electromagnetic field in which the electric field is purely transverse to some axis of reference, while the TM mode corresponds to a configuration in
which the magnetic field is purely transverse to that axis. In our configuration of a horizontally stratified earth, the natural choice is to take the $z$-axis as axis of reference. Hence, the vertical electric field corresponds to the TM mode, while the vertical magnetic field corresponds to the TE mode. When the TE and TM modes are known the whole electromagnetic field is known. Now, we want expressions for the vertical component of the electric and magnetic fields since they can be solved for independently in the layered configuration and the horizontal components of the electric and magnetic fields follow from these two. Elimination of the horizontal components of the electric and magnetic field strengths gives the wave equations for the vertical components,

\begin{align}
(\partial_z^2 - \Gamma^2)\tilde{E}_z &= \zeta \tilde{E}_z + \eta^{-1} \partial_z (jk_T \cdot \tilde{J}_T - \partial_z \tilde{J}_T^z) \quad (4.31a) \\
(\partial_z^2 - \Gamma^2)\tilde{H}_z &= jk_T \times \tilde{J}_T^z \quad (4.31b)
\end{align}

with $\Gamma = (k_T \cdot k_T + \gamma^2)^{1/2}$ and $\Re\{\Gamma\} \geq 0$. In view of (4.25), the corresponding Green’s function is the solution of the modified Helmholtz equation

\begin{equation}
(\partial_z^2 - \Gamma^2)\tilde{G} = -\delta(z) \quad (4.32)
\end{equation}

whose well known solution is

\begin{equation}
\tilde{G}(z) = \frac{\exp(-\Gamma |z|)}{2\Gamma} \quad (4.33)
\end{equation}

In view of equations (4.31a), (4.31b), (4.25) and (4.33), the vertical components of the electric and magnetic fields are given by

\begin{align}
\tilde{E}_z &= (-\zeta \tilde{J}_T^z - \eta^{-1} \partial_z [jk_T \cdot \tilde{J}_T^z - \partial_z \tilde{J}_T^z])\tilde{G}(z) \quad (4.34a) \\
\tilde{H}_z &= -jk_T \times \tilde{J}_T^z \tilde{G}(z) \quad (4.34b)
\end{align}

Collecting the results and carrying out the necessary differentiations with respect to $z$ we can express the vertical components of the electric and magnetic fields in terms of the tensor Green’s functions as

\begin{align}
\tilde{E}_z &= \tilde{G}_{z,T}^{EJ} \cdot \tilde{J}^e \quad (4.35a) \\
\tilde{H}_z &= \tilde{G}_{z,T}^{HJ} \cdot \tilde{J}^e \quad (4.35b)
\end{align}

where the corresponding tensor components of the Green’s functions are found to be

\begin{align}
\tilde{G}_{z,T}^{EJ} &= -\eta^{-1} jk_T \partial_z \tilde{G} = \frac{jk_T}{\eta} \Gamma \text{sign}(z) \tilde{G} \quad (4.36a) \\
\tilde{G}_{z,T}^{EJ} &= (\zeta + \eta^{-1} \partial_z \partial_z)\tilde{G} = \eta^{-1} k_T^2 \tilde{G} - \eta^{-1} \delta(z) \quad (4.36b) \\
\tilde{G}_{z,T}^{HJ} &= -jk_T \times_T \tilde{G} \quad (4.36c)
\end{align}
where \( k_ρ = (k_x^2 + k_y^2)^{1/2} \). The sign function is defined as

\[
\text{sign}(z) = \begin{cases} 
-1 & \text{for } z < 0 \\
0 & \text{for } z = 0 \\
1 & \text{for } z > 0 
\end{cases}
\]  

(4.37)

Observe that a vertical electric dipole only excites TM modes, while horizontal electric dipoles excite both TM and TE modes. The horizontal components of the electric field are found from the vertical electric and magnetic fields and the source term as

\[
\tilde{E}_T = \frac{jk_T}{\eta k_ρ^2} [j k_T \cdot \tilde{J}_T - \partial_z (\eta \tilde{E}_z + \tilde{J}_z^e)] + \frac{\zeta}{k_ρ^2} j k_T \times \tilde{H}_z
\]  

(4.38)

It is observed that the horizontal components of the electric field consist, in principle, of both TE and TM modes. We keep the separation of TE and TM modes in the representations of the horizontal components of the electric field. Substitution of the results of equations (4.34a) and (4.34b) in (4.38) and carrying out the necessary differentiations, yields the required expressions. Here we summarize only the final result for the total electric field vector,

\[
\tilde{E} = \tilde{G}^{TMEJ} \cdot \tilde{J}^e + \tilde{G}^{TEEJ} \cdot \tilde{J}^e
\]  

(4.39)

with the electric field related TM and TE mode Green’s tensors given by

\[
\tilde{G}^{TMEJ} = \begin{pmatrix}
\frac{j k_x j k_y}{2 k_ρ^2} & \frac{j k_x j k_y}{2 k_ρ^2} & \frac{j k_x \text{sign}(z)}{2 \eta} \\
\frac{j k_x j k_y}{2 k_ρ^2} & \frac{j k_x j k_y}{2 k_ρ^2} & \frac{j k_x \text{sign}(z)}{2 \eta} \\
-\frac{k_ρ^2}{2 \eta} & -\frac{k_ρ^2}{2 \eta} & \frac{k_ρ^2}{2 \eta} - \eta^{-1} \delta(z)
\end{pmatrix} \exp(-\Gamma |z|)
\]

(4.40a)

\[
\tilde{G}^{TEEJ} = \frac{\zeta}{2 k_ρ^2} \begin{pmatrix}
\frac{j k_y j k_y}{\eta} & -\frac{j k_x j k_y}{\eta} & 0 \\
-j k_x j k_y & j k_x j k_x & 0 \\
0 & 0 & 0
\end{pmatrix} \exp(-\Gamma |z|)
\]

(4.40b)

Combining all solutions, the total electric and magnetic field strengths in the upper half-space are obtained as

\[
\begin{bmatrix}
\tilde{E}_x \\
\tilde{E}_y \\
\tilde{E}_z \\
\tilde{H}_x \\
\tilde{H}_y \\
\tilde{H}_z
\end{bmatrix} = \tilde{G}^T \begin{bmatrix}
\tilde{J}_x^e \\
\tilde{J}_y^e \\
\tilde{J}_z^e
\end{bmatrix}
\]

(4.41)
where $\tilde{G}^\uparrow$ is defined as the upward (negative $z$-direction) Green’s function

$$\tilde{G}^\uparrow = \frac{e^{\Gamma z}}{2\Gamma}$$ \hspace{1cm} (4.42)

In a similar way for the lower half space where $z$ is positive, we have

$$\tilde{G}^\downarrow = \frac{e^{-\Gamma z}}{2\Gamma}$$ \hspace{1cm} (4.44)

### 4.5.2 Source above a layered stack

Here the total electric and magnetic field strengths in the upper half-space of the multilayered medium (see Figure 4.5) are derived. For the GPR antenna configuration considered in this study, i.e., monostatic TEM horn antenna, it is assumed that only the $x$-directed electric source term $J_{ex}$ is different from zero. Then from equation (4.31a) considered in the upper half space in between the source level and the first interface, a source free layer $n$, and the lower half space, the general solution for the vertical electric field is written as

\[
\tilde{E}_z^{\uparrow} = \tilde{G}_x \begin{bmatrix} J_{ex} \\ J_{ey} \end{bmatrix}
\]

where $\tilde{G}_x$ is defined as

$$\tilde{G}_x = \frac{e^{-\Gamma z}}{2\Gamma}$$ \hspace{1cm} (4.43)

\[
\tilde{E}_z^{\uparrow} = \tilde{G}_x = \frac{e^{-\Gamma z}}{2\Gamma}
\]

\[
\tilde{E}_z^{\downarrow} = \tilde{G}_x = \frac{e^{-\Gamma z}}{2\Gamma}
\]

\[
\tilde{E}_z^{\uparrow} = \tilde{G}_x = \frac{e^{-\Gamma z}}{2\Gamma}
\]

\[
\tilde{E}_z^{\downarrow} = \tilde{G}_x = \frac{e^{-\Gamma z}}{2\Gamma}
\]

where $\tilde{G}^\uparrow$ is defined as

### 4.5. Solution for Ground Penetrating Radar

\[
\tilde{E}_z^{\uparrow} = \frac{jk_x}{2\eta_1} J_{ex} \left[ \exp(-\Gamma_1 z) + R_1^{TM} \exp(\Gamma_1(z - 2z_1)) \right] \hspace{1cm} 0 < z < z_1
\]

\[
\tilde{E}_z^{\downarrow} = A_n^{TM} \exp(-\Gamma_n z) + B_n^{TM} \exp(\Gamma_n z) \hspace{1cm} z_{n-1} < z < z_n
\]

\[
\tilde{E}_z^{\uparrow} = A_N^{TM} \exp(-\Gamma_N z) \hspace{1cm} z > z_{N-1}
\]

where the factor $R_1$ is the total reflected field from the upper interface containing all the reflection and transmission contributions from the layered half space that is radiated into the upper half space. All interfaces are source free so we can use the conditions of equations (4.21a) and (4.21c). In the horizontal wavenumber domain, these conditions are for the vertical electric field
where the first condition comes from the continuity of the normal component of the total electric current (displacement and conduction currents), while the second condition follows directly from the continuity condition for the horizontal components of the electric field as can be seen from the expression of equation (4.38). In our configuration, the second condition is simplified to

\[
\lim_{z \downarrow z_n} \eta \partial_z \tilde{E}_{zn} = \lim_{z \uparrow z_n} \eta \partial_z \tilde{E}_{zn+1}
\]  

First we connect the fields at the interfaces \( z_n, n = 2, \cdots, N - 1 \), by imposing the above two conditions,

\[
\eta_n [A_n^T M \exp(-\Gamma_n z_n) + B_n^T M \exp(\Gamma_n z_n)] = \eta_{n+1} [A_{n+1}^T M \exp(-\Gamma_{n+1} z_n) + B_{n+1}^T M \exp(\Gamma_{n+1} z_n)]
\]  

\[
\Gamma_n [A_n^T M \exp(-\Gamma_n z_n) - B_n^T M \exp(\Gamma_n z_n)] = \Gamma_{n+1} [A_{n+1}^T M \exp(-\Gamma_{n+1} z_n) - B_{n+1}^T M \exp(\Gamma_{n+1} z_n)]
\]

Introducing the global reflection coefficient, \( R_{TM}^n \), at interface \( n \) and the layer thickness, \( h_{n+1} \), of layer \( n + 1 \) as

\[
R_{TM}^n = \frac{B_{TM}^n}{A_{TM}^n} \exp(2\Gamma_n z_n) \quad h_{n+1} = z_{n+1} - z_n
\]

we can express the global reflection coefficient \( R_{TM}^n \) in terms of \( R_{TM}^{n+1} \) as

\[
R_{TM}^n = \frac{r_{TM}^n + R_{TM}^{n+1} \exp(-2\Gamma_{n+1} h_{n+1})}{1 + r_{TM}^n R_{TM}^{n+1} \exp(-2\Gamma_{n+1} h_{n+1})}
\]

\[
r_{TM}^n = \frac{\eta_n \Gamma_n - \eta_{n+1} \Gamma_{n+1}}{\eta_{n+1} \Gamma_n + \eta_n \Gamma_{n+1}}
\]

where \( r_{TM}^n \) is the TM mode local reflection coefficient of the \( n \)th interface. This is an upward recursion formula for the global reflection of an \( N \)-layered half-space. In the lower half-space there are only down going waves, hence the global reflection coefficient at the lowest interface equals the local reflection coefficient at \( z = z_{N-1} : R_{TM}^{N-1} = r_{TM}^{N-1} \). This is equivalent to recognizing that in the absence of up-going waves in the lower half-space we have
4.5. Solution for Ground Penetrating Radar

\( B^T_M = 0 \) and consequently \( R^T_M = 0 \), which initializes the recursion scheme and directly sets \( R^T_{N-1} = r^T_{N-1} \). Now we have the field at the interface \( z_2 \), by upward recursion from \( z = z_{N-1} \), in terms of the global reflection coefficient \( R_2 \) and the unknown down-going wavefield amplitude \( A^T_2 \) and we need to connect the fields at the upper interface to solve for \( A^T_2 \) and \( R^T_1 \). Application of the interface conditions here leads to

\[
\eta_1 \frac{jk_x}{2\eta_1} J_x^e \exp(-\Gamma_1 h_1)(1 + R^T_1) = \eta_2 A^T_2 [1 + R^T_2 \exp(-2\Gamma_2 h_2)]
\]

(4.53a)

\[
\Gamma_1 \frac{jk_x}{2\eta_1} J_x^e \exp(-\Gamma_1 h_1)(1 - R^T_1) = \Gamma_2 A^T_2 [1 - R^T_2 \exp(-2\Gamma_2 h_2)]
\]

(4.53b)

Solving for \( R^T_1 \) yields

\[
R^T_1 = \frac{r^T_1 + R^T_2 \exp(-2\Gamma_2 h_2)}{1 + r^T_1 R^T_2 \exp(-2\Gamma_2 h_2)},
\]

(4.54)

which is expression for the global reflection coefficient as given in equation (4.52) with \( n = 1 \). Now the total vertical component of the electric field is, in between the source level and the upper interface, obtained as

\[
E_{z;1} = \frac{jk_x}{2\eta_1} J_x^e \left[ \exp (-\Gamma_1 z) + R^T_1 \exp (\Gamma_1 (z - 2z_1)) \right] \quad 0 < z < z_1
\]

(4.55)

A similar procedure for the vertical component of the magnetic field leads to

\[
H_{z;1} = \frac{jk_y}{2\Gamma_1} \left[ \exp (-\Gamma_1 z) + R^{TE}_1 \exp (\Gamma_1 (z - 2z_1)) \right] \quad 0 < z < z_1
\]

(4.56)

where the global and local TE-mode reflection coefficients at the first interface is given by

\[
R^{TE}_1 = \frac{r^{TE}_1 + R^{TE}_2 \exp(-2\Gamma_2 h_2)}{1 + r^{TE}_1 R^{TE}_2 \exp(-2\Gamma_2 h_2)},
\]

(4.57)

\[
r^{TE}_1 = \frac{\mu_2 \Gamma_1 - \mu_1 \Gamma_2}{\mu_2 \Gamma_1 + \mu_1 \Gamma_2}
\]

(4.58)

4.5.3 Response of the multilayered medium

Given the monostatic TEM horn antenna configuration and the Fraunhofer approximation, we assume the emitter and receiver to be point devices and located both at \( z = 0 \). The source reduces to the \( J_x^e \) component, and only the
Chapter 4. GPR design and modeling

$x$-directed electric field is assumed to be measured. The $x$-component of the electric field at $z = 0$ is computed by substituting (4.55) and (4.56) in (4.38) as

$$
\tilde{E}_{x,z=0} = \left( \frac{k_x^2}{\eta_1 k_p^2} - \frac{k_y^2 \zeta_1}{2 \Gamma_1 k_p^2} \right) J_x^e - \left( \frac{\Gamma_1 k_x^2 R_{TM}^2 - \zeta_1 k_x^2 R_{TE}^2}{2 \eta_1 k_p^2} \right) \exp \left( -2 \Gamma_1 z_1 \right) J_x^e
$$

As shown in Section 4.3.3, the radar-antenna-multilayered medium system is modeled as linear systems in series and parallel (see Figure 4.2). Parameter $S_{11}$ is measured and is related to the response of the multilayered medium by (4.3). Therefore, the incident field is not measured, only the backscattered field is measured for a unit strength source ($J_x^e = 1$). Accordingly, we define the response of the multilayered medium considering only the upgoing polarization modes as

$$
\hat{G}_{xx} = \left[ k_x^2 \left( \frac{\Gamma_1 R_{TM}^2}{2 \eta_1 k_p^2} + \frac{\zeta_1 R_{TE}^2}{2 \Gamma_1 k_p^2} \right) \exp \left( -2 \Gamma_1 z_1 \right) \right]
$$

### 4.6 Inverse Spatial Fourier Transformation

#### 4.6.1 Transition to polar coordinates

Since the configuration is invariant along the $\hat{x}$ and $\hat{y}$ directions, the transition to polar coordinates reduces the number of inverse Fourier integrals. In order to bring to the fore the computational benefit of the monostatic mode compared to a bistatic mode of operation, we derive hereafter the spatial Green function for the general case where the source and receiver points are not especially the same in the $x, y$-plane. Polar coordinates $(\rho, \theta)$ are introduced according to

$$
x = \rho \cos(\theta) \quad (4.61)
y = \rho \sin(\theta) \quad (4.62)
$$

where $\rho$ and $\theta$ are therefore equal to

$$
\rho = \sqrt{x^2 + y^2} \quad \theta = \arctan \left( \frac{y}{x} \right) \quad (4.63)
$$

In a similar way, $(k_\rho, k_\theta)$ are introduced according to

$$
k_x = k_\rho \cos(k_\theta) \quad (4.64)
k_y = k_\rho \sin(k_\theta) \quad (4.65)$$
4.6. Inverse Spatial Fourier Transformation

so that

\[ \text{dk}_x \text{dk}_y = k_\rho \text{dk}_\rho \text{dk}_\theta \]  

(4.66)

and

\[ k_\rho = \sqrt{k_x^2 + k_y^2} \quad k_\theta = \theta - \arctan \left( \frac{k_y}{k_x} \right) \]  

(4.67)

Then, equation (4.60) can be written as

\[ \tilde{G}_{xx}^1 = \cos^2(k_\theta) \tilde{g}_1(k_\rho) + \tilde{g}_2(k_\rho) \]  

(4.68)

where

\[ \tilde{g}_1(k_\rho) = \left( \frac{\Gamma_1 R^{TM}}{2\eta_1} + \frac{\zeta_1 R^{TE}}{2\Gamma_1} \right) \exp \left( -2\Gamma_1 z_1 \right) \]  

(4.69)

and

\[ \tilde{g}_2(k_\rho) = -\frac{\zeta_1 R^{TE}}{2\Gamma_1} \exp \left( -2\Gamma_1 z_1 \right) \]  

(4.70)

are defined such that they are independent of \( k_\theta \).

Therefore, using the trigonometric identity

\[ \cos(k_\theta) \cos(\theta) + \sin(k_\theta) \sin(\theta) = \cos(k_\theta - \theta) \]  

(4.71)

the inverse spatial Fourier transform (4.26) can be written as

\[ G_{xx}^1(\rho, \theta) = G_{xx,1}^1(\rho, \theta) + G_{xx,2}^1(\rho, \theta) \]  

(4.72)

with

\[ G_{xx,1}^1(\rho, \theta) = \left( \frac{1}{2\pi} \right)^2 \int_0^{+\infty} \int_0^{2\pi} \cos^2(k_\theta) \cdot \exp \left( -jk_\rho \rho \cos(k_\theta - \theta) \right) \text{dk}_\theta \tilde{g}_1(k_\rho)k_\rho \text{dk}_\rho \]  

(4.73)

and

\[ G_{xx,2}^1(\rho, \theta) = \left( \frac{1}{2\pi} \right)^2 \int_0^{+\infty} \int_0^{2\pi} \exp \left( -jk_\rho \rho \cos(k_\theta - \theta) \right) \text{dk}_\theta \tilde{g}_2(k_\rho)k_\rho \text{dk}_\rho \]  

(4.74)

By changing the variable of integration \( k_\theta \) to \( \varphi \) defined by \( \varphi = k_\theta - \theta \), (4.73) becomes

\[ G_{xx,1}^1(\rho, \theta) = \left( \frac{1}{2\pi} \right)^2 \int_0^{+\infty} \int_{-\theta}^{2\pi-\theta} \cos^2(\varphi + \theta) \cdot \exp \left( -jk_\rho \rho \cos(\varphi) \right) \text{d}\varphi \tilde{g}_1(k_\rho)k_\rho \text{dk}_\rho \]  

(4.75)
and (4.74) becomes

\[ G_{xx, 2}^1(\rho, \theta) = \left( \frac{1}{2\pi} \right)^2 \int_0^{+\infty} \int_{-\theta}^{2\pi - \theta} \exp(-j\rho \theta \cos(\varphi)) \, d\varphi \, \tilde{g}_2(\rho) \, k_\rho \, dk_\rho \]  

(4.76)

The integration can be reduced to a one-dimensional integral over the radial component \( k_\rho \) with the help of the first kind Bessel functions \( J_n(\cdot) \) defined as

\[ J_n(x) = \left( \frac{-j}{2\pi} \right)^{n/2} \int_0^{2\pi} \exp(-jx \cos(\varphi)) \cos(n\varphi) \, d\varphi \]  

(4.77)

where \( n \) denotes the order of the Bessel function. Substituting in (4.75) the following trigonometric identity

\[ \cos^2(\varphi + \theta) = \cos^2(\varphi) \cos^2(\theta) + \sin^2(\varphi) \sin^2(\theta) - \cos(\varphi) \cos(\theta) \sin(\varphi) \sin(\theta) \]  

(4.78)

and using the following relations

\[ \frac{1}{2\pi} \int_0^{2\pi} \exp(-j\rho \theta \cos(\varphi)) \cos^2(\varphi) \, d\varphi = \frac{1}{2} [J_0(k_\rho \rho) - J_2(k_\rho \rho)] \]  

(4.79a)

\[ \frac{1}{2\pi} \int_0^{2\pi} \exp(-j\rho \theta \cos(\varphi)) \sin^2(\varphi) \, d\varphi = \frac{1}{2} [J_0(k_\rho \rho) + J_2(k_\rho \rho)] \]  

(4.79b)

\[ \frac{1}{\pi} \int_0^{2\pi} \exp(-j\rho \theta \cos(\varphi)) \cos(\varphi) \sin(\varphi) \, d\varphi = 0 \]  

(4.79c)

the second integral in (4.75) yields

\[ \frac{1}{2\pi} \int_{-\theta}^{2\pi - \theta} \cos^2(\varphi + \theta) \exp(-j\rho \theta \cos(\varphi)) \, d\varphi = \frac{1}{2} [J_0(k_\rho \rho) - J_2(k_\rho \rho)] \cos^2(\theta) + \frac{1}{2} [J_0(k_\rho \rho) + J_2(k_\rho \rho)] \sin^2(\theta) \]  

(4.80)

and then (4.75) becomes

\[ G_{xx, 1}^1(\rho, \theta) = \frac{1}{4\pi} \int_0^{+\infty} \left( [J_0(k_\rho \rho) - J_2(k_\rho \rho)] \cos^2(\theta) \right) \]  

\[ + [J_0(k_\rho \rho) + J_2(k_\rho \rho)] \sin^2(\theta) \, \tilde{g}_1(\rho) \, k_\rho \, dk_\rho \]  

(4.81)

that can be further simplified to

\[ G_{xx, 1}^1(\rho, \theta) = \frac{1}{4\pi} \int_0^{+\infty} [J_0(k_\rho \rho) - J_2(k_\rho \rho) \cos(2\theta)] \, \tilde{g}_1(\rho) \, k_\rho \, dk_\rho \]  

(4.82)
which is a Sommerfeld type integral (i.e., semi-infinite range integral with Bessel functions as kernels) that has to be evaluated numerically. The second integral in (4.76) yields directly

\[ G_{\uparrow xx}(\rho, \theta) = \frac{1}{2\pi} \int_0^{+\infty} J_0(k_\rho \rho) \tilde{g}_2(k_\rho) k_\rho dk_\rho \] (4.83)

which is also a Sommerfeld type integral.

For our specific configuration of the monostatic configuration (\( x = 0 \) and \( y = 0 \)), we have a further reduction to a single ordinary integral

\[ G_{\uparrow xx}(\rho = 0, \theta) = \frac{1}{8\pi} \int_0^{+\infty} \left( \frac{\Gamma_1 R^{TM}}{\eta_1} - \frac{\zeta_1 R^{TE}}{\Gamma_1} \right) \exp (-2\Gamma_1 z_1) k_\rho dk_\rho \] (4.84)

4.6.2 Numerical evaluation of the integral

The computation of integral (4.84) is easily performed using Gauss’ type quadrature rules available in standard mathematical libraries. Figure 4.6 illustrates the fast convergence of the integrand, which is due to the monostatic antenna configuration (the Bessel functions vanish in equations (4.82) and (4.83)). As a result, the evaluation of the integral is faster, which constitutes a valuable advantage when performing inverse modeling. For evaluating the integral, the integration path is deformed in the complex plane to avoid the integrand singularities (guided-wave poles and branch points) using Cauchy’s integral theorem. The integral is generally evaluated as a sum of series of partial integrals over finite subintervals over \((0, a)\) where the integration path is deformed, and over \((a, +\infty)\) where the integration path is real (tail integral) [Michalski, 1998].

4.7 Simulations and Measurements

4.7.1 Frequency response of the TEM horn

In Section 4.3.4, we have determined the position of the virtual source-receiver point of the antenna. Then, we can now compute the frequency response function \( G_{\uparrow xx}(\omega) \) for any known configuration of the multilayered medium. Simulations were done using the code of Slob [2000]. For the particular purpose of determining the frequency response of the antenna, we performed radar measurements with the antenna in air above a metal sheet since the configuration is then well-known. Equation (4.4) can therefore be solved for \( H(\omega) \).

We determined \( H(\omega) \) for the virtual source being at 40 cm above the metal sheet. Figure 4.7 represents the frequency response \( H(\omega) \) computed in the
Figure 4.6. Real and imaginary part of the integrand in the complex $k_\rho$ plane. The elliptical integration path used to avoid the singularities is shown on the projection plane.
Figure 4.7. Frequency response $H(f)$ and impulse response $h(t)$ of the antenna computed considering, respectively, 0.8 GHz and 1.5 GHz as lower cut-off frequency.
ranges 0.8-4 GHz and 1.5-4 GHz, respectively, and the corresponding time domain impulse responses $h(t)$. First, we can observe in the frequency domain high oscillations of the frequency response between 0.8 and 1.5 GHz. These oscillations can be attributed to the worst performance of the antenna in this frequency range, and to the fact that the multilayered medium response function does not accurately represent the modeled system in this frequency range. This can be due to reflections from surrounding objects since the antenna is less directive with decreasing frequency. The assumption of an infinite horizontally layered medium may then break down. The effect of this last explanation appears clearly when considering the corresponding impulse response in the time domain. The large oscillations around 1 ns constitute the transient region and are due to multiple reflections occurring in the antenna system. This ringing is caused only by the backscattered field. At the time interval between 2 and 4 ns, we observe the second and third order reflections which attenuate with time, this is the resonance region. But between 6 and 7 ns, in the tail region which must normally decay exponentially, an unexpected oscillation appears which should not be part of the antenna system response. It is likely to result from a measured wave reflection coming from outside the antenna and that is not modeled in $G^{xx}$. The antenna frequency response plays then the role of rectifying the forward model to fit to the measured data. When considering only frequencies higher than 1.5 GHz, this oscillation disappears. In fact, with increasing frequency, the directivity of the TEM horn increases and the horizontally multilayered medium approximation holds better. Therefore the forward model is expected to perform better for higher frequencies. The atypical observed oscillation may stem from the finite dimensions of the metal sheet which is modeled as horizontally infinite, from obstacles near the experimental setup, or from ringing between the antenna and the metal sheet. Also, the absolute value of the reflection coefficients might not be exactly equal to 1, as normally assumed in the model when considering a PEC.

### 4.7.2 Reflection on a metal sheet

We used the so determined antenna frequency response to predict the radar signal for other heights of the antenna above the metal sheet for which measurements have been also performed. Model predictions and measurements are illustrated on Figure 4.8 for the virtual source being at 45 cm above the metal sheet. Clearly, the measurements are well reproduced by the model ($RMSE_{h=45\, \text{cm}} = 1.69 \times 10^{-2}$), particularly for the higher frequencies, as expected for the aforementioned reasons. Also, for higher frequencies, modeling the metal sheet as infinite in size is more correct. For larger heights, results are similar, but for smaller heights, the $RMSE$ increases when approaching the metal sheet ($RMSE_{h=25\, \text{cm}} = 2.36 \times 10^{-2}$). Simulated data and mea-
4.7. Simulations and Measurements

Figure 4.8. Predicted and measured radar signal for the antenna being at 45 cm above the metal sheet. The signal relative to the frequency response determination \((h = 40 \text{ cm})\) is also represented.

Measurements can also be compared directly in terms of the multilayered medium response function, which is actually the quantity of interest. Results are presented in Figure 4.9. Due to the transformations (4.2) and (4.4), discrepancies between simulations and measurements are more apparent, especially for the norm of \(G_{xx}^\uparrow\) for which large oscillations are observed. The phase is very well modeled up to about 1.7 GHz.

4.7.3 Inverse estimation of the antenna position

In order to see if the model prediction errors observed in previous section play an important role as regards to the system characterization, we used the noisy measured signals to estimate the corresponding heights of the antenna above the metal sheet by inversion of the forward model. The inversion was formulated by the classical least square problem. The objective function to be minimized was accordingly defined as follows

\[
\phi(h) = \left| G_{xx}^d - G_{xx}^m \right|^T \left| G_{xx}^d - G_{xx}^m \right|
\]  

(4.85)

where \(h\) is the unknown height of the virtual source point above the metal sheet, and \(G_{xx}^d = G_{xx}^d(f)\) and \(G_{xx}^m = G_{xx}^m(f, h)\) are the vectors containing, respectively, the observed and modeled response functions.
Figure 4.9. Predicted and measured multilayered medium response function for the antenna being at 45 cm above the metal sheet. The multilayered medium response function relative to the frequency response determination (h = 40 cm) is also represented.

Figure 4.10 shows the objective function pertaining to the measurements performed with the source being at 30.5 cm above the metal sheet. The global minimum of the objective function corresponds exactly (error less than 1 mm) to the real height of the antenna. Inversion results for the other heights present the same estimation accuracy. This suggests that the forward model represents sufficiently well the radar-antenna-multilayered medium system for this configuration. It is worth noting that the oscillatory behavior of the objective function can lead to optimization problems (local minima) when using an optimization algorithm to solve the inverse problem. A global search approach would be required.

4.7.4 Free space response of the antenna

An another way of validating our model is to consider both $H(\omega)$ and $H_i(\omega)$ as unknowns. These parameters characterizing the antenna can be determined by performing measurements at two different heights (a and b) above the metal sheet, resulting in a system of two linear equations as (4.3) to two unknowns that can be solved as

$$H_i(\omega) = S^{a}_{11}(\omega) - \frac{S^{b}_{11}(\omega) - S^{a}_{11}(\omega)}{G^a_{xx}(\omega) - G^{a}_{xx}(\omega)} G^{a}_{ux}(\omega)$$

(4.86)
4.8 Summary and Conclusions

In this chapter, a ground penetrating radar (GPR) system for characterizing the shallow subsurface by inverse modeling is proposed. It consists in an ultrawide band stepped frequency continuous wave (SFCW) radar combined with an off-ground dielectric filled TEM horn antenna used in monostatic mode. Particular attention was paid to design the system in accordance with forward and inverse modeling, requiring both simplicity and accuracy. Main advantages of the adopted radar configuration are: (i) it is suitable for real-time mapping, (ii) an SFCW radar allows to characterize accurately the antenna system and to control an ultrawide band, and (iii) the monostatic mode allows for a more simple and realistic forward modeling and leads, e.g., to faster Sommerfeld integral evaluation.

We fully described the solution of Maxwell’s equations for electromagnetic

Figure 4.10. Objective function to be minimized to estimate the height of the antenna above the metal sheet by inverse modeling. The star represents the real height of the antenna and correspond well with the global minimum of the objective function.

$$H(\omega) = \frac{S_{11}^b(\omega) - S_{11}^a(\omega)}{G_{xx}^{b\uparrow}(\omega) - G_{xx}^{a\uparrow}(\omega)}$$  \hspace{1cm} (4.87)

Figure 4.11 compares $H_i(\omega)$ determined by this way with $H_i(\omega)$ measured directly by performing a $S_{11}(\omega)$ measurement in free space conditions for which $G_{xx}^{\uparrow}(\omega) = 0$. We can observe that modeled and observed data are also well in accordance in this case.

4.8 Summary and Conclusions

In this chapter, a ground penetrating radar (GPR) system for characterizing the shallow subsurface by inverse modeling is proposed. It consists in an ultrawide band stepped frequency continuous wave (SFCW) radar combined with an off-ground dielectric filled TEM horn antenna used in monostatic mode. Particular attention was paid to design the system in accordance with forward and inverse modeling, requiring both simplicity and accuracy. Main advantages of the adopted radar configuration are: (i) it is suitable for real-time mapping, (ii) an SFCW radar allows to characterize accurately the antenna system and to control an ultrawide band, and (iii) the monostatic mode allows for a more simple and realistic forward modeling and leads, e.g., to faster Sommerfeld integral evaluation.

We fully described the solution of Maxwell’s equations for electromagnetic
waves propagating in horizontally layered media. Without loss of generality, the response function representing the backscattered field at the virtual source point of the antenna is specifically derived for our GPR configuration. The approximation of the point source and receiver for the antenna is expected to be valid when working in the far field of the antenna. By considering the antenna as a convolution operator, the antenna is modeled as a linear system and is fully characterized by its frequency responses.

For validating the model, an SFCW radar system has been implemented using a vector network analyzer. Measurements were performed above a metal sheet in the frequency range 0.8-4 GHz. The location of the virtual source point and the frequency response of the antenna were determined. Comparison of measurements and simulations using the electromagnetic point source model demonstrates the validity of the model for the simple configurations investigated. Finally, we were able to estimate accurately the elevation of the antenna above a metal sheet from the measurements by solving the inverse problem.
Chapter 5

Estimating soil dielectric properties from monostatic GPR signal inversion in the frequency domain

Abstract    A new integrated approach for identifying the shallow subsurface dielectric properties from ground penetrating radar (GPR) signal is proposed. It is based on an ultrawide band (UWB) stepped frequency continuous wave (SFCW) radar combined with a dielectric filled TEM horn antenna to be used off-ground in monostatic mode. This radar configuration is appropriate for subsurface mapping and allows for an efficient and realistic modeling of the radar-antenna-subsurface system. Forward modeling is based on linear system response functions and on the exact solution of the three-dimensional Maxwell equations for wave propagation in a horizontally multilayered medium representing the subsurface. Subsurface parameters are estimated by model inversion using the Global Multilevel Coordinate Search optimization algorithm combined sequentially with the local Nelder-Mead Simplex algorithm (GMCS-NMS). Inversion of synthetic data and analysis of the corresponding response surfaces proved the uniqueness of the inverse solution. Laboratory experiments on a tank filled with a homogeneous sand subject to different water content levels demonstrated further the stability and accuracy of the solution towards measurements and modeling errors, particularly concerning the dielectric constant. Inversion for the electric conductivity led to less satisfactory results. This was mainly attributed to the characterization of the frequency response of the antenna and to the frequency dependence of the electric conductivity.

5.1 Introduction

Ground penetrating radar (GPR) is an increasingly used nearby remote sensing tool to detect buried objects and to characterize the subsurface structure and properties in a wide variety of applications [Davis and Annan, 1989; Meller, 1995; Daniels, 1996; Annan, 2002]. In the areas of unsaturated zone hydrology and water resources, GPR has been used to identify soil stratigraphy [Davis and Annan, 1989; Kang and Lu, 1993; Boll et al., 1996], to locate water table [Nakashima et al., 2001], to follow wetting front movement [Vellidis et al., 1997; Gloaguen et al., 2001], to measure soil water content [Du and Rummel, 1994; Greaves et al., 1996; Chanzy et al., 1996; Van Overmeeren et al., 1997; Weiler et al., 1998; Huisman et al., 2001; Rucker and Ferré, 2003], to assess soil salinity [al Hagrey and Müller, 2000], and also to support the monitoring of contaminants [Brewster and Annan, 1994; Darayan et al., 1998; Yoder et al., 2001]. Excellent review on GPR principles is given by Annan [2002] and a review on its application for measuring soil water content is given by Davis and Annan [2002].

The method relies on the relation between the soil constituents, particularly the water content [Topp et al., 1980; Tabbagh et al., 2000], and its dielectric properties, namely, the magnetic permeability, the dielectric permittivity, and the electric conductivity, which are the fundamental variables governing GPR electromagnetic wave propagation. In particular, the water content exhibits a monotonic and highly correlated dependence on the dielectric permittivity. Dielectric contrasts create partial wave reflections which are picked up by the radar system [Daniels, 1996].

Generally, GPR signal analysis is performed using ray-tracing based techniques and tomographic inversion techniques [Goodman, 1994; Cai and McMechan, 1995]. The most commonly used method to identify the depth dependent dielectric constant, which governs wave propagation speed, is the common midpoint (CMP) method [e.g., Mayne, 1962; Garambois et al., 2002]. With this method, stacking velocity fields are extracted from multi-offset radar soundings at a fixed central location. Wave propagation velocities in the ground can be obtained using the Pythagorean theorem or by tomographic inversion. For instance, Nakashima et al. [2001] applied the CMP method to estimate the groundwater level in an environment with multiple reflectors occurring at different depths. They were able to estimate the vertical dielectric constant distribution from the interval velocities obtained from the CMP. Yet, CMP-derived velocity estimates are generally characterized by low resolution and high uncertainty [Tillard and Dubois, 1995]. The success of the measurements depends on the presence of clearly reflecting layers in the soil. Moreover, the method is not appropriate for real-time mapping as it requires
several measurements for a single profile characterization.

To circumvent this last limitation, Du and Rummel [1994], and more recently, Huisman et al. [2001], focused on the velocity of the ground wave for which the propagation distance is known a priori. The ground wave is the signal traveling directly from source to receiving antenna though the upper centimeters of the soil. When the ground wave has been identified using several measurements with increasing antenna separations, the ground wave velocity can be determined from measurements with a fixed antenna separation (Single Trace Analysis; STA). However, Huisman et al. [2001] observed that STA leads to higher uncertainties on the wave speed estimation compared to multiple measurements and suggested to use GPR with multiple receivers for mapping applications. Besides, only the first centimeters of the soil are characterized, which restrict strongly applications in agriculture since crop roots develop mainly in the first soil meter. A last drawback of this approach is the effect of small scale vertical heterogeneities on the average velocity determined from the ground wave.

The dielectric structure of the subsurface is also obtainable from GPR data acquired with cross-hole tomographic acquisition geometries. This technique transmits direct electromagnetic energy from a transmitting antenna in one borehole to a receiving antenna in another borehole over several transmitting/receiving locations. Borehole data can also be processed using ray-tracing techniques or tomographic inversion. But the method can not be used in a mapping application since wells are required.

The main limitations of the existing characterization methods arise from the strongly simplifying assumptions with respect to the antennae radiative properties and electromagnetic wave propagation phenomena. As a result, only a part of the information contained in the GPR signal is utilized, usually the propagation time. Whereas tomographic inversions of travel times are well established, ray-based inversions of amplitudes depend critically on the complex directive properties of the radar antennae [Holliger et al., 2001]. This hampers the accurate quantitative identification of the absolute subsurface dielectric properties.

Resorting to the physical and mathematical basis of GPR wave propagation is necessary to estimate simultaneously both the depth dependent soil dielectric permittivity and electric conductivity. The relation between the subsurface constitutive parameters and the measured electromagnetic field is governed by Maxwell’s equations. Reconstruction of the unknown constitutive parameters from the known field appeals to inverse modeling. Inverting electromagnetic data has been a major challenge in applied geophysics for many years [Spagnolini, 1997; Lazaro-Mancilla and Gomez-Treviño, 2000]. Successful inversion is challenging since it involves rigorous forward modeling of the three-dimensional GPR-subsurface system, which is furthermore computationally...
very time-consuming. Moreover, the inverse problem should satisfy elemental well-posedness conditions. Nevertheless, inversion is becoming a rational choice due to the ever increasing power of computers [Sasaki, 2001].

In the present study, a new integrated approach for identifying the shallow subsurface water content from GPR signal inversion is investigated. Using the GPR system and GPR-subsurface electromagnetic model presented in Chapter 4 [Lambot et al., 2003e], model inversion is carried out iteratively using the Global Multilevel Coordinate Search optimization algorithm in sequential combination with the local Nelder-Mead Simplex algorithm (GMCS-NMS) [Huyer and Neumaier, 1999; Lambot et al., 2002]. We examine the well-posedness of the inverse problem for both synthetic data and real data acquired in controlled laboratory conditions for a homogeneous sand subject to different water content levels. GPR signal inversion results are compared with time domain reflectometry (TDR) measurements. To our knowledge, the proposed integrated approach constitutes a first attempt in water resources research to provide a tool being substantially appropriate for subsurface mapping and having the potential to provide simultaneously the depth dependent dielectric constant and electric conductivity.

5.2 Materials and Methods

The ground penetrating radar system and the radar-antenna-subsurface model used in this study are fully described in Chapter 4.

5.2.1 Model inversion

Subsurface parameter identification by inverse modeling is a nonlinear optimization problem which consists in finding the parameter vector $b = [\varepsilon_n, \sigma_n, h_n]$, $n = 1 \cdots N$, so that an objective function $\phi(b)$ is minimized, $N$ being the number of layers in the subsurface model. In the particular case where no prior information on the parameters is taken into account and assuming observation errors to be normally distributed, independent, and homoscedastic, the maximum likelihood theory reduces to the classical least squares problem. The objective function to be minimized was accordingly defined as follows

$$\phi(b) = \left| \mathbf{G}^{*}_{xx} - \mathbf{G}^T_{xx} \right| \left| \mathbf{G}^*_{xx} - \mathbf{G}^T_{xx} \right|$$

(5.1)

where $\mathbf{G}^{*}_{xx} = G^{*}_{xx}(\omega)$ and $\mathbf{G}^T_{xx} = G^T_{xx}(\omega, b)$ are the vectors containing, respectively, the observed and simulated response functions. Since these response functions are complex functions, the difference between observed and modeled data is expressed by the amplitude of the errors in the complex plane.
Objective function (5.1) relates indirectly the response function of the multilayered medium to its constitutive parameters. However, as in most electromagnetic inverse problems, this function is highly nonlinear and is characterized by an oscillatory behavior and a multitude of local minima. This complex topography hampers inevitably traditionally used local optimization algorithms to converge to the global minimum, i.e., the solution of the inverse problem. Therefore, an efficient global approach is needed. Following the approach of Lambot et al. [2002], we use the Global Multilevel Coordinate Search (GMCS) algorithm [Huyer and Neumaier, 1999] combined sequentially with the classical Nelder-Mead Simplex algorithm (NMS) [Lagarias et al., 1998] to minimize (5.1).

5.2.2 Experiments description

Measurements. Laboratory experiments were conducted at the Royal Military Academy of Bruxelles (Belgium). The frequency response function \( H_f(\omega) \) of the antenna was determined by performing a \( S_{11} \) measurement in free space, for which \( G_{xx}(\omega) \) is equal to zero in equation (4.3). \( H(\omega) \) was determined by performing a \( S_{11} \) measurement with the antenna in air above a metal sheet for which \( G_{xx}(\omega) \) can be readily computed using the electromagnetic model. Equation (4.3) was then solved for \( H(\omega) \). For additional details on the characterization of the antenna properties, refer to Chapter 4.

Radar measurements were carried out in controlled laboratory conditions on a homogeneous sand subject to seven different water content levels ranging from dry to wet conditions. The sand was packed horizontally in a 1.45 m \( \times \) 1.30 m area tank made of wood. The thickness of the sand layer varied from about 11 cm to 14 cm, as a function of the imposed water content level. Below the sand layer, a horizontal metal sheet was installed to control the bottom boundary conditions in the electromagnetic model. Indeed, materials underneath this metal sheet have no influence on the measured backscattered signal. The antenna was situated at about 30 cm above the sand surface.

Starting from dry conditions, the different water content levels were imposed successively by adding water on the sand, and by mixing manually sufficiently long to obtain a homogeneous distribution of the water within the whole sand layer. Subsequently to each radar measurement, three juxtaposed vertical time domain reflectometry (TDR) measurements were performed in the area just beneath the antenna, and then, three 100 cm\(^3\) samples were collected at the same locations for determining the actual volumetric water content by means of the standard oven-drying method.

Analysis. Synthetic data inversions were performed after the real data inversions. Seven sets of synthetic data were generated using the estimated param-
Chapter 5. Soil dielectric properties from GPR signal inversion

Parameters from the inversion of the seven real experiments and the corresponding configurations. The inversion of synthetic data aims to investigate the uniqueness of the solution of the inverse problem, and also to verify that the adopted optimization approach is able to find correctly and accurately the global minimum of the objective function. This approach has the benefit that one knows exactly the true solution of the inverse problem.

Parameters to be optimized were the three which characterize a single sand layer, namely, the dielectric constant ($\varepsilon_r'$), the electric conductivity ($\sigma$), and the thickness ($h$). In reality, dielectric parameters are frequency dependent with the dependence described by Debye’s equation. Frequency dispersion mechanisms are principally electronic and ionic lattice polarizations for solids, whereas the main frequency dispersion mechanism is the Debye rotating dipole relaxation for free dipolar molecules [West et al., 2003]. These mechanisms operate mainly at characteristic frequencies well above 1 GHz, and so do not give rise to much frequency dispersion in the TDR and GPR frequency ranges [Heimovaara, 1994]. However, other relaxation mechanisms operate in a mixture of solids and polar liquids due to bound water and Maxwell-Wagner effects. Nevertheless, the relaxation frequencies encountered in most porous media [Cambell, 1992] are either beyond the upper limit of TDR and GPR bandwidths (relaxation of free soil water at frequencies above 2 GHz) or in the lower range of the bandwidths (relaxation of bound water and Maxwell-Wagner relaxation at frequencies below 10 MHz). Accordingly, [Weerts et al., 2001; Huisman et al., 2002] observed that for TDR, taking into account the frequency dependence of the dielectric permittivity did not greatly improve the fit between measured and modeled waveforms and that a frequency independent apparent permittivity adequately describes the TDR measurements made in a sandy soil. We also consider in this study an inverse modeling analysis in which the frequency dependent dielectric parameters are replaced by frequency independent effective parameters.

Generally, sensitivity and stability analyses are also performed on synthetic data to demonstrate the well-posedness of an inverse problem. However, in the present study, such analyses were not done directly since it relies heavily on the knowledge of the expected measurement and modeling errors which are difficult, if not impossible, to quantify. Stability of the solution was examined directly using real data.

5.3 Results and Discussions

5.3.1 Response surface analysis

Uniqueness and stability of the inverse solution were first investigated using response surfaces of the objective function which partially reveal the struc-
5.3. Results and Discussions

ture of the inverse problem, i.e., the presence of a well-defined solution, the occurrence of local minima, and also qualitatively parameter sensitivities and correlations. Response surfaces are two-dimensional contour plots representing the objective function as a function of two parameters, while all the other parameters are held constant at their true value. In our study, they represent therefore only cross sections of the full three-dimensional parameter space.

Inversions took place in a very large parameter space \( (2 < \varepsilon'_r < 25; 1 \times 10^{-5} < \sigma < 1 \times 10^{-1} \text{Sm}^{-1}; 0 < h < 0.25 \text{ m}) \) which contained largely all the solutions corresponding to the seven considered scenarios. Figure 5.1 shows the response surfaces of the logarithm of the objective function pertaining to both synthetic error free data and real data, for the three different parameter planes \( \varepsilon'_r - \sigma, \varepsilon'_r - h, \sigma - h \). The range of each parameter has been divided into 100 discrete values resulting in 10000 objective function calculations for each contour plot.

For synthetic data (left-handed contour plots), each response surface shows a well-defined global minimum corresponding to the true parameter values. This illustrates partially the uniqueness of the solution for the given model configuration. A unique solution reveals that the frequency response function of the multilayered medium contains sufficient information so as to estimate simultaneously all parameters of interest. It is worth noting the nonlinear and oscillatory behavior of the objective function resulting in the presence of numerous local minima. This imposes inevitably the use of a global and efficient optimization approach for minimizing the objective function.

The \( \varepsilon'_r - \sigma \) and \( \sigma - h \) response surfaces exhibit an elliptical minimum parallel to the \( \sigma \) axis. This suggests that these two parameter pairs are uncorrelated, which is advantageous for their inverse identification. However, the model is visibly less sensitive to \( \sigma \). \( \varepsilon'_r \) and \( \sigma \) are uncorrelated because they govern independently wave propagation velocity and attenuation, respectively. The banana shape contour plot in the \( \varepsilon'_r - h \) space suggests an important negative correlation between these parameters. This stems from the fact that a similar signal can be obtained for either a low dielectric constant (high propagation velocity) with a high layer thickness, or a high dielectric constant (low propagation velocity) with a low layer thickness. Indeed, in both cases the propagation time through a layer can be the same. We would like to emphasize here, that as a consequence of the nonlinearity of the Green function with respect to the dielectric parameters, parameter sensitivity and correlation are dependent of the parameter values. For instance, in the \( \sigma - h \) plane, \( h \) is not very sensitive in a wide range for the higher values of \( \sigma \), whereas it is very sensitive around the global minimum. In fact, when \( \sigma \) is high, the signal is strongly attenuated throughout the layer, and the picked up signal contains less information regarding layer thickness.

Response surfaces pertaining to real data exhibit mostly the same general
Chapter 5. Soil dielectric properties from GPR signal inversion

Figure 5.1. Response surfaces of the objective function logarithm $\log_{10}(\phi(b))$ in the $\varepsilon'_r - \sigma$, $\varepsilon'_r - h$, and $\sigma - h$ parameter planes. Left-handed figures correspond to numerically generated error free data ($\phi(b)$), and right-handed figures correspond to real data ($\phi^*(b)$). The white star represents the global minimum of the objective function.
5.3. Results and Discussions

shape as synthetic response surfaces. More important is the unchanged position of the global minimum, which demonstrates the excellent stability properties of the inverse problem towards measurements and modeling errors. This can be attributed to the filtering effect of the used Green’s function, so no artificial smoothing is required. As expected, the values of the objective function are higher and the global minimum regions are flatter, resulting in an increase in parameter uncertainty. This flattening and the occurrence of much more local minima, especially in the $\varepsilon'_{r} - h$ plane, is unfavorable to the optimization task which will require more function evaluations to find the global minimum accurately.

Error sources in real data inversions are mainly to be attributed to the difference between the model and the reality. Figure 5.2 illustrates the measured and modeled complex Green function for the first water content level. We observe that, while the phase is well modeled, large errors occur in the amplitude. Their origin stems mainly from the determination of the antenna frequency response functions, particularly $H(\omega)$. Also, the approximation of an infinite perfect electric conductor for the metal sheet may fail, particularly for the lower frequencies. To overcome these problems, we recommend further studies to determine more accurately the frequency response of the antenna (see Chapter 6).

5.3.2 Water content estimation

Inversions of synthetic data for the seven scenarios supported response surface observations and all three unknown parameters ($\varepsilon'_{r}, \sigma, h$) were exactly retrieved by the GMCS-NMS optimization method with about 2900 objective function evaluations. This demonstrates at the same time the uniqueness of the inverse solution for this single layer configuration and the good performances of GMCS-NMS. However, three-dimensional GMCS-NMS inversions of real data led to local minima due to the higher complexity of the objective function topography. The true global minimum of each scenario was identified by fixing parameter $h$ to its true measured value, reducing thus the dimensionality of the optimization problem to two. The solution was then found after about 700 iterations. Nonetheless, extensive objective function evaluations proved the uniqueness of the solution in the three-dimensional space, as supported by the response surface analysis. The encountered optimization problem can be solved by either reducing modeling error and smoothing thus the objective function, or by increasing considerably the maximum number of objective function evaluations in the optimization process. Moreover, prior information on the parameters could be included by constraining more the parameter space.

Figure 5.3 represents the inversely estimated dielectric constant as a func-
Chapter 5. Soil dielectric properties from GPR signal inversion

Figure 5.2. Measured and modeled Green’s function for the water content level $\theta = 0.0031$ m$^3$ m$^{-3}$.

Figure 5.3. Dielectric constant ($\varepsilon_r'$) as a function of water content ($\theta$). Square and triangular markers pertain, respectively, to GPR and TDR measurements, dotted line represents Topp’s model, and solid line is a third-degree polynomial equation fitted to GPR measurements.
5.3. Results and Discussions

Fitting a soil specific empirical model similar to Topp’s equation [Topp et al., 1980] to the data led to a standard deviation of 0.0036 \( m^3 m^{-3} \) for the error on the water content. The observed standard deviation is mainly due to errors related to the water content levels \( \theta = 0.177 \) and \( \theta = 0.203 \). We can observe the same behavior for TDR measurements for these two levels. That means that these two more important errors are likely to stem mainly from gravimetric measurement errors or from the variation of the sand density after manual mixing. To further check the consistency, the fitted model is compared with Topp’s equation. A good agreement exists between both except in the highest range where a maximum divergence of about 0.03 \( m^3 m^{-3} \) is seen in water content prediction. Yet, it is important to emphasize here that since we do not know the real relation between the dielectric constant and the volumetric water content for this specific soil, we cannot prove that the inversely estimated dielectric constant is the real one, even for TDR measurements.

It is worth mentioning that volumetric water content was taken as the average water content of the three collected samples for each scenario. The variation of the water content amongst the three samples for the same level was less than \( \theta = 0.01 m^3 m^{-3} \), indicating a good homogeneous distribution of the water within the sand layer after manual mixing.

The difference between GPR and TDR measurements can be partly attributed to the difference in the frequency range in which TDR and GPR operate. Since the dielectric constant is frequency dependent, both instruments measure actually a different effective dielectric constant. Weiler et al. [1998] also observed such a difference. Also, the systematic character of the difference may be due to an error in TDR calibration or may be inherent to the used software. Indeed, different travel time analysis methods can lead to differences as high as 0.04 \( m^3 m^{-3} \) for the same waveform (extreme ways to perform travel time analysis) [Huisman et al., 2002]. Finally, the setting of the travel time analysis parameters is usually determined by the user, who visually checks whether analysis is performed correctly. However, it is difficult to obtain a set of travel time analysis parameters that does not need to be changed during the processing of TDR measurements over a wide range of soil water contents. We didn’t change these parameters in this study. It is worth to note that the TDR measurement of the dielectric constant was not possible for the two lower water content levels since the shape of the TDR waveform was not appropriate for the used travel time analysis algorithm. There is no such restriction when inverting GPR signal. This is of practical interest for water monitoring in arid regions for instance.
5.3.3 Electric conductivity estimation

Although a reasonable correlation between TDR and GPR was found ($r^2 = 0.90$), results pertaining to the estimation of the electric conductivity are less satisfactory, as illustrated in Figure 5.4. Possible reasons related to GPR measurements are threefold. First, as observed in the response surfaces, this parameter is less sensitive compared to the others, resulting in a higher uncertainty for its estimation. Second, in contrast to the dielectric constant, the estimation of this parameter relies very much on the error on the amplitude of the signal, which is quite important in this specific antenna calibration case. Indeed, the electric conductivity governs mainly the attenuation of the electromagnetic waves within the propagation medium. Finally, the electric conductivity is strongly dependent of the frequency. This makes the comparison between GPR and TDR not really significant and explains partly with TDR measurements errors the difference of one order of magnitude between the two methods. TDR derived electric conductivity relies heavily on the TDR software calibration, on the probe contact with the sand, and on the electric conductivity itself.

5.4 Summary and Conclusions

Commonly used methods to characterize the subsurface by means of GPR technology suffer from important limitations for their application. We propose in this study a new integrated approach for identifying the shallow subsurface water content from GPR signal. It is based on an ultrawide band (UWB) stepped frequency continuous wave (SFCW) radar combined with a dielectric filled TEM horn antenna to be used off-ground in monostatic mode. This radar configuration is appropriate for subsurface mapping and allows for an efficient and realistic modeling of the radar-antenna-subsurface system [Lambot et al., 2003e]. Forward modeling is based on linear system response functions and on the exact solution of the three-dimensional Maxwell equations for wave propagation in a horizontally multilayered medium representing the subsurface. Subsurface parameters are estimated by model inversion using the Global Multilevel Coordinate Search optimization algorithm in sequential combination with the local Nelder-Mead Simplex algorithm (GMCS-NMS).

We have examined the theoretical applicability of the inverse modeling method for a single soil layer configuration using synthetic data. Response surface analysis and synthetic inversions demonstrated simultaneously the uniqueness of the inverse solution and the appropriateness of the adopted optimization scheme.

We implemented the proposed radar system and performed laboratory experiments on a tank filled with a homogeneous sand layer subject to different water content levels. Results demonstrated further the stability and accuracy
5.4. Summary and Conclusions

of the solution towards measurement and modeling errors, particularly concerning the dielectric constant. Using a soil specific calibration, the standard deviation of the error on water content prediction was equal to 0.0036 m$^3$m$^{-3}$. Inversion for the electric conductivity led to less satisfactory results. This was mainly attributed to the characterization of the frequency response of the antenna and to the strong frequency dependence of the electric conductivity. Finally, some limitations were encountered for minimizing objective functions constructed from real data due to their increased nonlinearity.

Clearly, an inverse modeling approach for GPR signal analysis is an interesting alternative to travel time analysis because it is based on the underlying physics, it is fully automated, and it uses all the information contained in the signal. This information is required to estimate simultaneously the dielectric constant and the bulk electric conductivity. We will further focus on the improvement of the antenna characterization to reduce modeling errors, on the parameterization of the optimization algorithm, and on the investigation of configurations closer to field conditions, e.g., two layer configuration or a continuous variation of the dielectric properties with depth.

Figure 5.4. Electric conductivity measured by GPR ($\sigma_{GPR}$) as a function of electric conductivity measured by TDR ($\sigma_{TDR}$).
Chapter 6

Accurate modeling of GPR signal for an accurate characterization of the subsurface dielectric properties*

Abstract The possibility to estimate accurately subsurface dielectric properties from ground penetrating radar (GPR) signal using inverse modeling is obstructed by the appropriateness of the forward model describing the GPR-subsurface system. In this study, we improved the recently developed approach of Lambot et al. [2003c, e] whose success relies on a stepped frequency continuous wave (SFCW) radar combined with an off-ground monostatic TEM horn antenna. This radar configuration enables realistic and efficient forward modeling. We included in the initial model (i) the multiple reflections occurring between the antenna and the soil surface using a positive feedback loop in the antenna block diagram, and (ii) the frequency dependence of the dielectric properties using a local linear approximation of the Debye model. The model was validated in laboratory conditions on a tank filled with a two-layered sand subject to different water content levels. Results showed remarkable agreement between the measured and modeled Green’s functions. Model inversion for the dielectric constant demonstrated further the accuracy of the method. Inversion for the electric conductivity led to less satisfactory results. However a sensitivity analysis demonstrated the good stability properties of the inverse solution, and put forward the necessity to reduce the remaining clutter by a factor 10. This may partly be achieved through a better characterization of the antenna transfer functions, and by performing measurements in an environment without close extraneous scatterers.

6.1 Improved antenna model

Based on the model of Lambot et al. [2003c, e], we propose to model the radar-antenna-air-subsurface system using the block diagram represented in Figure 6.1. The previous model has been improved by adding the block $H_f(\omega)$ with a positive feedback connection in parallel with the block representing the air-subsurface system. Accordingly, the resulting transfer function, expressed in the frequency domain, is given by

$$S_{11}(\omega) = \frac{Y(\omega)}{X(\omega)} = H_i(\omega) + \frac{H_t(\omega)G_{xx}^1(\omega)H_r(\omega)}{1 - H_f(\omega)G_{xx}(\omega)}$$  \hspace{1cm} (6.1)

where $Y(\omega)$ and $X(\omega)$ are, respectively, the received and emitted signals at the VNA reference plane; $H_i(\omega)$, $H_t(\omega)$, $H_r(\omega)$, and $H_f(\omega)$ are, respectively, the complex return loss, transmitting, receiving, and feedback loss transfer functions of the antenna; and $G_{xx}^1(\omega)$ is the transfer function of the air-subsurface system modeled as a multilayered medium. This relationship is referred to as the antenna equation in the frequency domain.

Due to the variations of impedance between the antenna feed point, antenna aperture, and air, multiple wave reflections occur within the antenna. The return loss transfer function $H_i(\omega)$ represents the part of this ringing, measured at the reference plane, that is independent of the backscattered electromagnetic field $G_{xx}^1(\omega)$. $H_i(\omega)$ can thus be measured directly by performing $S_{11}(\omega)$ measurements in free space conditions for which $G_{xx}^1(\omega) = 0$. The transmitting and receiving transfer functions describe the antenna gain and phase delay between the measurement point and the source and receiver virtual point. Equation (6.1) can be simplified by defining $H(\omega) = H_t(\omega)H_r(\omega)$, reducing by this way the number of transfer functions to be determined. The positive feedback loop with transfer function $H_f(\omega)$, similarly to $H_i(\omega)$, accounts for the variations of impedance between the antenna feed point, antenna aperture, and air, which creates a part of the backscattered field to be reflected again toward the subsurface. This leads to multiple wave reflections between the antenna and the subsurface.

The two remaining unknowns $H(\omega)$ and $H_f(\omega)$ in (6.1) can be readily determined by performing $S_{11}(\omega)$ measurements with the antenna located at two different heights ($a$ and $b$) above a metal sheet. For these simple configurations, the theoretical transfer functions $G_{xx}^1(\omega)$ are known accurately. This results in
two equations as (6.1) to two unknowns that can be solved analytically as

\[
H_f(\omega) = \frac{S^{b}_{11}(\omega) - S^{a}_{11}(\omega)}{G^{[b]}_{xx}(\omega)} \]  
\[
H(\omega) = \frac{S^{a}_{11}(\omega)}{G^{[a]}_{xx}(\omega)} - S^{a}_{11}(\omega)H_f(\omega) \]  

Figure 6.2 illustrates the effect of transformation (6.1) on measurements performed with the antenna located at different heights above a metal sheet. For convenience, measured frequency domain data are presented here in the time domain using the inverse discrete fast Fourier transform. In the \( s_{11}(t) \) signal, we observe clearly the wave reflections occurring within the antenna, between 0 and 2 ns. The reflection at the metal sheet level appears between 4 and 6 ns. Finally, the second order reflection at the metal sheet, due to the feedback loss of the antenna, occurs between 8 and 11 ns. In the filtered \( g_{xx}^{T}(t) \) signal, only the response of the metal sheet is visible. This illustrates the appropriateness of the block diagram presented in Figure 6.1 to model accurately the monostatic antenna system. Let’s note that the slight ripples on the time domain signal are caused by the inverse Fourier transform since only the frequency signal between 1 and 3 GHz was measured.
6.1 Frequency dependence of the electric conductivity

In this chapter, we improve the subsurface model by considering the imaginary part of the complex dielectric permittivity (see equation (4.13)) to be frequency dependent. Since a limited frequency range is intentionally considered here (1 GHz to 2 GHz), and to limit the number of unknowns in the inverse problem to ensure well-posedness, we approximate locally the apparent electric conductivity \( \sigma = \sigma' + \omega \varepsilon'' \) in (4.15) using a linear model

\[
\sigma(f) = \sigma_{1\text{GHz}} + a(f - 10^9) \tag{6.4}
\]

where \( \sigma_{1\text{GHz}} \) is the reference apparent electric conductivity at 1 GHz, and \( a \) is the linear variation rate of \( \sigma(f) \). Limiting the maximum frequency to 2 GHz is moreover in favor of the Fraunhofer approximation (see Section 4.3.2).

6.3 Experiment Description

6.3.1 Setup

Laboratory experiments were conducted at the Royal Military Academy of Bruxelles (Belgium). In contrast to the studies reported in Chapter 4 and Chapter 5, the antenna used in this study consisted in a linear polarized double ridged broadband TEM horn (BBHA 9120 D, Schwarzbeck Mess-Elektronik). We chose this commercial antenna for its higher gain compared to the previously used dielectric filled one (results not shown). Antenna dimensions are 22 cm length and 14 cm \( \times \) 24 cm aperture area. Its nominal frequency range is 1-18 GHz and its isotropic gain ranges from 6 dBi to 18 dBi. Reflections from antenna terminal and from the edges of the antenna panels are minimized.
through an appropriate resistive loading of the antenna panels using the commonly used Wu-King profile [Wu and King, 1965], which emulates conductivity profiles within antenna panels that scale hyperbolically with the distance from the terminal. Parameter $S_{11}$ was measured sequentially at 126 stepped operating frequencies over the range 1-2 GHz with a frequency step of 8 MHz. The frequency response functions $H_i(\omega)$, $H(\omega)$, and $H_f(\omega)$ of the antenna were determined as described in Section 6.1.

Radar measurements were carried out in controlled laboratory conditions on a tank filled with a two-layered disturbed sandy soil. The volumetric water content of the bottom layer was fixed at about $0.10 \, m^3 \, m^{-3}$, whereas the top layer was subject to nine different water content levels, ranging from 0 to 0.26 $m^3 \, m^{-3}$. The sand was packed horizontally in a $1.45 \, m \times 1.30 \, m$ area tank made of wood. The thickness of the bottom layer was equal to 13 cm, whereas the thickness of the top sand layer varied from about 10 cm to 14 cm, as a function of the imposed water content level. Below the sand layer, a horizontal metal sheet was installed to control the bottom boundary conditions in the electromagnetic model. Indeed, materials underneath this metal sheet have no influence on the measured backscattered signal. The antenna was situated at about 40 cm above the sand surface.

6.3.2 Measurements and analysis

Starting from dry conditions, the different water content levels were imposed successively by adding water on the sand, and by mixing manually sufficiently long to obtain a homogeneous distribution of the water within the whole sand layer. Subsequently to each radar measurement, three juxtaposed vertical time domain reflectometry (TDR) measurements were performed in the area just beneath the antenna, and then, three 100 cm$^3$ samples were collected at the same locations for determining the actual volumetric water content by means of the standard oven-drying method at 105 °C.

Given the adopted forward model, the electromagnetic parameters to be optimized are the dielectric constant $\varepsilon'_r$, the reference electric conductivity ($\sigma_{1GHz}$), and parameter $a$. To limit the dimensionality of the inverse problem, parameters of the bottom layer were inversely estimated before setting up the second sand layer in the tank. They were then used as fixed parameters in the forward model for the characterization of the top layer. The thickness of the layers were directly measured and also used as fixed parameters during inversion. Inversions took place in a large parameter space ($2.5 < \varepsilon'_r < 15$; $1 \times 10^{-3} < \sigma_{1GHz} < 1 \times 10^{-1} \, Sm^{-1}$; $1 \times 10^{-12} < a < 1 \times 10^{-10} \, Ssm^{-1}$) which contained all the solutions corresponding to the nine considered scenarios. In this study, we restricted the dimensionality of the inverse problem to better investigate the validity of the forward model and the stability of the
inverse solution, without having to deal with optimization issues for higher dimensions. Well-posedness and optimization issues has been handled in [Lambot et al., 2003c].

6.4 Results and Discussion

6.4.1 Effect of the frequency dependence

Figure 6.3 represents the measured and modeled complex Green’s functions pertaining to the single sand layer characterization. Two scenarios are considered: (i) no frequency dependence of the electric conductivity is assumed, and (ii) the frequency dependence is taken into account according to (6.4). Let’s note that we consider here frequencies till 3 GHz to better illustrate the effect of the frequency dependence on the signal. Higher frequencies are not represented since the signal is not accurately modeled. This can be due to the fact that at these frequencies, the Fraunhofer approximation is no more valid.

First we observe that even when dispersion is not considered, both the amplitude and phase of the soil response function are relatively well modeled. In contrast, for the same one-layered configuration, the amplitude was not well reproduced in the study of Lambot et al. [2003c]. Including the soil-antenna ringing in the antenna equation as a positive feedback loop has greatly improved the forward model, especially regarding the amplitude modeling. Part of the improvement of the results may also stem from the better performances (higher gain) of the BBHA 9120 D antenna compared to the previously used dielectric-filled TEM horn antenna developed by Scheers [2001].

Accounting for electric dispersion enhances further the fitting of the model to the measured Green’s function. The phase is closely reproduced, except around 2.1 GHz. This last discrepancy, as well as the phase discrepancies observed in the no-dispersion case, stem from the fact that the Green function tends to zero at these frequencies. In this case, small errors on the real and imaginary parts of the Green function can result in large errors on the phase. This is an artifact of representing the complex data in modulus and phase.

The linear dispersion model seems quite appropriate to describe the observed Green’s function, particularly in the range 1-2 GHz. Two kinds of error characterize the modeling of the amplitude: (i) local clutter, and (ii) general trend. The origin of the local variations is mainly to be attributed to the determination of the antenna frequency response functions, particularly $H(\omega)$ and $H_f(\omega)$. The smoothness of $H_1(\omega)$ suggests that this transfer function is accurately determined (results not presented). In contrast, both $H(\omega)$ and $H_f(\omega)$, indirectly determined, present similar local variations. This clutter is likely to arise from the approximation of an infinite perfect electric conductor (PEC) for the metal sheet used for the antenna characterization, as well as from the
6.4. Results and Discussion

Figure 6.3. Measured and modeled Green’s function for the antenna being in air above a single sand layer. The model in left-handed figure assumes no frequency dependence of the electric conductivity whereas the model in right-handed figure assumes a linear frequency dependence following equation (6.4).

scattering from extraneous objects present in the laboratory. These problems could be minimized by characterizing the antenna in an anechoic chamber and using a larger metal sheet as infinite PEC.

The exact origin of the global mismatch is much more difficult to bring to light. It should stem from the different hypothesis used in the forward model, mainly, (i) the far-field approximation, (ii) the virtual source and receiver point of the antenna which is assumed to be at a fixed position (actually, its position changes with frequency, the high frequencies being emitted nearer the feed point, and the low frequencies being emitted in the proportionally larger part of the antenna), (iii) the fact that only the $x$-component of the electric field is assumed to be measured and that only an $x$-directed current source is present, and (iv) the linear frequency dependence of the electric conductivity and the frequency independence of the dielectric permittivity. In view of the higher amplitude of the modeled $G_{xx}$ compared to the measured one between 2 and 3 GHz, we may conclude that dispersion of the electric conductivity, which governs mainly electromagnetic wave attenuation, is not perfectly linear, but of a higher order in this frequency range. Let’s note finally that discrepancies may also stem from the finite size of the sand box and extraneous scatterers present in the laboratory.

6.4.2 Water content estimation

Given the apparently not linear behavior of dispersion in the range 1-3 GHz, we restricted the considered frequency band to 1-2 GHz, in which the local linear approximation seems quite well appropriate. Figure 6.4 shows, in both the frequency and time domains, the measured and modeled Green’s func-
tions pertaining to the water content levels WC2 ($\theta = 0.04 \text{ m}^3\text{m}^{-3}$) and WC9 ($\theta = 0.26 \text{ m}^3\text{m}^{-3}$) of the top sand layer. In these configurations, electromagnetic wave propagation phenomena are relatively complex as infinite wave reflections occur simultaneously in the air layer, in the top layer, and in the bottom layer. For the WC2 scenario, the observed Green’s function is remarkably well reproduced by the forward model. As aforementioned, the larger phase errors occur when the absolute value of the Green function is small. We can observe from the time domain representation that all three reflection interfaces are visible, which means that the picked up wave has well propagated in the two sand layers without too much attenuation.

For the WC9 case, larger discrepancies are observed, particularly concerning the amplitude. However, the general trend is still well modeled. Time domain data, as well as the behavior of the phase in the frequency domain, indicate that the backscattered signal originates mainly from the soil surface interface. Also, the behavior of the amplitude becomes progressively linear at higher frequencies. This is due to the higher dielectric contrast between the air layer and the sand layer for this water content level, and to the fact that the wave is also strongly attenuated, particularly when increasing frequency.
Figure 6.5 represents the inversely estimated dielectric constant as a function of the nine different water content levels. Results are very consistent. Fitting a soil specific empirical model (third order polynomial) similar to Topp’s equation [Topp et al., 1980] to the data led to a standard deviation of 0.0070 m$^3$m$^{-3}$ for the error on the predicted water content, which is very satisfying. For TDR measurements, the observed standard deviation is 0.0032 m$^3$m$^{-3}$. Differences observed between TDR and GPR, as well as the observed errors, are partly to be attributed to the different measurement scales, given the observed spatial variability of the actual water content inside layers. Indeed, the three collected samples for each scenario indicated stochastic heterogeneity with absolute variations reaching $0.01 - 0.02$ m$^3$m$^{-3}$, values well in accordance with the observed standard deviations.

The difference in the operating frequencies can also explain the mismatch between TDR and GPR, particularly in view of the systematic lower values of the GPR derived dielectric constant for the higher water content levels. Weiler et al. [1998] also observed such a difference. With increasing frequency the water molecules become progressively too slow to follow the fast alternating electric field. The polarizability decreases and the energy applied is absorbed. The relaxation frequency of free water is equal to 17 GHz, but lower values are observed for bound water [Hilhorst, 1998]. Therefore, TDR and GPR may actually measure different effective dielectric constants.

For the lower water content ($\theta = 0.00$ m$^3$m$^{-3}$), the analysis of the TDR signal is expected to be not very accurate since the shape of the waveform is not appropriate (the TDR signal is not sufficiently attenuated) for the used travel time analysis algorithm [Or et al., 1998]. The perfect agreement between TDR and GPR for the three water content levels ranging from 0.04 to 0.12 m$^3$m$^{-3}$ indicates that dielectric dispersion is negligible in these cases. It further points out that the setting of the travel time analysis parameters for TDR has been done correctly. This constitutes an important step in using TDR [e.g., Huisman et al., 2002]. There is no such restriction when inverting GPR signal.

### 6.4.3 Electric conductivity estimation

As illustrated in Figure 6.6, results pertaining to the estimation of the electric conductivity are less satisfactory. The standard deviation of TDR measurement errors, considering a second order polynomial fitted to the TDR derived electric conductivity as reference, is found to be $3.6 \times 10^{-4}$ Sm$^{-1}$, whereas the standard deviation of GPR measurement errors is one order of magnitude higher and equal to $3.6 \times 10^{-3}$ Sm$^{-1}$. Let’s note that electric conductivities measured by TDR and GPR are of the same order of magnitude, and that the errors are rather randomly distributed than systematic. That means that discrepancies are likely to stem mainly from measurements and modeling errors,
Figure 6.5. Dielectric constant ($\varepsilon_r'$) of the upper sand layer as a function of its water content ($\theta$). Square and triangular markers pertain, respectively, to GPR and TDR measurements, dotted line represents Topp’s model, and solid line is a third-degree polynomial equation fitted to GPR measurements.

Figure 6.6. Electric conductivity as a function of the water content. Left-handed figure represents, in comparison with TDR measurements, the electric conductivity $\sigma_{1GHz}$ (see equation (6.4)). Right-handed figure represents the estimated frequency dependence of the electric conductivity for GPR measurements.
6.4. Results and Discussion

instead of frequency dispersion. As shown by Lambot et al. [2003c], the electric conductivity is less sensitive compared to the dielectric constant, resulting in a higher uncertainty for its estimation, and a higher sensitivity toward measurement and modeling errors (instability).

The frequency dependence functions $\sigma(f)$ shown in Figure 6.6 indicates that frequency dispersion increases with the water content level. For WC9 for instance, the apparent electric conductivity is multiplied by more than 10 between 1 GHz and 2 GHz. This is due to the out of phase polarization component $\omega\varepsilon''$ in equation (4.14) denoting polar relaxation phenomenon. These results are in accordance with the systematic lower values of the GPR derived dielectric constant compared to TDR for the highest water content levels.

6.4.4 Sensitivity analysis

In order to investigate the relation between the accuracy of the GPR derived material properties and the accuracy of the modeled Green’s function, we performed a sensitivity analysis. A synthetic Green’s function was generated for a configuration similar to the WC2 scenario. Then we added errors to the synthetic data and performed inversions to estimate back the original electromagnetic parameters, whose true values are known exactly. To be realistic, we considered the error observed for the WC2 case. Then we defined the relative response error ($RRE$) as the ratio between the added error and the error observed for the actual WC2 case. We considered $RRE$ ranging from 0 to 3, to represent all error levels observed for the nine laboratory experiments.

Results are presented in Figure 6.7. We can observe, as expected, that the absolute error on the inversely estimated dielectric constant, $\Delta\varepsilon'_r$, remains negligible, even for $RRE = 3$. This means that the proposed model is sufficiently accurate so as to estimate this property with a very good accuracy. In contrast, the electric conductivity is less stable toward measurement and modeling errors and $RRE$ values ranging from 1 to 3 lead to absolute errors $\Delta\sigma_{1GHz}$ of about $1.5 \times 10^{-3}$ Sm$^{-1}$ to $5 \times 10^{-3}$ Sm$^{-1}$, as effectively observed in Figure 6.7 for the real experiments.

It is worth noting the linear behavior of the sensitivity functions in Figure 6.7. This illustrates the good stability properties of the inverse solution, i.e., the solution depends continuously on the error on the response function. Let’s note that no error on $G_{z,x}$ leads to no error on the estimated parameters, which demonstrates the uniqueness of the solution. To get the same accuracy as for TDR, we still have to reduce measurement and modeling errors by a factor 10. As aforementioned, this may partly be achieved by characterizing the antenna properties in an anechoic chamber, and by performing measurements in absence of extraneous backscatters. But also, some underlying forward model assumptions may also be questioned.
Chapter 6. Accurate modeling of GPR signal

Figure 6.7. Absolute parameter estimation error as a function of the relative response error (RRE) on the Green function.

6.5 Summary and Conclusions

The only way to take up the challenge of mapping quantitatively both dielectric and electric profiles using GPR is to resort to inverse modeling, since in this case, the entirety of the information contained in the GPR signal is utilized. However, the success of the method relies heavily on the accuracy with which the forward model represents the actual GPR-subsurface system.

In the follow-up of the works reported by Lambot et al. [2003c, e], this study tackles the issue of the forward model. This last is improved by considering additional mechanisms that were not initially accounted for, namely, the multiple wave reflections occurring between the antenna and the soil surface, and the frequency dependence of the electric conductivity. The antenna-subsurface ringing was modeled by adding a positive feedback loop in the antenna block diagram, and dispersion was described by a local linear approximation of the Debye model. We validated the improved model in laboratory conditions for a two-layered sand subject to different water contents. We also used a linear polarized double ridged broadband TEM horn antenna with a higher gain to have a better signal-to-noise ratio.

The description of the radar signal was significantly improved when considering these additional phenomena. Both amplitude and phase of the radar signal are now accurately modeled. This resulted in an accurate estimation of the soil dielectric permittivity, and in a significantly better estimation of the electric conductivity. A sensitivity analysis led to the conclusion that the clutter level still has to be decreased by a factor 10 to enable an accurate estimation of the electric conductivity. This may be achieved by taking care to minimize the effect of ambiguous clutter from extraneous object scattering, and by improving the forward model, particularly concerning the antenna. Results pointed out the importance of considering the frequency dependence of
the electric conductivity, which is significant at high water content levels. To a lesser extent, we observed also a slight frequency dependence of the dielectric permittivity.
Chapter 7

Measuring the water retention curve of a sandy soil using an off-ground monostatic GPR

Abstract In the follow-up of the works reported by Lambot et al. [2003c, d], we explore the possibility of measuring a continuous soil moisture profile from the inversion of ground penetrating radar (GPR) signal. Hypothetical experiments were conducted to demonstrate the well-posedness of the inverse problem for the specific case of identifying a soil moisture profile in hydrostatic equilibrium with a water table. In this case, the profile agrees with the water retention curve of the soil. The analysis subsequently extends to an actual case study in controlled outdoor conditions on a large tank filled with sand. Encouraging results were obtained since the soil moisture profile in the sand was relatively well estimated. However, the inverse solution suffers from a lack of stability since the operating frequency range of the used radar (800-4000 MHz) was not appropriate. Even for shallow investigations (0-70 cm), very low frequencies (50-250 MHz) would have been required for an accurate and reliable characterization of such a profile. Nevertheless, high frequencies allowed for an accurate estimation of the surface (0-30 cm) soil moisture, which rises particularly promising perspectives of GPR in agricultural and humanitarian demining applications.

Chapter 7. Measuring the water retention curve using GPR

7.1 Model Configuration

In this study, the dielectric properties vary continuously with depth. A continuous dielectric profile can be obtained by considering layers with $h_n \to 0$ in Figure 4.5 (page 72). The sand is subject to an hydrostatic equilibrium with a water table, and consequently, the dielectric profile agree with the water retention curve, since the dielectric permittivity is directly related to the water content [Topp et al., 1980]. The water retention curve of the sand is assumed to be described by the well-known van Genuchten model [van Genuchten, 1980]:

$$\theta(h) = \theta_r + (\theta_s - \theta_r) \left[1 + |\alpha h|^n\right]^{-m}$$

(7.1)

where $\theta_r$ and $\theta_s$ are, respectively, the residual and saturated water content ($L^3 L^{-3}$); $\alpha (L^{-1})$ and $n (-)$ are curve shape parameters which are, respectively, inversely related to the air entry value and the width of the pore size distribution; $m = 1 - 1/n (-)$ is restricted by Mualem’s condition with $n > 1$; and $h$ is the pressure head. Note that in hydrostatic equilibrium, the pressure head is related to the depth $z$ by $|h| = z_w - z$, where $z_w$ is the depth of the water table.

Since the relations between the volumetric water content of the sand, the dielectric permittivity, and the electric conductivity are monotonic and almost linearly increasing [Topp et al., 1980; Rhoades et al., 1990], the dielectric profile can be described using a similar equation to the van Genuchten model, that is, we define

$$\varepsilon_r'(h) = \varepsilon_{r,r}' + (\varepsilon_{r,s}' - \varepsilon_{r,r}') \left[1 + |\alpha h|^n\right]^{-m}$$

(7.2)

where $\varepsilon_{r,r}'$ and $\varepsilon_{r,s}'$ are, respectively, the dielectric constant of the dry and water saturated soil, and $\alpha (L^{-1})$, $n (-)$, and $m = 1 - 1/n (-)$ are curve shape parameters.

Similarly, the electric conductivity profile can be defined as

$$\sigma(h) = \sigma_r + (\sigma_s - \sigma_r) \left[1 + |\alpha h|^n\right]^{-m}$$

(7.3)

where $\sigma_r$ and $\sigma_s$ are, respectively, the electric conductivity of the dry and water saturated soil, and $\alpha (L^{-1})$, $n (-)$, and $m = 1 - 1/n (-)$ are curve shape parameters.

In this study, the magnetic permeability $\mu$ is equal to the magnetic permeability of free space $\mu_0$. The thickness of the layers in the model configuration (Figure 4.5) is set to 1 cm. It can be shown that a finer resolution is not required for frequencies lower than about 3.5 GHz (results not presented). Given the large number of layers in the configuration model, evaluation of the Green function is computationally time consuming (about 3 minutes for 301 frequencies and 67 layers on a Pentium 1400 GHz). It is therefore important to limit
the number of parameters to be optimized in the inversion process. Parameters $\varepsilon'_{r,r}$ and $\varepsilon'_{r,s}$ were determined, respectively, from the dry and saturated water contents using the sand specific petrophysical relation established in the study of Lambot et al. [2003d] for GPR (see Figure 6.5, page 114). This relation yields:

$$\varepsilon'_{r} = 63.05 \theta^2 + 23.88 \theta + 2.37$$  \hspace{1cm} (7.4)

Parameter $\sigma_r$ is fixed to zero. Parameters $\alpha$ and $n$ in (7.2) and (7.3) are assumed to be the same. This approximation is expected to be valid given the link between both properties, and should not result in large estimation errors since, as shown in Lambot et al. [2003d], the Green function is very much less sensitive to the electric conductivity than to the dielectric permittivity.

It is well known that in the operating frequency range of GPR, soil materials can exhibit significant dispersive properties, i.e., the complex effective dielectric permittivity of the soil is function of frequency [Hipp, 1974; Hallikainen et al., 1985; Heimovaara et al., 1996; Teixeira et al., 1998]. In the frequency range of interest (0.8-1.8 GHz), Lambot et al. [2003d] observed that the dielectric constant of the sand was almost independent of the frequency, whereas the electric conductivity showed a clear frequency dependence. Since we focus mainly in estimating the dielectric profile, we consider in this study an effective electric conductivity independent of the frequency.

Given the forward model and its parameterization, model inversion consists in finding the parameter vector $\mathbf{b} = [\alpha, n, \sigma_s]$ so that objective function (5.1) is minimized.

### 7.2 Numerical Experiments

For analyzing the well-posedness of the inverse problem dealt with in this study, synthetic Green’s functions were generated for five different scenarios. The benefit of this numerical approach is that the true parameter values are known and that the response function is perfectly described by the electromagnetic model. The hypothetical dielectric profiles are represented in Figure 7.1, as well as the corresponding Green’s functions, and cover a large range of possible cases. A realistic electric profile (not presented) has been determined from the dielectric profile using Rhoades’ model [Rhoades et al., 1976]

$$\sigma(\theta) = (a\theta^2 + b\theta)\sigma_w + \sigma_r$$  \hspace{1cm} (7.5)

where $\theta$ is the water content (m$^3$ m$^{-3}$), $\sigma_w$ is the soil solution electric conductivity (S/m), $\sigma_r$ is the electric conductivity of dry soil (S/m), and $a$ and $b$ are soil specific empirical parameters. We took $a = 1.85$, $b = 3.85 \times 10^{-2}$.
Chapter 7. Measuring the water retention curve using GPR

Figure 7.1. Dielectric profiles (left) pertaining to the five synthetic scenarios, \( z \) being the depth and \( \varepsilon_r' \) being the dielectric constant, and corresponding Green’s functions (right).

\[
\sigma_w = 0.075 \text{ S/m, and } \sigma_r = 5.89 \times 10^{-4} \text{ S/m, which are typical values for sandy soils [Amente et al., 2000]. The water content in (7.5) was determined from the dielectric constant using Topp’s model [Topp et al., 1980]. Inversions were performed considering the frequency range 0.8-1.8 GHz with a frequency step of 8 MHz. The lower frequency corresponds to the lower cut-off frequency of the radar system used in this study.}
\]

Figure 7.2 represents the objective functions pertaining to scenarios S2, S3, S4, and S5 (S1 leads to similar results). The considered parameter space includes simultaneously all scenarios and has been divided into 100 discrete values, resulting in 10000 objective function calculations for each contour plot. A star represents the known global minimum of the objective function, which corresponds in every case exactly to the solution obtained by inversion of the synthetic Green functions using GMCS-NMS. These results demonstrate the identifiability of the model parameters and the uniqueness of the inverse solution for this model configuration. That means that sufficient information is theoretically contained in the Green function to estimate the dielectric profile. Parameters \( \alpha \) and \( n \) are generally negatively correlated. For S2, S4, and S5 scenarios, the model is less sensitive to \( n \) than to \( \alpha \), in contrast to scenario S3. The presence of local minimum regions in the objective functions imposes the use of a global optimization approach.

It is worth noting that the amplitude and phase of the Green’s functions represented in Figure 7.1 are not very much different for some scenarios. That means that the inverse problem may suffer from a lack of stability when subject to measurements and modeling errors. Moreover their frequency dependence is almost linear in this frequency range. This indicates that most of the information in the Green’s function arise from a single reflector, namely, the air-subsurface interface.
7.3 Outdoor Experiment

7.3.1 Description

From a mathematical point of view, the objective of the outdoor experiment was to investigate the stability properties of the inverse problem, i.e., the sensitivity of the inverse solution in relation to actual modeling and measurement errors. Outdoor experiments were conducted at the TNO facilities in Den Haag (The Netherlands). Measurements were performed on a 1.5 m deep and 3 m × 10 m area tank filled with sand. The benefit of this outdoor test site, compared to laboratory conditions, is that there is no metallic and a few non-metallic objects in the surroundings of the tank, minimizing by this way ambiguous clutter from extraneous object scattering. Moreover, the dimensions of the tank make the approximation of an infinite horizontally multilayered medium much more realistic, compared to laboratory scale experiments.

The sand was subject to a hydrostatic equilibrium with a water table imposed at 67 cm depth. Evaporation was prevented using a plastic sheet set up at the soil surface. The saturated zone extended from 150 cm depth to 67 cm.
depth. Given the operating frequency range, the saturated zone constituted the lower half space in the electromagnetic model, since electromagnetic waves are expected to be completely absorbed in this layer. The experimental conditions at the TNO are closely representative of field conditions in partially saturated sandy soils.

The antenna system consisted in a linear polarized double ridged broadband TEM horn (BBHA 9120 A, Schwarzebeck Mess-Elektronik). Antenna dimensions are 22 cm length and 14 cm × 24 cm aperture area. Its nominal frequency range is 0.8-5 GHz. Parameter $S_{11}$ was measured sequentially at 1601 stepped operating frequencies over the range 0.8-4 GHz with a frequency step of 2 MHz. However, only the range 0.8-1.8 GHz with a frequency step of 8 MHz was used for the inversions. The frequency response functions $H_i(\omega)$, $H(\omega)$, and $H_f(\omega)$ of the antenna were determined as described in Lambot et al. [2003d], by performing $S_{11}$ measurements in free space conditions (with the antenna oriented toward the sky) and at two different heights above a metal sheet.

Subsequently to the radar measurements, 300 cm$^3$ soil samples were collected along the soil profile for determining the actual volumetric water content by means of the standard oven-drying method at 105 °C. Given the hydrostatic equilibrium, the water profile corresponds to the water retention curve of the sand.

### 7.3.2 Results and discussions

Figure 7.3 represents the GPR derived and directly measured water retention curves of the sand, which agree fairly. The GPR derived water content has been computed from the dielectric constant using the sand specific relation represented in Figure 6.5 (page 114). The larger discrepancies, as high as about 0.05 m$^3$m$^{-3}$, are observed in the middle of the profile. For the lower pressure heads, as expected, the curves fit well, since the saturated dielectric constant is assumed to be known and is a fixed parameter. The water content is also well estimated for the higher pressure heads, which correspond to the shallowest 30 cm of the sand. Errors are inferior to 0.025 m$^3$m$^{-3}$. This stems from the fact that most of the information contained in the observed Green function originates from the reflection at the air-sand interface. This is expressed in Figure 7.4 representing the observed and modeled Green function, in both the frequency and time domains. The linear behavior of both the amplitude and phase of the frequency domain Green function signifies that the soil surface is by far the main reflector. This was also observed for the numerical experiments and is confirmed by the time domain representation of the Green function, for which a linear time gain has been applied to make more apparent the possible reflections arising later in time.
7.3. Outdoor Experiment

![Water retention curve (WRC) of the sand. The dash line represents van Genuchten’s model fitted to the ground truth data.](image)

Significant differences are observed between the measured and modeled Green functions. They may originate from different error sources: (i) the different hypothesis underlying the electromagnetic antenna and subsurface models, (ii) the characterization of the antenna frequency response functions, (iii) the fact that the actual dielectric profile is not as continuous as assumed, due to the inherent presence of heterogeneities in the sand tank, and (iv) the presence of ambiguous clutter. In the study of Lambot et al. [2003d], it was shown that the model was very accurate for describing the radar signal. Only some improvements were required to enhance the estimation of the electric conductivity. In the present study, results are less satisfactory, especially for the modeling of the Green function pertaining to the metal sheet measurements used for the characterization of the antenna properties (not presented). This may stem from the different antenna used in this study, which is also a linear polarized double ridged broadband TEM horn, but with a different lower cut-off frequency (800 MHz instead of 1000 MHz) in order to obtain more information from deeper in the subsurface. It is possible that the antenna model is less appropriate for this antenna. Also, the presence of ambiguous clutter at the TNO facilities may also account for the observed discrepancies.

Discontinuities in the subsurface properties are also clearly present. This is expressed by the oscillatory behavior of the error in the frequency domain Green function (see Figure 7.4) which is typical of two- or three-layered media. This is further apparent in the time domain representation of the Green function. A reflection occur just under the air-soil interface. This discontinuity...
Chapter 7. Measuring the water retention curve using GPR

Figure 7.4. Measured and modeled Green’s function represented in both the frequency domain (left) and the time domain (right).

is also apparent in Figure 7.3 for the gravimetric measurements. Reflections arising later in time may be attributed to errors in the antenna frequency response functions and ambiguous clutter.

Figure 7.5 represents the modeled Green function in a lower frequency range (50-800 MHz). Oscillations are now visible and indicate that this is the part of the spectrum that really contains the information from the zone between the water table and the soil surface. The shape of the dielectric profile dealt with in this study and the presence of saturating water lead to strong attenuation of the high frequencies, even in a low electrically conductive sandy soil and for shallow investigations (0-67 cm).

7.4 Summary and Conclusions

This chapter tackles the issue of estimating a continuous dielectric profile in soil using GPR. In particular, we investigate the feasibility of measuring a dielectric profile in a sandy soil in hydrostatic equilibrium with a water table. In this case, the dielectric profile corresponds to the water retention curve of the sand. Compared to other existing GPR characterization methods, the benefit of the adopted approach is that information from the ground is obtained from a single GPR measurement with a monostatic antenna to be used off-ground. This ensures a high degree of mobility which is necessary for low-cost, rapid, and high resolution mapping of the subsurface hydrologic properties.

As shown with the synthetic examples in this study, the radar signal contains sufficient information so as to estimate with uniqueness such a continuous dielectric profile. The outdoor experiment demonstrated however that the inverse solution may not be stable when the operating frequency range is too high. The reason is that such dielectric profiles attenuate very much high frequen-
cies. This is why the presence of water renders generally poor GPR results [Vandenberghhe and Overmeeren, 1999]. Although we deal in this study with the shallow 0-70 cm subsurface, frequencies as low as 50 to 250 MHz would have been required. Further research will focus on the joint use of low and high frequency antennae for estimating moisture content of shallow subsurface systems.

Nevertheless, the estimation of the water retention curve of the sand was fairly good. This is because a priori knowledge on the profile was assumed, that is, the depth of the water table and the dielectric properties of the saturated sand were assumed to be known. It is worth noting that the used operating frequency range (800-1800 MHz) allowed for an accurate estimation of the shallowest 30 cm of the soil. This rises interesting perspectives in mapping the shallow subsurface, which is particularly relevant in the calibration of methods that use satellite images to map the surface soil moisture, as well as in humanitarian demining applications.

Figure 7.5. Modeled Green’s function in the frequency range 50-800 MHz.
Chapter 8

Summary, conclusions, and perspectives

8.1 Hydrodynamic Inversion

Hydrodynamic inverse modeling is the only way to allow for a field scale effective characterization of the unsaturated soil hydraulic properties. Further, using only water content data as input in the inversion is attractive since this variable is obtainable using remote sensing techniques. Indeed, it is highly correlated to the dielectric permittivity, which governs electromagnetic wave propagation velocity.

In chapter 2 [Lambot et al., 2002], we proposed a new inverse modeling procedure which is based on this idea. Hydraulic parameters are estimated from soil moisture time series monitored at different depths during a natural infiltration event subject to in-situ boundary conditions. A sensitivity analysis allowed to design the location of the water content monitoring sensors in an optimal way. Then, we demonstrated carefully the well-posedness of the given inverse problem. In particular, we showed theoretically using synthetic numerical experiments that soil moisture time series constitute enough information so as to ensure a unique solution of the inverse problem. We showed subsequently that hydraulic parameters can still accurately be determined if reasonable and plausible measurement errors on the water content data are present.

In this chapter, emphasis was given to the optimization of the objective function in the inversion procedure. Formulated by the classical least squares problem, the objective function is minimized using the advanced Global Multi-level Coordinate Search algorithm (GMCS) [Huyer and Neumaier, 1999] that we combined sequentially with the classical Nelder-Mead Simplex algorithm (NMS) [Lagarias et al., 1998]. We have introduced this optimization method in the area of unsaturated zone hydrology since it is suited for solving accurately and efficiently complex nonlinear problems. Actually, the objective functions encountered in hydrodynamic inverse modeling are inherently characterized by a relatively complex topography including many local minima and discontinuities. In this case the classically used gradient based optimization methods are not appropriate.
The GMCS algorithm is an intermediate between purely heuristic and stochastic optimization methods. In contrast to purely heuristic methods, like Genetic algorithms for instance, the convergence of GMCS toward the global minimum is ensured if the user defined maximum number of iterations is sufficiently large. Unlike many stochastic methods that operate only at the global level and are therefore quite slow, GMCS contains local enhancements that lead to quick convergence once the global part of the algorithm has found a point in the basin of attraction of the global minimum. The combination GMCS-NMS allows for a faster convergence towards the solution. We showed using the synthetic scenarios that the combination GMCS-NMS was strongly competitive compared to GMCS alone, NMS alone, as well as compared to a Genethic algorithm. We used the same optimization approach in the inversions of the electromagnetic model as well.

The inverse identification of soil hydraulic properties was further tested on real data. In this case, measurement errors are lumped with modeling errors, which are often hard to quantify, and the inverse problem may suffer from instability. In chapter 3 [Lambot et al., 2003a], we evaluated the overall inverse modeling procedure using the flow observed under laboratory conditions. Laboratory infiltration experiments were conducted on four different soil columns, including an artificial homogeneous sand and three undisturbed agricultural soils collected in the experimental fields of the Agricultural Research Center of Gembloux (Belgium). Soil moisture was monitored using time domain reflectometry (TDR). To avoid the flaw of an inappropriate forward model parameterization, we used three different models for describing the water retention curve and the hydraulic conductivity function, namely, the Mualem-van Genuchten model [Mualem, 1976; van Genuchten, 1980], Assouline’s model [Assouline et al., 1998; Assouline, 2001], and the decoupled van Genuchten-Brooks and Corey combination [Fuentes et al., 1992].

All three models produced similar results. The inversely estimated water retention curves, as well as the saturated conductivity, agreed relatively well with the hydraulic properties obtained by the traditional direct methods. The saturated conductivity was largely overestimated in one case, since the explored moisture range was too small. Water content times series were very well modeled for the homogeneous sand and a sandy loam, but results were less satisfactory for two more structured silt loam soils. It is worth noting that water transfer prediction based on the directly measured hydraulic properties led in every case to very large errors. The major part of the observed discrepancies was partly attributed to the different scales of characterization, and to some extent to conceptual limitations in the forward transport model, which does not consider hysteresis, air entrapment, preferential flow, and all heterogeneities inherent to agricultural soils.

In particular, issues were encountered to characterize the initial conditions
8.2 Ground Penetrating Radar and Electromagnetic Inversion

In the flow model. Since TDR returns only point values for the water content, it was necessary to characterize the initial conditions in terms of pressure head. In this case, when an hydrostatic equilibrium is reached, initial conditions for the entire profile can be obtained easily and accurately from point pressure head measurements using linear interpolation and extrapolation. That can not be done with the water content. The problem with pressure head, however, is that measurements are not possible in dry conditions for non-sandy soils.

To mitigate to this, we propose investigating in future ways to use water content profiles as initialization in the inverse procedure. An entire water content profile is potentially available from ground penetrating radar (GPR) measurements (see Chapter 7). Provided that the flow models describe adequately the hydrodynamic behavior of soils, we can therefore conclude that the proposed inversion method is promising for identifying the effective subsurface unsaturated hydraulic properties at the field scale using remote sensing.

8.2 Ground Penetrating Radar and Electromagnetic Inversion

Traditionally used GPR systems and signal analysis methods suffer from a series of drawbacks since dielectric profiles are only obtainable using a number of measurements for a single profile characterization, and the antennae must be in contact with the ground, or descended in separated wells. Moreover, only the dielectric permittivity is generally measured. The only way to take up these restrictions is to resort to inverse modeling, since in this case, the entirety of the information contained in the GPR signal is utilized.

In chapter 4 [Lambot et al., 2003e], we proposed a new integrated approach to allow for such a characterization. The GPR system consists in an ultrawide band (UWB) stepped frequency continuous wave (SFCW) radar combined with a TEM horn antenna to be used off-ground in monostatic mode, thereby ensuring a high degree of mobility. This radar configuration allows further for an efficient, accurate, and purely conceptual mathematical description of the system, which enables the use of advanced inverse modeling techniques to identify the ground parameters. Additionally, in contrast to the commonly used time domain systems, an UWB may be covered, and consequently, more information from the ground can be obtained.

We developed a simple model to relate the radar measurements to the response of the ground. It describes the antenna which is viewed as a filtering convolution operator. It consists in a linear system composed of elementary model components in series and parallel, accounting each for a specific electromagnetic propagation phenomenon. Then, given the off-ground monostatic mode, we model realistically and in an effective way the subsurface by means
Chapter 8. Summary, conclusions, and perspectives

of a three-dimensional horizontally multilayered medium, for which we derived the exact solution of Maxwell’s equations, namely, the Green’s function referred as to the ground response.

In chapter 5 [Lambot et al., 2003c], we examined the theoretical feasibility of identifying subsurface parameters by inverting synthetic Green’s functions. After conclusive results, we tested the overall approach under controlled laboratory conditions for a single sand layer subject to different water content levels. An SFCW radar system was implemented using a vector network analyzer (VNA). We obtained accurate results for the estimation of the dielectric permittivity. Using a soil specific calibration, the standard deviation of the error on water content prediction was equal to 0.0036 m^3 m^{-3}. Yet, the electric conductivity was not well estimated. This was attributed to the fact that the forward model did not describe very well the amplitude of the Green function. Only the phase, related to the wave propagation velocity, was well modeled.

In view of this, we improved the antenna model, and we further accounted for the frequency dependence of the electric conductivity in the subsurface model [Lambot et al., 2003d] (Chapter 6). We included in the antenna block diagram the effect of the multiple reflections occurring between the soil surface and the antenna. By doing this, results were significantly improved, and the modeled and measured complex Green functions agreed closely, even for a more complex two-layered configuration. The electric conductivity was more accurately determined, but still important differences compared to TDR were observed. It was mainly attributed to the ambiguous clutter of extraneous object scattering in the laboratory.

In chapter 7 [Lambot et al., 2003b], we extended the method for estimating a continuously variable dielectric profile. We analyzed the specific case of a sandy soil in hydrostatic equilibrium with a water table. In this case, the dielectric profile corresponds to the water retention curve of the sand. We showed through synthetic examples that the radar signal may contain sufficient information so as to estimate with uniqueness such a continuous dielectric profile. An outdoor experiment demonstrated however that the inverse solution may not be stable when the operating frequency range is too high. The reason is that such dielectric profiles attenuate very much high frequencies. Hence, the presence of water reduces the performance of GPR soundings. Although we deal in this study with the shallow 0-70 cm subsurface, frequencies as low as 50 to 250 MHz would have been required. Nevertheless, the water retention curve of the sand was fairly well estimated since prior information on the depth of the water table and its dielectric permittivity was introduced. It is worth noting that the used operating frequency range (800-1800 MHz) allowed for an accurate estimation of the shallowest 30 cm of the soil, with a negligible sensitivity to deeper depths. This rises interesting perspectives in mapping the shallow subsurface, which is particularly relevant in the calibration of methods that use
satellite images to map the surface soil moisture, as well as in humanitarian demining applications.

Clearly, the developed GPR based approach for hydraulic characterization of soil constitutes a valuable alternative to the commonly used GPR methods. The most important advance is that we have a purely conceptual model which emulates remarkably well the radar-antenna-subsurface system. Henceforth, it is already usable in controlled laboratory conditions for characterizing material properties. Moreover, the new antenna model may already be used in field applications to analyze properly the radar signal. Yet this research limits to the development of some new concepts that have to be progressively improved and validated in conditions closer to the reality. In particular, more research is needed to further investigate the effects of realistic complications, such as more complex dielectric profiles, topographic roughness of the air-soil interface, and stochastic heterogeneity of the electric material parameters in the subsurface. An important improvement to bring on to the system would be the used of an additional monostatic antenna to cover a wider frequency band, so as to obtain much more information from the ground.

Also, further efforts must be allocated to find the optimal tuning of the radar system, to upgrade the performances of the radar antenna, to improve the forward modeling of the radar-antenna-subsurface system, and finally, to optimize the inversion procedure to estimate more accurately and more effectively the soil functional properties. A better theoretical understanding of the relationships between functional agronomic and environmental variables, referred to as petrophysical relations, and the measured dielectric properties is also required to enable valuable applications.

8.3 Further Perspectives

The synthetic and laboratory scale studies presented in this thesis prove a valuable potential of GPR for practical applications. The GPR information processing flow chart as presented in Figure 1.3 (page 6) may constitute a unique tool in the field of agricultural and environmental engineering for characterizing the variability of the multiple soil properties. This flow chart can still be completed using additional sources of information that have to be integrated appropriately. For instance, electromagnetic induction may be included to improve the identification of the electric conductivity. Analyzing the GPR signal in the time domain may provide information on the subsurface stratigraphy (e.g., soil depth), which can be included in the electromagnetic model as well as in the hydrodynamic model. Weather conditions may give information on the shape of the dielectric profile, which can serve as a priori knowledge in the electromagnetic inversion. Measurements of the optical properties of crop
leaves combined with a GPR assessment of the electric conductivity of the soil solution may provide valuable information on the soil-plant nutrient status.

Actually, this fundamental research can not yet provide information regarding the achievable performances, in terms of accuracy, of the proposed GPR sensing method for field conditions. For instance, they will depend, among many other factors, on the effect of soil roughness or the presence of plants. The absence of strong reflectors (dielectric interfaces) may also reduce the performances, in particular to identify a continuous dielectric profile. Accuracy issues and requirements in precision agriculture or other domains are also not evident [e.g., Sudduth et al., 2001; Zhang et al., 2002]. It depends on the specific application, and on the sensitivity of the models that are used in relation to the errors on their inputs, i.e., the GPR derived data. For instance, in hydrodynamic inverse modeling (see Chapter 2), an error of $0.01 \text{ m}^3\text{m}^{-3}$ in the water content is completely acceptable for identifying accurately the subsurface hydraulic properties. Also, the accuracy requirements depend on the variability of the soil properties within a field. For instance, the electric conductivity map depicted in Figure 1.2 would require an accuracy of at least 0.01 S/m to be drawn. All these issues are far beyond the scope of this study which aims mainly at providing a new technology with the highest accuracy as possible, so that it can be used in a range of applications as wide as possible. For example, it could be used also to support humanitarian landmine identification [Lambot et al., 2003f].


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International Conferences

A. Oral presentations


B. Poster presentations


C. Contributions as co-author


About the author

Sébastien Lambot was born in Dinant, Belgium, on June 9, 1976. In 1999, he obtained a degree in Agricultural Engineering, with a specialization in Génie Rural, at the Faculty of Agricultural Sciences at the Université catholique de Louvain (UCL, Belgium). In 1998, he followed a one week training in Morocco on water management and irrigation systems. He realized his Master Thesis in relation to precision agriculture by developing an original system for spreading organic fertilizers with an optimized distribution within cropped fields. Supervised by Professor Benoit Raucent (Department of Mechanics, UCL), the project was conducted in collaboration with Agrimat s.a. (Belgium) and the Agronomic Research Center of Gembloux (Belgium). It was selected by the Commission "Machines et Produits” at the Mecanic Show 99 (Libramont, Belgium).

In 1999, he obtained a four years FRIA (Fonds pour la Recherche dans l’Industrie et l’Agriculture) PhD grant. He started his PhD research programme at the Department of Environmental Sciences and Land Use Planning at UCL under supervision of Professor Marnik Vanlooster. His PhD project aims at developing hydrogeophysical characterization techniques of soil using ground penetrating radar, thereby implementing an interdisciplinary fundamental research programme supporting applications in agricultural and environmental engineering, but also in geophysical engineering for humanitarian landmine detection.

During this project, he participated to a European Research and Development Project (Optidis, QLK5-1999-01238, Development of an optical detection system for diseases in field crops with a view to reduce pesticides by targeted application). Given the interdisciplinary nature of his research, cooperation was established with the Microwave Laboratory of UCL (Belgium), with the Royal Military Academy of Bruxelles (Belgium), which collaborated already within the frame of a humanitarian demining project (HUDEM), and finally with the Applied Earth Science department at the Delft University of Technology (TUDelft, The Netherlands). In 2002, he spent two months at TUDelft, under supervision of Dr. Evert Slob, to be trained and guided in the field of electromagnetic wave propagation in soils.

In 2003, he obtained a two year European Marie Curie Intra-European Fellowship (2004-2005) to pursue his research in the field of hydrogeophysics at TUDelft.