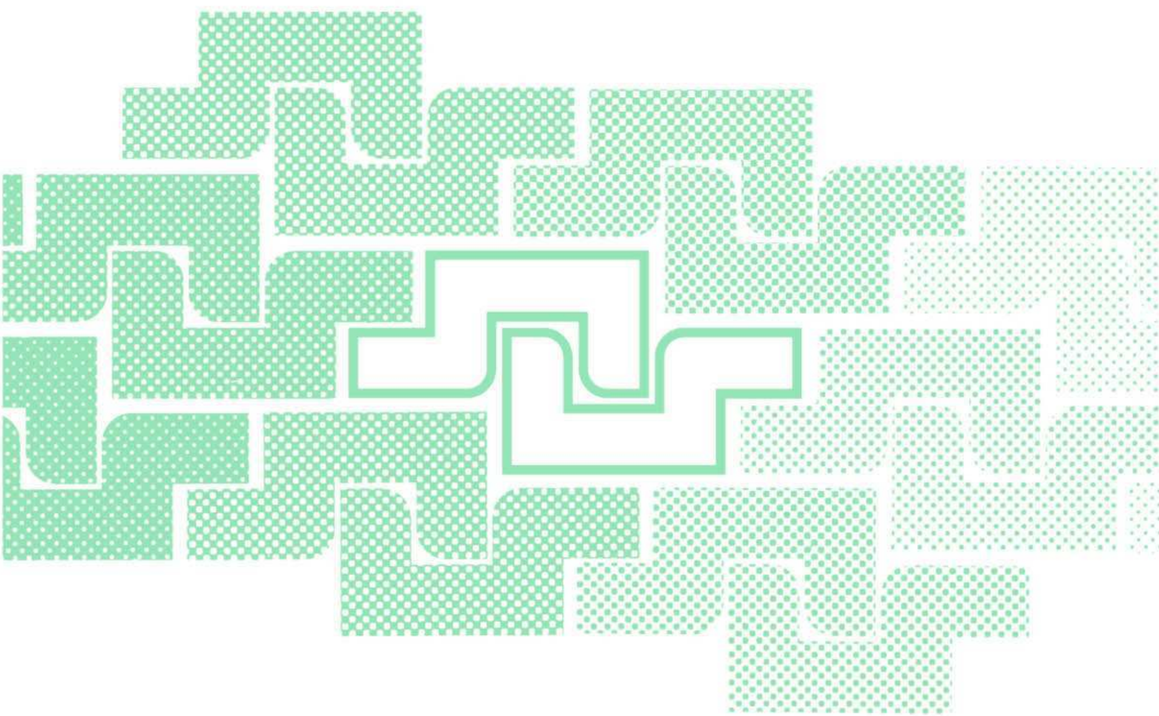

Applied Hydrogeophysics

Edited by

Harry Vereecken, Andrew Binley, Giorgio Cassiani,
André Revil and Konstantin Titov

NATO Science Series

IV. Earth and Environmental Sciences – Vol. 71

Applied Hydrogeophysics

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1. APPLIED HYDROGEOPHYSICS

Harry Vereecken, Andrew Binley, Giorgio Cassiani, Andre Revil,
and Konstantin Titov

1.1. Introduction

Soils and groundwater are important natural resources that sustain life on Earth. In the last century, the enormous expansion of industrial and agricultural activities has led to an increased environmental pressure on these systems. Soils and groundwater are extremely important because they yield much of our water resources and sustain food production for humanity. Agricultural activities consume nearly 80% of the fresh water used throughout the world, and the majority of this water is used for irrigation. In many countries aquifers are used as the major source of water for this purpose. Irrigation of cropland has greatly increased food production, but has also had some drawbacks due to the amount of water drawn from aquifers. Some of the major problems related with irrigation are excessive leaching of nutrients and pesticides, depletion of aquifers, ground subsidence, and soil salinization.

The vadose zone, being the subsurface environment between soil surface and groundwater, also serves as the repository for municipal, industrial and government waste. In Europe, more than 1.5 million sites are estimated to be potentially contaminated (EEA, 2000). These sites consist of military, industrial and waste disposal sites that are either abandoned or still under operation. The total number of identified sites that have been explicitly identified is about 21,000. The estimated total clean-up costs are at least in the order of 100 billion Euros.

As safe and effective use of the subsurface environment is a major challenge facing our society, there is a great need to improve our understanding of the shallow subsurface and the groundwater systems. As the subsurface is impossible to ‘observe’ directly, methods are needed to reveal its physical and hydrological properties, in addition to the hydrochemical characteristics of fluids stored and flowing through it. Traditional borehole-based sampling is often limited because of the localized knowledge often derived from such measurements and the disturbance induced to samples. As in the oil and mining industry, geophysical methods may offer a means of addressing this problem, by providing a spatially extensive, non-invasive means of investigating the subsurface. In the past, applications of geophysical methods in

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groundwater and vadose zone hydrology have mainly focused on mapping geological structures (e.g. clay/sand layers, bedrock valleys, etc), delineation of aquifer boundaries, mapping of fracture zones, etc. In summary, the focus has been for a long time on the "geometrical" characterization of the subsurface. For such purposes standard methods are presently available and well-documented in the literature.

Recently, increased attention has been given to the use of geophysical methods to derive parameters and state variables characterizing especially surface near groundwater systems and soils (Vereecken et al., 2002, 2004; Rubin and Hubbard, 2005). This approach has also similarities with the experience of the oil industry, having as an objective the "petrophysical" characterization of the subsurface. Research in this direction is mainly driven by the fact that geophysical methods allow continuous mapping in space and time of geophysical properties which can be transferred to parameters or variables characterizing the aquifer system (e.g. water content, porosity, flow velocity). Classical approaches like drilling and coring have shown their limitations in capturing this spatial and temporal variability. Characterizing spatial and temporal variability of aquifers is, however, a key factor determining e.g. success of water management strategies or predicting pollution risks to water supply systems.

Hydrogeophysical methods and approaches are presented in the recent book *Hydrogeophysics* edited by Yoram Rubin and Susan Hubbard (2005). That book is the first to deal explicitly with geophysical methods for hydrological and hydrogeological processes. It addresses in depth the fundamentals of hydrogeological characterization as well as the fundamentals of geophysical characterization. A series of case studies and emerging technologies in the field of hydrogeophysics are also presented.

In *Applied Hydrogeophysics* we follow up on the material presented in *Hydrogeophysics* but focus on the applications of hydrogeophysical methods to the understanding of hydrological processes and environmental problems dealing with the flow of water and the transport of contaminants. This book, unlike its predecessor, is therefore organized mainly in hydrological process-driven chapters, rather than in methodological chapters. We feel that this structure is suitable particularly to the understanding of the end user and the professionals that want to make use of the new hydrogeophysical techniques for their specific field of application. In addition, this structure gives a more pronounced practical touch to the book. Hence the title *Applied Hydrogeophysics*.

The book is the outcome of a successful NATO Advanced Research Workshop held in St. Petersburg, 25–29 July, 2004 entitled "Soils and groundwater contamination: Improved risk assessment based on integrated hydrogeological and geophysical methods." The objectives of the meeting were to critically evaluate the state of the art in hydrogeophysics for the assessment of risks related to soil/groundwater contamination, to promote the interaction between soil scientists, hydrologists, hydrogeologists and geophysicists from all over the world; and to identify goals for future research. Specific attention was given to the applications of hydrogeophysical methods and techniques to problems arising in the use and management of soil and groundwater systems.

In the following we present a brief summary of the context and content of the various chapters.

1.2. Brief Overview

The book is organised in 12 chapters. The chapter of Linde et al. (Chapter 2) discusses the choices that must be made in estimating hydrogeophyiscal parameters. The authors identify three different methods presently available in the literature: direct mapping, integration methods and joint inversion methods. Direct mapping refers to the transformation of a geophysical model into hydrogeological model. A typical example is the estimation of water content data using ground penetrating radar. In integration methods the geophysical inversion is performed independently from the hydrogeological data and it includes the well-known methods such as cokriging and Bayesian estimation. The joint inversion methods aim to simultaneously invert geophysical and hydrogeophysical data. In their chapter, Linde et al. present the state of the art cases for each of these three methods.

The chapter by Yeh et al. on the hydrogeophysical use of sequential successive linear estimator (SSLE) and electrical resistivity tomography (ERT) introduces the SSLE as a promising alternative procedure for the inversion of ERT measurements. The SSLE is a geostatistically based cokriging-like approach. However, unlike the classical cokriging, the SSLE is able to tackle the nonlinear relationship between electrical potentials and the electrical conductivity. After a description of the SSLE, several synthetic case studies and a field application using the SSLE are given. The examples show the ability of the SSLE to condition the inverse procedure by a priori knowledge about the structure of the electrical conductivity as well as independent point measurements of the electrical conductivity in the subsurface. As expected, the conditioning of the inverse procedure reduces the ill-posedness of the inverse problem and therefore enhances the quality of the inversion results. Furthermore the SSLE features a quantification of the estimate of the electrical conductivity that is essential for decision making based on inversion results.

The chapter by Cassiani and others on unsaturated zone processes presents the basic concepts of non-invasive determination and monitoring of the temporal and spatial variation of volumetric moisture content in soils under natural and experimental conditions. Knowledge of soil moisture dynamics and its spatial distribution is important in many hydrological processes such as soil water flow, infiltration, surface runoff, and soil evaporation. Moreover, soil water content and water flow play a critical role in a number of environmental processes such as soil and subsoil contamination, catchment hydrology, flood generation, slope stability, water resources and agricultural management. Typical measurements techniques of soil water content such as soil coring combined with gravimetric determination and time domain reflectometry (TDR) only provide local and spatial discontinuous information of soil moisture content and are often destructive and highly invasive. The authors illustrate in their chapter the value of ground-penetrating radar (GPR) and electrical resistivity tomography for investigating water flow and soil water content dynamics in a non-invasive and spatially distributed manner. In particular, the analysis of time lapse measurements, provides a means of determining vadose zone structural properties from dynamic hydrogeophysical signals. The authors present examples dealing with the use of cross-hole GPR and vertical radar profiling to monitor natural infiltration, and cross-hole monitoring of a tracer injection using GPR and ERT.

Chapter 5 (Kemna et al.) deals with the use of hydrogeophysical methods to characterize solute transport in soils and groundwater. It gives an outline of the conceptual and mathematical models that are generally used for the description and modelling of transport processes in porous media such as soils, aquifer sediment and karstic and fractured media. The relationship between the spatial and temporal moments of solute concentrations to transport parameters and heterogeneity of the hydraulic conductivity is outlined. The chapter focuses on hydrogeophysical approaches to characterize solute transport and solute mapping such as ERT, GPR and Radio-Magnetic Tellurics (RMT). Results are shown for a tracer monitoring experiment at the Krauthausen test site in Germany. At this site tracer tests with high and low conductive tracer solutions were performed to study the role of heterogeneity on solute transport. Applications of hydrogeophysical methods are also presented for the case of solute transport in fractured aquifers at various sites in the US, Switzerland and UK. For the unsaturated zone, applications of hydrogeophysical methods, such as cross-borehole radar tomography, high-resolution borehole resistivity and radar profiling are presented for studying the temporal dynamics and spatial variation of moisture content in a sandstone aquifer at a UK site. Finally, the chapter presents current developments and an outlook in the development and use of hydrogeophysical methods and techniques for improving our understanding of solute transport processes.

The chapter by Atekwana et al. (Chapter 6) presents research in a novel discipline aimed at understanding the impact of microbial activity and processes on geophysical properties of earth materials. The chapter demonstrates the effect of microbial activity on properties such as texture, surface area, pore size and pore geometry, tortuosity, cementation, formation factor and elastic moduli. In addition, chemical properties may be changed by microbial activity and that may lead to alteration of e.g. ionic strength, ionic charge density and ionic mobility of the fluid phase, leading to variations in electrical conductivity. The chapter presents results from laboratory experiments exploring microbe-sediment-geophysical relationships using direct current resistivity, induced polarization, self-potential and seismic methods. Examples of the applications of these geophysical methods to detect microbial activity are presented for different field sites that are contaminated with hydrocarbons.

French et al. present in Chapter 7 various examples of geophysical methods that have been used to characterize water flow and transport processes in the subsurface environments located in the cold regions of Russia, Norway and Switzerland. In permafrost areas, water supply and changes in mechanical properties due to changes in permafrost are major issues. Applications of electromagnetic sounding are presented for the case of leakage from frozen dams, the detection of taliks, cryopegs and ground ice at Yamal Peninsula, and saltwater injection into permafrost areas. Surface tomographic electrical resistivity methods are presented that allow the determination of infiltration and the characterization of solute transport. Studies on the drainage conditions beneath a glacier conducted with resistivity techniques are also disucssed. The authors address the difficulties encountered when applying these geophysical methods to characterize hydrological processes in cold regions. These problems are, for example, related to the grounding and calibration of geophysical measurements with respect to hydrological state variables, such as water content, but also to variations in temperature and phase transitions that may affect geophysical properties. A combination of all these elements may hamper the interpretation of geophysical measurements. The authors suggest that combining conventional methods with geophysical methods may overcome these problems.

Goldman and Kafri (Chapter 8) discuss the applications of time domain electromagnetic (TDEM) measurements for detecting the geometry and bulk resistivity of seawater intrusion into granular and carbonate coastal aquifers. Many of these aquifer systems are located in the Mediterranean coastal areas of southern Spain, southern France, Greece, the Adriatic coastal areas but also the southern Atlantic coast of the USA. The authors provide evidence that TDEM permits more reliable estimates of the porosity of those parts of the aquifers were saltwater has intruded. The method, however, requires calibration with respect to available hydrological data such as water levels, salinities and porosities.

In Chapter 9, Revil et al. discuss the theory and application of self-potential (SP) methods to environmental problems. The physics underlying the self-potential signals are associated with both ground water flow (streaming potential) and redox processes (electro-redox effect). The authors present various applications of the self-potential method, including the determination of hydraulic conductivity and storativity of aquifers using the electrical response during a pumping test, the monitoring of water flow in the vadose zone, the study of landslides, and the delineation of contaminant plumes in shallow aquifers. Recently, self-potential tomography (or electrography) methods have been developed, allowing imaging of subsurface properties. The inversion of self-potential signals is similar to that developed in medical imaging where electro-encephalographic signals are inverted to locate the source of epilepsy and electrophysiological activity of the brain.

Geophysical methods for investigating subsurface engineered barriers, used for containment and remediation, are presented in the Chapter 10 by Slater and Binley. These structures provide unique geophysical targets and are typically characterized by strong geophysical signatures associated either with the barrier itself, or the flow of liquids through them. The authors discuss the use of geophysical methods for the investigation of subsurface engineered containment structures (landfill liners/covers, waste tanks/storage ponds, containment barriers and caps) and flow through structures (permeable reactive barriers). Characterization and monitoring requirements are first introduced, followed by an in-depth analysis of the applicability of geophysical measurements for the following purposes: (1) verification that design specifications are met during installation; (2) characterization of variation in the physical properties of such barriers; (3) monitoring of liquids (leaks) through containment barriers; (4) evaluation and monitoring of geochemical processes occurring in flow through reactive barriers. Recent examples of the application of geophysical technologies to such studies of engineered barriers are presented. The authors present recommendations for future geophysical research on these unique targets.

In the chapter of Meju a consistent and process-based geoelectrical framework for the investigation of non-engineered landfill sites is presented. His approach is based on concepts derived from geotechnics and contaminant biogeochemistry and takes into account the complex geometry of landfill sites, the heterogeneous material composition and the attendant biogeochemical processes occurring in landfills. The main tenet of the approach is that geoelectrical response of landfill sites will vary in relation to significant changes in the chemistry of subsurface pore fluids and that these responses can be observed with hydrogeophysical methods such as electrical and electromagnetic methods (e.g. DC-resistivity techniques, Transient Electromagnetics (TEM) and Radio Magnetic Telluric soundings (RMT)). The chapter provides various interesting case studies that illustrate the various aspects of the proposed conceptual geoelectrical model as well as a discussion of emerging methods and challenges in the field of land-fill characterization.

In Chapter 12, Shestopalov et al. present data on groundwater contamination from Chernobyl-sourced radionuclides (^{137}Cs and ^{90}Sr) within the Chernobyl Exclusion Zone and Kyiv region. Measurable concentrations of these radioisotopes exist not only in the soil water and shallow groundwater, but also in regional aquifers down to a depth of 100 m and more. Experimental and modeling studies have shown that groundwater contamination mainly enters the upper aquifer by preferential pathways occurring at different scales. Depression-related vertical preferential flow zones occur widely in the floodplain terraces of the Dnieper and Ukrainian Polesye regions, and their role in the penetration of Chernobyl-sourced radionuclides through the soil-unsaturated zone into the aquifer system has been studied in detail. An experimental study of radionuclide distribution in deposits and groundwater also reveals the influence of other types of preferential flow zones on the total contamination in the geological environment. To account for the preferential flow zones it is necessary to obtain more reliable assessments of possible groundwater contamination and protectability. A new concept is proposed to assess groundwater protectability and vulnerability, based on a typology approach, using field experiment assessments and modeling. Application of this methodology enables maps to be drawn of groundwater protectability and vulnerability for ^{137}Cs within the Kyiv region of the Dnieper basin. The relative share of the input from depressions in the overall groundwater recharge and radionuclide contamination is assessed.

1.3. Outlook

Throughout *Applied Hydrogeophysics*, current limitations and future challenges are highlighted. Given the rapid development of the field of hydrogeophysics, we anticipate significant advances in the near future. The development of improved joint-inversion approaches will allow better constraints of hydrological models using geophysical methods; Chapters 2 and 3 point towards a number of such approaches. This will require comprehensive datasets containing both hydro-geological and geophysical information at high spatial and temporal resolution in order to develop and validate such approaches. The appreciation of links between biogeochemical and geophysical properties of the subsurface, as outlined in Chapter 6, has immense future potential for understanding groundwater contamination mechanisms, including the monitoring of contamination and remediation. Examples illustrated in Chapters 5, 7, 8, 10, 11 and 12 also illustrate how hydrogeophysics may offer new tools for monitoring subsurface processes, particularly for the determination of vulnerability of important groundwater resources. Methodological development, driven by the hydrological community, is likely to offer better tools for determining hydrological properties of the subsurface. Chapter 9 reveals how new approaches using self potential may give insight into water and chemical fluxes within the subsurface, i.e., quantities of direct value to the hydrologist. New methods, also targeting directly the hydrological processes and properties, such as surface magnetic resonance imaging, are advancing in their development and we anticipate exciting new findings in the near future.

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2. HYDROGEOPHYSICAL PARAMETER ESTIMATION APPROACHES FOR FIELD SCALE CHARACTERIZATION

Niklas Linde, Jinsong Chen, Michael B. Kowalsky, and Susan Hubbard

2.1. Introduction

The potential benefits of including geophysical data in hydrogeological site characterization have been stated numerous times (e.g. Ezzedine et al., 1999; Hubbard et al., 1999; Chen et al., 2001; Hubbard and Rubin, 2005). The principle reason for the growing interest in using geophysical methods in hydrogeological studies is that geophysics may provide spatially distributed models of physical properties in regions that are difficult to sample using conventional hydrological wellbore methods (e.g. Butler, 2005). The geophysical models often reveal more details compared with hydrogeological models derived from hydrogeological data, such as pump tests and observations of hydraulic heads. Furthermore, geophysical methods are less invasive compared with hydrogeological methods and they are comparatively cheap. Therefore, geophysical surveys can improve hydrogeological characterization if we could relate the geophysical and hydrogeological properties in an appropriate way. The added value of including geophysics in hydrogeological characterization has become increasingly accepted and several published case studies clearly show the worth of including geophysics for different applications and data types (e.g. see reviews by Hyndman and Tronicke, 2005; Goldman et al., 2005; Daniels et al., 2005). However, the success of a given hydrogeophysical case-study is dependent on many different factors and it is often difficult to develop an opinion a priori about the applicability of a method at another site or for another application. Here, we discuss some of the choices that need to be considered in a characterization effort and point out similarities and fundamental differences between different hydrogeophysical parameter estimation approaches presented in the literature.

The integration of hydrogeological and geophysical data sets is a complex process that often entails consideration of several different factors, such as:

- the measurement support volume is dependent on the characterization method;
- the models have space-varying resolution that depend on the data type, survey design, geological characteristics, and other factors;

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- the effects of measurement errors and simplified assumptions are difficult to assess;
- an infinite number of models can often explain a finite number of noisy data.

Because of non-uniqueness, we need to state a preference for a certain type of model (e.g. the smoothest, the least number of model parameters, etc.) and it is not always clear how this preference affect the outcome of an investigation. Our problem of hydrogeophysical parameter estimation is further complicated because relationships between geophysical and hydrogeological parameters are often:

- non-unique;
- poorly understood; and
- non-stationary.

Reviews of petrophysical relationships for hydrogeophysical investigations are given by Lesmes and Friedman (2005) and Pride (2005).

In Section 2.2, we discuss some critical choices that should be considered prior to the hydrogeophysical parameter estimation effort, such as: project objectives and available data (Section 2.2.1); model parameterization (Section 2.2.2); petrophysical relationships (Section 2.2.3); a priori information (Section 2.2.4); optimization or Monte Carlo methods (Section 2.2.5), objective functions (Section 2.2.6); and at which stage to establish the link between geophysics and hydrogeology (Section 2.2.7). We discuss three categories of hydrogeophysical parameter estimation, which we refer to as direct mapping (Section 2.3), integration methods (Section 2.4), and joint inversion methods (Section 2.5). We acknowledge that not all research falls cleanly into a single category. For example, McKenna and Poeter (1995) used a geostatistical indicator simulation to define zonation. Nonetheless, we find that this classification scheme is useful for the purposes of this review, and we give several case-studies to illustrate the merits and limitations of these categories (Section 2.3–2.5). We conclude this chapter with a summary and outlook discussion (Section 2.6).

We hope that this chapter will help the reader in considering the factors important for hydrogeophysical characterization, and in developing a hydrogeophysical parameter estimation approach for their specific problem of interest.

2.2. Critical Choices

Throughout this chapter we group available data into geophysical and hydrogeological data. These data are further grouped into measurements of system properties (e.g. permeability) and measurements of state variables (e.g. apparent resistivity, seismic travel-times, hydraulic head, and breakthrough times of tracer). Strictly speaking, measurements of system properties in hydrogeological site-characterization do not exist because these measurements are typically obtained by measuring other state variables from which an estimate is derived using a relationship that is valid under certain conditions (e.g. Butler, 2005). Rather, measurements of system properties denote estimates that have been made outside our estimation procedure and we must assume that they are known to a certain degree of accuracy.

2.2.1. PROJECT OBJECTIVES AND AVAILABLE DATA

The need for information about the structure of hydrogeological system properties occurs in many applications and at different scales. The objectives, site characteristics, and available geophysical and hydrogeological data vary on a case-by-case basis, and attempts to estimate hydrogeological system properties using geophysical data must take these characteristics into account. In this chapter, we consider these characteristics as given (e.g. we do not consider experimental design). Instead, we attempt to provide some guidance on how to formulate a hydrogeophysical parameter estimation method that matches specific objectives and provides a level of detail that can be resolved given the available data. In practice, other factors related to available budget, expertise, and computational facilities will be influential in determining the approach taken.

2.2.2. MODEL PARAMETERIZATION

Model parameterization depends on the research objectives and the available data. Regularization is a necessary step towards defining a well-posed inverse problem (e.g. Tikhonov and Arsenin, 1977). We must find ways to constrain model space in order to obtain meaningful results. We consider three approaches to model parameterization: zonation (e.g. Carrerra and Neuman, 1986a, b, c); geostatistical (e.g. Hoeksema and Kitanidis, 1984; Dagan, 1985); and Tikhonov regularization approaches (e.g. Tikhonov and Arsenin, 1977; Constable et al., 1987).

Zonation is used in applications where we assume that the earth can be divided into a number of zones where the variations of a property within the zones are small compared with the variations between the zones. Possible applications where a zonation approach could be justified are the delineation of sand from interbedded clay layers or sediments from the underlying bedrock. The advantage of the zonation approach is that the number of model parameters can be relatively small and smoothness constraints in the inversion may thus be avoided. Auken and Christensen (2004) demonstrated that this approach is preferable when mapping large-scale hydrogeological units in sedimentary environments using electrical methods. Such an approach also allows straightforward incorporation of borehole logs (Auken and Christensen, 2004). The zonation approach is probably the best approach when geological structure is apparent and formation boundaries are distinct (McLaughlin and Townley, 1996). However, the influence of the model parameterization is strong in zonation approaches and it might be difficult to reach conclusive results (e.g. Constable et al., 1987). Hydrogeological inversion codes that fall into this category are non-linear regression models such as the freely available UCODE (Hill, 1992) and MODFLOWP (Poeter and Hill, 1998), where regularization is imposed through model parameterization and/or by keeping certain model parameters fixed.

The geostatistical parameterization assumes that the parameter of interest is a spatial random variable with a certain correlation structure and sometimes a deterministic trend (e.g. Gómez-Hernández, 2005). This correlation structure typically includes a variance and integral scales that might vary in different directions (i.e., anisotropy). The geostatistical approach thereby decreases the number of effective parameters through spatial correlations and a known variance. A geostatistical parameterization is probably preferable when the parameters of interest vary in more or less random fashion and there is no clearly defined structure (McLaughlin and Townley, 1996).

The dominant approach to geophysical inversion is to use a fine grid discretization, where regularization is achieved through smoothing (i.e., finding the model that fits the data with minimum structure), damping (i.e., finding the model that fits the data and is the closest to an initial model) or a combination of smoothing and damping (Tikhonov and Arsenin, 1977; Maurer et al., 1998). Maurer et al. (1998) showed that a known mean and spatial correlation structure of a system property can be described by a combination of smoothing and damping; thereby, indicating a strong similarity between Tikhonov regularization approaches and geostatistics. However, the perspective is quite different. Tikhonov regularization is imposed to find a unique model (i.e., to make an ill-posed inverse problem well-posed). However, in geostatistical formulations the model covariance structure is honoured because it is assumed to describe real characteristics of the site. Damping has recently also been introduced in geostatistics (Kitanidis, 1999).

Our brief discussion on model parameterization shows that some understanding of the site characteristics is helpful in determining an appropriate model parameterization (e.g. Auken and Christensen, 2004). From this we can infer that the resulting models are not just determined by the data, but also by seemingly innocent choices of model parameterization and regularization.

2.2.3. THE PETROPHYSICAL RELATIONSHIP

How are geophysical and hydrogeological properties related? This is one of the most difficult questions in the efforts of hydrogeophysical parameter estimation. We should strive to choose a representation of the petrophysical relationship that reflects our understanding. This leads us to consider petrophysical relationships that are either:

- physically or empirically based;
- intrinsic or model-based;
- parameterizable or non-parameterizable;
- unique or non-unique; and
- stationary or non-stationary.

Below we briefly describe these petrophysical relationship characteristics. Since it is not within the scope of this chapter to provide detailed descriptions of physically based and empirical petrophysical relationships, the reader is referred to reviews given by Mavko et al. (1998), Lesmes and Friedman (2005), and references therein.

2.2.3.1. *Physically or Empirically Based Petrophysical Relationship*

Let us consider the problem of inferring water saturation in the vadose zone using radar data. In low loss material and for radar frequencies the EM wave velocity v (m/s) is related to the dielectric constant through (Davis and Annan, 1989):

$$v \approx \frac{c}{\sqrt{\kappa}}, \tag{1}$$

where c is the EM wave velocity in free space (3×10^8 m/s) and κ is the effective dielectric constant. An approximate value of the effective dielectric constant can be calculated using the so-called complex resistive index method (CRIM) (Tinga et al., 1973; Alharthi and Lange, 1987; Roth et al., 1990):

$$\kappa = \left[(1-\phi)\sqrt{\kappa_\mathrm{s}} + S_\mathrm{w}\phi\sqrt{\kappa_\mathrm{w}} + (1-S_\mathrm{w})\,\phi\sqrt{\kappa_\mathrm{a}}\right]^2, \tag{2}$$

where ϕ is porosity, S_w is water saturation, κ_s, κ_w, and κ_a are the dielectric constants for the solid, water, and air components of the soil, respectively. By combining Equations (1–2) we can estimate the water saturation if we have an estimate of porosity, radar velocity, and the permittivity of the earth material:

$$S_\mathrm{w} = \frac{\left(\frac{c}{v} + (\phi-1)\sqrt{\kappa_\mathrm{s}} - \phi\sqrt{\kappa_\mathrm{a}}\right)}{\phi\left(\sqrt{\kappa_\mathrm{w}} - \sqrt{\kappa_\mathrm{a}}\right)}. \tag{3}$$

Using a physically based approach, it is straightforward to relate uncertainties in the petrophysical models' parameters with uncertainties in the resulting models. As an example, we show confidence limits of water saturation for the

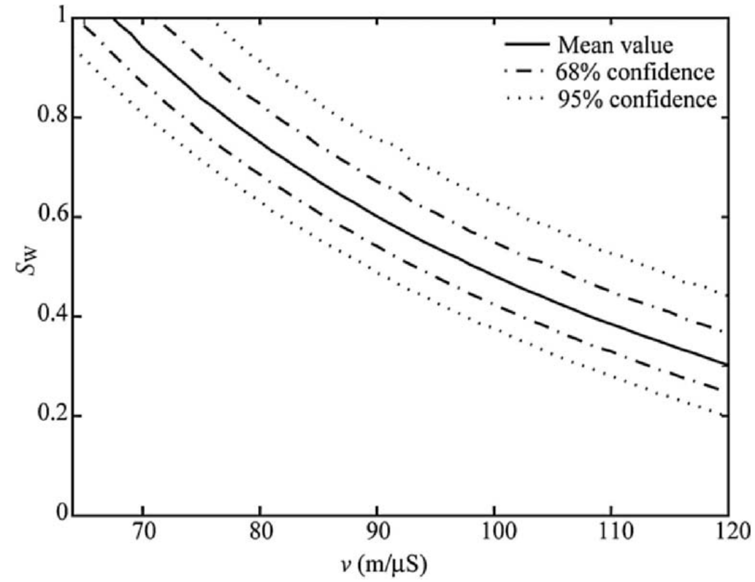

Figure 1. A petrophysical model between radar velocity υ and water saturation S_w based on the CRIM model. The resulting confidence intervals are shown assuming normally distributed random errors in the radar velocity, porosity, and the effective dielectric constant of the solid

case where it is assumed that κ_s, ϕ, and υ are normally distributed, where κ_s has a mean of 4 and a standard deviation of 1, ϕ has a mean of 0.35 and a standard deviation of 0.02, and that υ has a standard deviation of 1 m/µs (Figure 1). We see that substantial prediction errors in the estimation of saturation occur, even when parameters are well-defined and the structure of the petrophysical model is assumed to be known. For this example, the dominating cause of uncertainty is the uncertainty of κ_s.

Most often, we rely on semi-empirical relationships (such as Archie's law; Archie, 1942) or purely empirical relationships (such as a linear regression between log electrical conductivity and log permeability measurements; Purvance and Andricevic, 2000a). These relationships are much more difficult to work with because (1) we need to estimate a site-specific relationship and (2) we have limited understanding of the validity of this relationship away from the calibration points. However, this is often the only possibility and several successful case studies are given in the literature (e.g. Purvance and Andricevic, 2000b; Hubbard et al., 2001).

2.2.3.2. *Intrinsic or Model-Based Petrophysical Relationship*

We define the intrinsic petrophysical relationship as the relationship between the true geophysical and hydrogeological system properties; and we define the model-based petrophysical relationship as the relationship between our geophysical and hydrogeological model parameters. The intrinsic relationship is unknown to us. Laboratory analysis might provide a good estimate, although it may be difficult to scale the relationship for use at the field scale (e.g. Moysey and Knight, 2004). Day-Lewis and Lane (2004) compared the correlation between a synthetic slowness (i.e., the inverse of velocity) structure and the estimated slowness structure derived from a hypothetical radar survey. They showed that the linear correlation coefficients between these two structures were space-varying, significantly less than one, a function of acquisition errors, survey geometry, and regularization. This implies that the model-based petrophysical relationship is different from the intrinsic petrophysical relationship and that it might be non-stationary even if the intrinsic petrophysical relationship is stationary. This is problematic, because:

- if we use a physically based relationship, such as Equation (3), or a close approximation of the intrinsic relationship based on laboratory analysis, its predictive power will be significantly decreased if we use it to relate our estimated geophysical model with hydrogeological properties and it might give biased results;
- an empirical relationship estimated by regression of collocated hydrogeological data and estimated geophysical parameters will not be strictly valid throughout the model domain even if all properties except the geophysical and hydrogeological system properties of interest are kept constant; and
- relationships that we establish in the field are not only a function of hydrogeological characteristics, but also of acquisition errors, survey geometry, and regularization of the inverse problem. These campaign-related errors reduce the validity of the developed relationships for use at other sites.

How large are these potential errors compared with other error sources and with regard to the accuracy needed to meet specific project objectives? It is not always necessary to have very detailed models and the effects discussed above might be insignificant in certain applications, such as mapping of the interface between salt and freshwater in coastal aquifers where the electrical formation factor is determined using borehole information and applied to large scale resistivity models. However, these effects are probably significant if we attempt to provide high-resolution characterization at the local scale in order to predict solute transport.

2.2.3.3. *Weak or No Parameterization of the Petrophysical Relationship*

In some cases, a relationship between a geophysical and a hydrogeological system property may not exist or it may be very weak. For example, Pride (2005) stated that there is no theoretical basis for a universal relationship between seismic velocity and permeability in porous media. However, site specific models may exist (Pride, 2005; Hubbard et al., 2001; Hyndman et al., 2000), although they may vary within short distances (Prasad, 2003). It has been argued that the logarithm of electrical conductivity and the logarithm of permeability have a linear relationship, but the slope is site-specific and it is very sensitive to clay content (Purvance and Andricevic, 2000a).

In cases where the petrophysical relationships are weak, zonation approaches (see Section 2.2.2) can potentially be useful to determine the geometry of hydrofacies. Borehole information and tracer test data can subsequently be used to estimate the hydrogeological system properties of these zones (e.g. Hyndman et al., 1994; Hyndman and Gorelick, 1996; McKenna and Poeter, 1995, see also Section 2.5.1). Such an approach is useful when different facies have distinctly different geophysical properties because under such circumstances the determination of facies becomes relatively insensitive to errors in the geophysical data acquisition and the subsequent inversion. Alternatively, if we use a geostatistical parameterization or an Occam type of inversion we could impose restrictions on the model space. An example was provided by Gallardo and Meju (2004) who jointly inverted seismic refraction data and surface dc resistivity data by restricting the model space of the two models to models where the cross-gradients, **t**, of the models were zero. The cross-gradient in the case of one geophysical model, $\mathbf{m}_{\mathrm{g}}$, and one hydrogeological model, $\mathbf{m}_{\mathrm{h}}$, is defined as

$$\boldsymbol{\tau} = \nabla \mathbf{m}_{\mathrm{g}} \times \nabla \mathbf{m}_{\mathrm{h}} \tag{4}$$

This approach has yet not been incorporated in hydrogeophysics, but it is promising because structural similarity between models is emphasized instead of a petrophysical relationship that is difficult to justify in many applications.

In short, the representation of the petrophysical relationship is one of the most difficult tasks in hydrogeophysical parameter estimation. A precautionary attitude is recommended.

2.2.4. A PRIORI INFORMATION

A priori information is information about characteristics of the models that we get from other sources of information rather than the actual geophysical or hydrogeological data. Prior information in deterministic inversions is used to define bounds of possible models, such as ensuring that velocities are positive, or that the electrical resistivities are below 10,000 Ohm-m in a sedimentary basin. These bounds should ideally represent information that is known without doubt. Stochastic inversion theory takes an additional step by assigning a probability distribution of the possible values of the model parameters before any measurements are made (e.g. Tarantola, 1987).

A priori information is sometimes used to tune the model to get agreeable features of the solution or make it well-posed. This violates a pure use of a priori information, but might be a good place to incorporate subjectivity, if needed. We agree with the ironic comment made by Jackson (1979) in discussing the use of a priori information to resolve non-uniqueness: “One disadvantage of the technique is that the assumptions which lie hidden in the abstractness of most methods are in this method left naked for the world to see.” An excellent tutorial to the use of a priori information is Scales and Tenorio (2001), and Malinverno and Briggs (2004) provided a discussion on how hierarchical and empirical Bayes can be used to avoid assuming that the probability distribution function is known.

2.2.5. OPTIMIZATION OR MONTE CARLO METHODS

Local optimization methods are the most common parameter estimation approaches and model uncertainties are typically evaluated around the solutions that minimize the objective function. Uncertainty is thus often described in terms of a standard deviation of the estimated model parameters or through sensitivity analysis of what parameters are better resolved than others. Furthermore, in a deterministic approach only uncertainties in the data are assumed. Uncertainty estimates performed in this way are often over-optimistic. Another form of uncertainty arises if the problem is strongly non-linear because it might result in local minima. There are ways to decrease non-linearity, such as transformation of the data, weighting, and alternative parameterizations of the models. We can also assess the existence of local minima by trying different initial and prior models (e.g. Oldenburg and Li, 1999). Even if we find the global minimum it does not mean that we can disregard other local minima. An alternative is to carry out a global search to derive the posterior pdf of all model parameters. Markov chain Monte Carlo Methods (MCMC) are often performed for computational efficiency using the Metropolis-Hastings algorithm (e.g. Mosegaard and Tarantola, 1995) or Gibb’s sampling (e.g. Chen et al., 2003), as will be described in Sections 2.4.3 and 2.5.3.

2.2.6. OBJECTIVE FUNCTIONS

In this section, we discuss common objective functions used in different estimation procedures. The treatment is cursory and it is mainly given to illustrate in a simple fashion how different methods are interconnected and to provide relevant references. We also spend some time discussing Occam’s inversion because of its widespread use in geophysical inversion. Geophysical inverse theory is treated by Menke (1984), Parker (1994), and Tarantola (1987); an excellent review of hydrogeological inversion is given by McLaughlin and

Townley (1996). A formalized treatment of stochastic forward and inverse modeling in hydrogeophysics is given by Rubin and Hubbard (2005).

The data fit χ_d^2 is often defined as

$$\chi_d^2 = (\boldsymbol{d} - \mathbf{F}[\mathbf{m}])^{\mathrm{T}} \mathbf{C}_{\mathrm{d}}^{-1} (\boldsymbol{d} - \mathbf{F}[\mathbf{m}]), \tag{5}$$

where $\boldsymbol{d}$ is an $N \times 1$ data vector (e.g. seismic travel times, mass fractions of tracer); **F** is a forward model operator; $\mathbf{C}_{\mathrm{d}}^{-1}$ is the inverse of the data covariance matrix. It is commonly assumed that the data are uncorrelated, rendering the $\mathbf{C}_{\mathrm{d}}^{-1}$ a diagonal matrix that contains the inverses of the estimated variances of the observation errors; thus, more reliable data carry larger weight when evaluating the data fit. Our data covariance matrix can either be estimated or assumed to take certain values if the method does not allow an error estimate. There is an implicit assumption of Gaussian errors in this formulation of the data fit. This is neither the only nor necessarily the best description of data fit, but it is without doubt the most commonly used. Huber (2003) provided a review of robust statistics and Finsterle and Najita (1998) discussed robust estimation in hydrogeology.

A general description of the model norm assuming that the model parameters have a Gaussian distribution is

$$\chi_m^2 = (\mathbf{m} - \mathbf{m}_0)^{\mathrm{T}} \mathbf{C}_{\mathrm{m}}^{-1} (\mathbf{m} - \mathbf{m}_0), \tag{6}$$

where $\mathbf{m}_0$ is an a priori model of size $M \times 1$; and $\mathbf{C}_{\mathrm{m}}^{-1}$ is the inverse of the model covariance matrix, which characterizes the expected variability and correlation of model parameters. However, the model covariance matrix is often unknown and it might be restrictive to damp the model to be close to an a priori model, if no good a priori model exists. Therefore, other model norms are typically defined using different measures of roughness (Constable et al., 1987), e.g. based on the first derivatives of the model

$$R_1 = (\boldsymbol{\partial}\mathbf{m})^{\mathrm{T}}(\boldsymbol{\partial}\mathbf{m}), \tag{7}$$

where ∂ is an $M \times M$ matrix, which for 1-D models is given by

$$\boldsymbol{\partial} = \begin{bmatrix} 1 & & & \\ -1 & 1 & & 0 \\ & \cdots & \cdots & \\ & 0 & -1 & 1 \end{bmatrix} \tag{8}$$

The data fit and measures of model structure can be combined to formulate the most common objective functions.

A weighted least-squares objective function (Equation (5)) is used when we do not have any a priori information and when the inverse problem is well-posed without adding a regularization term. However, this is typically