PhD Thesis - Informing groundwater models with near-surface geophysical data

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1 author:

Daan Herckenrath
Queensland Government

Technical University of Denmark

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Daan Herckenrath

DTU Environment
Department of Environmental Engineering

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Address:	DTU Environment Department of Environmental Engineering Technical University of Denmark Miljoevej, building 113 DK-2800 Kgs. Lyngby Denmark
Phone reception:	+45 4525 1600
Phone library:	+45 4525 1610
Fax:	+45 4593 2850
Homepage:	http://www.env.dtu.dk
E-mail:	reception@env.dtu.dk

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Preface

The work presented in this PhD thesis, entitled "Integration of groundwater models and near-surface geophysical data", was conducted at the Department of Environmental Engineering at the Technical University of Denmark (DTU) under the supervision of Associate Professor Peter Bauer-Gottwein (DTU) and Associate Professor Esben Auken (Aarhus University). The PhD research project was conducted in the period November 2008 to November 2011 and was funded by DTU and the Danish Agency for Science and Innovation. The study included an external stay of two months at the Department of Geophysics at Stanford University under supervision of Professor Rosemary Knight and an intensive collaboration with the Geophysics Department at Aarhus University under supervision of Associate Professor Esben Auken.

This PhD thesis comprises a synopsis and three papers that were submitted to international, ISI-indexed scientific journals:

I. Herckenrath, D., Legaz-Gazoty, A., Fiandaca, G., Auken, E., Christensen, M., Balicki, M. and P. Bauer-Gottwein, Sequential and Coupled Hydrogeophysical Inversion of a Groundwater Model using Geoelectric and Transient Electromagnetic Data, *Journal of Hydrology*, submitted.

II. Herckenrath, D., Odlum, N., Nenna, V., Auken, E., and P. Bauer-Gottwein, Calibrating salt water intrusion models with Time-Domain Electromagnetic Data, *Ground Water*, submitted.

III. Herckenrath, D., Behroozmand, A., Christiansen, L., Auken, E., and P. Bauer-Gottwein, Coupled hydrogeophysical inversion using time-lapse magnetic resonance sounding and time-lapse gravity data for hydraulic aquifer testing: potential and limitations, *Water Resources Research*, in review.

The papers are not included in this online-version, but can be obtained from the library at DTU Environment. Contact library@env.dtu.dk or
Department of Environmental Engineering
Technical University of Denmark,
Miljøvej, Building 113
DK-2800 Kgs. Lyngby
Denmark

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Without the comforting, inspiring and refreshing presence of family, friends, supervisors and colleagues this book would probably be worse. Thanks.

Daan Herckenrath

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Summary

Over the past decade geophysical methods have gained an increased popularity due to their ability to map hydrologic properties. Such data sets can provide valuable information to improve hydrologic models. Instead of using the measured geophysical and hydrologic data simultaneously in one inversion approach, many of the previous studies apply a Sequential Hydrogeophysical Inversion (SHI) in which inverted geophysical models provide information for hydrologic models. In order to fully exploit the information contained in geophysical datasets for hydrological purposes, a coupled hydrogeophysical inversion was introduced (CHI), in which a hydrologic model is part of the geophysical inversion. Current CHI-research has been focussing on the translation of simulated state variables of hydrologic models to geophysical model parameters. We refer to this methodology as CHI-S (State). In this thesis a new CHI-approach was developed, called CHI-P (Parameter), which applies coupling constraints between the geophysical and hydrologic model parameters.

A CHI-P was used to estimate hydraulic conductivities and geological layer elevations for a synthetic groundwater model using Time-Domain Electromagnetic (TDEM) data and for a real-world groundwater model using geo-electric data. For the synthetic study, the CHI-P resulted in improved parameter estimates and a reduction in parameter uncertainty for both the hydrologic and the geophysical model, when compared with a SHI. For the real-world groundwater model, parameter uncertainty could not be reduced significantly, but the CHI-P resulted in more consistent parameter estimates between the groundwater model and the geophysical model. To our knowledge, CHI-P is the first CHI method that can be applied to inform large-scale groundwater models with near-surface geophysical data.

In another study, we successfully applied a CHI-S to estimate parameter values of a saltwater intrusion model with TDEM data. Considering the small number of estimable parameters, data fit and parameter uncertainty, the salt water intrusion model provided an excellent interpretation of the geophysical data. The CHI-S yielded a geophysical model that could never be obtained with a separate geophysical inversion. Furthermore, we applied a CHI-S to evaluate the potential for time-lapse relative gravimetry (TL-RG) and magnetic resonance sounding (TL-MRS) to improve the estimation of aquifer properties during an aquifer pumping test. This was done, taking in account a number of practical issues that might limit the sensitivity of these techniques with respect to the estimated

aquifer properties. For this purpose a virtual pumping test was used with synthetic observation data. In contrast to the prior assumptions, the conclusions suggest that both geophysical techniques have a potential to improve the estimation of aquifer properties. In the analyses, TL-MRS outperformed TL-RG data and parameter uncertainty could be reduced with ca. 30 % for most of the scenarios that were investigated.

Dansk sammenfatning

I det seneste årti har geofysiske metoders vundet stor udbredelse i kortlægning af hydrologiske egenskaber. Disse teknikker kan levere data med høj opløsning, som kan korreleres med hydrologiske egenskaber og bruges til at forbedre hydrologiske modeller. I stedet for at benytte en fælles kalibrerings-metode, hvor de geofysiske målinger og hydrologiske data er brugt samtidig, kan mange af de nuværende undersøgelser anvende en Sequential Hydrogeophysical Inversion (SHI), hvor geofysiske modeller giver information til hydrologiske modeller. For at udnytte det fulde potentiale af geofysiske datasæt med hensyn til hydrologiske formål, blev en Coupled Hydrogeophysical Inversion (CHI) indført, hvor en hydrologisk model er en del af den geofysiske inversion. Aktuel CHI-forskning har fokuseret på oversættelse af simulerede tilstandsvariable i hydrologiske modeller til geofysiske modelparametre. Vi henviser til denne metode som CHI-S (State). I denne afhandling en ny CHI-strategi blev udviklet, kaldet CHI-P (Parameter), som baserer sig på koblingsbindinger mellem geofysiske og hydrologiske modelparametre.

En CHI-P blev anvendt til at estimere hydraulisk permeabilitet og geologisk lag-tykkelse for henholdsvis en syntetisk grundvandsmodel ved hjælp af Time-Domain Elektromagnetic (TDEM) data og en eksisterende grundvandsmodel ved hjælp af geo-elektriske data. I den syntetiske undersøgelse resulterede CHI-P i forbedrede parameter værdier og en reduceret parameterusikkerhed i både den hydrologiske og den geofysiske model, når man sammenligner med en SHI. For den eksisterende grundvandsmodel, kan parameterusikkerheden ikke reduceres tilsvarende, men CHI-P resulterede i mere konsekvente parameterestimater mellem grundvandsmodellen og den geofysiske model. Så vidt vides, er CHI-P den første CHI metode, der kan anvendes til at informere regionale grundvandsmodeller om geologiske egenskaber ud fra geofysiske data.

I en anden undersøgelse har vi med succes anvendt en CHI-S til at estimere parameter værdier af en saltvandsindtrængningsmodel med TDEM data. Under hensyntagen til det lille antal parametre, datafit og parameterusikkerhed, gav saltvandindtrængningsmodellen en fremragende fortolkning af de geofysiske data. CHI-S resulterede i en geofysisk model, der aldrig ville kunne opnås med en separat geofysisk inversion. Derudover har vi anvendt en CHI-S for at evaluere potentialet for time-lapse relativ gravimetri (TL-RG) og magnetisk resonans sounding (TL-MRS) for at forbedre estimater af grundvandsmagasinets egenskaber i løbet af en pumpetest. En række praktiske problemer, der kan

begrænse følsomheden af disse teknikker med hensyn til det estimerede grundvandsmagasins egenskaber blev herunder taget i regning. Til dette formål anvendte vi en virtuel pumpetest med syntetiske observationsdata. I modsætning til tidligere antagelser tyder konklusionerne på, at begge geofysiske teknikker har potentiale til at forbedre estimering af grundvandsmagasinets egenskaber. I analyserne har TL-MRS klaret sig bedre end TL-RG data, og parameterusikkerheden kunne reduceres med ca. 30 % for de fleste af de scenarier, der blev undersøgt.

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1 Introduction

Groundwater resources suffer from an increasing pressure due to increasing water demands for domestic, agricultural and industrial use. To develop optimal management strategies, essential background information is needed about the geology and the present hydrologic state of an area. Three core disciplines can be identified to characterize the hydrogeological properties of a region, which are geology, geophysics and hydrogeology. Typically geologists and geophysicists characterize the geological setting of an area, where geologists typically process and interpret available borehole and outcrop information, while geophysicists try to map geological structures using surface geophysical methods such as seismic, electromagnetic and geo-electric methods. Finally, hydrogeologists develop quantitative tools to describe relevant hydrologic processes and assess the impact of different groundwater management strategies.

Over the past decade geophysical methods, have gained an increased popularity because of their ability to map hydrologic properties as well. For example methods such as ground penetrating radar (GPR) and magnetic resonance sounding (MRS) are used to map moisture content [*Legchenko et al.*, 2002; *Huisman et al.*, 2003], while electromagnetic (EM) techniques are used to map salt water intrusion in coastal aquifers [M*acaulay and Mullen*, 2007]. If interpreted separately, these geophysical datasets only provide images of a certain hydrologic property in space or time. However, the methods do not provide an explanation with regards to the physical processes underlying the distribution of the mapped hydrologic property, which is essential to make predictions for the hydrologic system under different management scenarios. For this purpose hydrologic models are needed.

The emerging use of geophysical methods for hydrogeological imaging has yielded a new field of research, called hydrogeophysics. [*Rubin and Hubbard*, 1999] and [*Vereecken*, 2006] are the first books in which geophysics and hydrologic models are consistently brought together. A topic that is given specific interest is the inversion method[1] used to estimate geophysical models

[1] Inversion: Physical theories allow us to make predictions. Given a complete description of a physical system, we can predict the outcome of some measurements using a model. The inverse problem consists of using the actual measurements to estimate the values of model parameters that characterize the physical system [modified form *Tarantola*, 2005]. In the inversion process model parameter values are changed until the difference between the actual measurements and model simulations is minimal.

and parameters of hydrologic models. [*Ferré et al.*, 2009] and [*Hinnell et al.*, 2010], provide an overview of inversion frameworks that can be used to inform hydrologic models with geophysical data. Two specific types of inversion frameworks are a sequential hydrogeophysical inversion approach (SHI) and a coupled hydrogeophysical inversion approach (CHI). The main difference between both methods is that a SHI does not take into account the hydrologic model when performing a geophysical inversion.

This PhD research was part of RISKPOINT, a project funded by the Danish Council for Strategic Research, which aims to create a risk assessment tool to identify and prioritize clean up and management of point sources of contamination to groundwater. To provide an indication of the magnitude of this problem, there are ca. 13000 documented sites with contamination in Denmark and an additional 14000 sites where soil contamination is suspected [*Miljøstyrelsen*, 2009]. One of the objectives of this project is to evaluate the hydrological and hydrochemical interactions between groundwater and surface water with the ultimate goal to develop optimal management strategies.

Within the overall framework of the RISKPOINT-project, this PhD research was focused on the use of SHI and CHI to constrain, calibrate and validate numerical models of water flow and solute transport. Numerical models typically suffer from the lack of accurate and sufficiently resolved input and calibration data. Geophysical methods have the potential to provide essential information for flow and transport models over a range of scales [e.g. *Kemna et al.*, 2002; *Thomsen et al.*, 2004; *Chambers et al.*, 2004].

1.1 Previous work

Numerous papers have been published about the inclusion of geophysical data for hydrogeological site characterization. Examples are the delineation of landfills [*Radulescu et al.*, 2007; *Meju*, 2000], mapping tracer concentrations [*Singha and Gorelick*, 2005 and 2006] and the estimation of the spatial correlation structure of hydraulic properties [*Hubbard et al.*, 1999, *Day-Lewis et al.*, 2005]. The main reason for the increasing interest in using geophysical methods in hydrogeological studies is that geophysics provides spatially distributed models of physical properties in regions that are difficult to sample using conventional hydrological sampling methods [*Butler*, 2005]. *Hinnell et al.* [2010] and *Ferré et al.* [2009] discuss the different types of hydrogeophysical inversion approaches that can be used and *Hinnell et al.* [2010] provide a comprehensive list of references to case study applications using different types of coupling approaches. For example, geostatistical methods have been employed to estimate hydrologic parameter distributions based on the correlation structures found in inverted geophysical images [*Cassiani et al.*, 1998; *Hubbard et al.*, 1999; *Yeh et al.*, 2002; *Chen et al.*, 2004]. *Hyndman and Gorelick* [1996], *Chen et al.* [2006] and *Linde et al.* [2006] are examples of studies where hydrologic structures and parameter distributions are being estimated using geophysical and hydrologic data at the same time. Other studies use geo-electric [*Kemna et al.*, 2002; *Vanderborght et al.*, 2005; *Cassiani et al.*, 2006] and electromagnetic data [*Binley et al.*, 2001; *Day-Lewis et al.*, 2003; *Lambot et al.*, 2004; *Looms et al.*, 2008; *Knight*, 2001; *Huisman et al.*, 2003], e.g. GPR, to monitor temporal changes in water content or solute concentrations.

Many previous studies use a SHI in which first a geophysical model is estimated after which the hydrologic model is informed with the geophysical model. *Hinnell et al.* [2010], *Ferré et al.* [2009], *Kowalsky et al.* [2005], *Pollock and Cirpka* [2010] and *Lambot et al.* [2006, 2009], however, describe a CHI, in which a hydrological model is part of the geophysical inversion process and a single objective function is minimized which includes both a geophysical and hydrological component. In other words, both the geophysical and the hydrologic model and their associated observations are used to constrain one another.

1.2 Aim of this study

The vast majority of previous CHI-studies perform a geophysical inversion by estimating parameters of a hydrologic model in order to fit geophysical measurement data. This is done by translating simulated hydrologic state variables (moisture content, concentration) to geophysical parameter distributions to simulate a geophysical signal that can be compared with the measurement data. This is not the only way to perform a CHI. Another approach to perform a CHI would be to couple parameters of the geophysical model with parameters of the hydrologic model. A limitation of most previous studies is the small spatial scale of CHI case study applications. Moreover, the CHI frameworks by *Hinnell et al.* [2010], *Kowalsky et al.* [2005] and *Lambot et al.* [2009] do not allow for the separate estimation of geophysical model parameters which cannot be linked to the hydrologic model. This can be a significant limitation as a hydrologic model may not have a sufficiently detailed spatial resolution to represent near-surface variations in geophysical model parameters.

This research aims to develop new general CHI methods to address the previously mentioned limitations. The need for such a general framework can best be described by an example: At many sites globally large, high-resolutions airborne EM datasets have been collected to map salt water intrusion and geological properties on a regional scale [*Auken et al*., 2008; *Macaulay and Mullen*, 2007]. At the same time regional-scale groundwater models are available to establish a regional overview of the present state and future trends in the available groundwater resources and salt water intrusion [e.g. *Henriksen et al.*, 2003; *Langevin*, 2003a]. A consistent framework to integrate the potential wealth of geophysical information into these models is lacking. With this question in the back of our mind, the aim of this research is to:

- develop a new CHI-approach to estimate hydraulic properties for regional groundwater models using electromagnetic and geo-electric data
- apply a CHI to estimate parameters of salt water intrusion model based on electromagnetic data
- apply a CHI to evaluate the use of time-lapse gravity and magnetic resonance sounding data for aquifer pumping test monitoring

The latter objective pertains to a different spatial scale, but aquifer pumping tests are used to estimate typical values for the hydraulic properties of an aquifer, which are important to inform larger scale groundwater models with.

1.3 Structure of the thesis

This thesis provides a synopsis of the three papers that are found in Chapter 9. All the remaining chapters in this book have the purpose to introduce the different methods that are used in the papers and put them into a scientific and application-oriented context. Chapter 2 gives an overview of common hydrologic models that are used to simulate groundwater water flow and solute transport in the saturated zone, together with a brief summary of common geophysical techniques that are used for mapping hydrologic properties. Chapter 3 lists the properties of the two field sites that were used in our investigations, while chapter 4 provides an overview of the inversion frameworks that were developed in this research. Chapter 5 gives a short overview of results that were obtained during this PhD study. Finally, chapters 6 and 7 summarize, respectively, the main conclusions of this research and a list of future research directions based on the work that is presented in this book.

2 Hydrologic models and geophysical methods

2.1 Hydrologic models

In this research only flow and solute transport in the saturated groundwater zone will be considered. To simulate groundwater flow we start from the continuity equation

$$-\nabla \cdot (\rho(c)\theta \vec{u}) - W\rho_s = \frac{\rho(c)\theta_s}{dt} \tag{2.1}$$

where W is the external flux per unit volume [T^{-1}], θ_s is the porosity [-] which we assume to be equal to the saturated water content, where $\rho(c)$ is the density of the water [-] and where ρ_s represents the density of the water associated with the external sinks and sources [-]. $\rho(c)$ depends on the concentration of the dissolved solutes c [ML^{-3}] in the groundwater. The pore velocity u [LT^{-1}] is calculated using Darcy's law

$$\theta_s \vec{u} = -\frac{K}{g}\left(\nabla\left(\frac{h}{\rho(c)}\right) + \vec{g}\right) \tag{2.2}$$

in which h is the hydraulic pressure [$ML^{-1}T^{-2}$], K [LT^{-1}] is the hydraulic conductivity of the subsurface and g the gravitational acceleration [L^2T^{-1}]. Solute transport is commonly simulated with a convection-diffusion equation together with some basic chemical reactions like adsorption to a solid phase and a first order rate reaction. Neglecting the inclusion of adsorption and reactions the convection-diffusion equation can be written as

$$\frac{\partial c}{\partial t} = \vec{u} \cdot \nabla c + \nabla \cdot (\mathbf{D} \cdot \nabla c) + Wc_s \tag{2.3}$$

where **D** is the dispersion tensor [L^2T^{-1}], and c_s is the solute concentration associated with the sink and sources W, which represents features such as drains, wells and surface water bodies.

For regional models, Equation 2.1 and 2.3 are often solved numerically, using groundwater modeling software such as MODFLOW [*Harbaugh and McDonald*, 2000] and the solute transport module MT3DMS [*Zheng and Wang*, 1999]. The results of MODFLOW are water fluxes and water levels, while MT3DMS calculates solute concentrations and solute fluxes. In paper **II** we simulate salt water intrusion, for which we take into account the groundwater flow component due to density differences which are caused by differences in salinity. This is done, by coupling equation 2.1 and 2.3 with an "equation of state", which provides a relationship between groundwater density and salt concentrations. This equation of state is formulated as follows

$$\rho(c) = \rho_f + 0.71c \tag{2.4}$$

where ρ_f represents the density of freshwater and c the salt concentration calculated with equation 2.3. Equation 2.4 is based on a linearized formulation derived by [*Baxter and Wallace*, 1916] which does not take into account temperature and pressure effects on the density of the water. In this research SEAWAT [*Langevin and Guo*, 2006] is used to perform simulations for variable-density groundwater flow.

In paper **III** we use an analytical hydrologic model to calculate the water table drawdown around a pumping well due to groundwater pumping. For aquifer pumping tests, the governing equations are the same as for saturated groundwater flow. Typically uniform aquifer properties and simple aquifer geometries are assumed, in order to use an analytical expression for the simulation of water table drawdown. Many studies [*Moench*, 1997; *Neuman*, 1972] have been dedicated to the derivation of the most complete analytical expression to capture all relevant hydrologic processes and pumping test design characteristics, as delayed drainage and borehole flow. Typical software packages for pumptest analysis are AQTESOLV [*Duffield*, 2007] and WTAQ [*Barlow and Moench*, 1999].

2.2 Hydrologic applications of geophysical methods

A wide variety of geophysical techniques is available. Many books provide a description of the underlying physics and applications for the various methods [e.g. *Telford et al.,* 1990]. The art of the geophysicist is to pick out a particular geophysical method that is most suitable, given its sensitivity for the property that needs be mapped, the scale that has to be represented and the environmental noise conditions that might interfere with the geophysical survey. In this paragraph we only provide a brief overview of the different techniques, after which we describe some major applications of geophysics to map hydrologic variables.

2.2.1 Basic classification of geophysical methods

Kearey et al. [2002] provide an excellent description of available geophysical methods. Table 2.1 is based on the classification used in this book and provides a basic classification of available techniques according to their underlying physics and indicates which physical property of the earth is estimated.

Table 2.1 Classification of geophysical techniques

Method	Measured data	Estimated property
Seismic	Travel time refracted/reflected seismic wave	Density and elastic moduli
Gravity	Gravitational field of the Earth in space and time	Density
Magnetic	Geo-magnetic field in space and time	Magnetic susceptibility
Nuclear magnetic resonance	Relaxation electromagnetic field	Fluid content and relaxation constants
Geo-electric	Earth resistance	Electrical resistivity
Induced polarization	Voltage decay	Electrical chargeability
Self potential	Electric potential	Electrical resistivity
Electromagnetic	Response to electromagnetic pulses	Electrical resistivity
Radar	Travel time of reflected radar	Dielectric constant

According to Table 2.1 many different physical properties of the subsurface can be estimated. In this thesis we only discuss their use with respect to hydrologic mapping. A much wider range of applications can be associated with geophysical techniques. For example, magnetic methods are used to detect iron ore bodies and seismic methods are employed to explore existing oil and gas reservoirs. Note Table 2.1 lists two properties, a measured quantity and an estimated property. For most geophysical techniques the estimated property is obtained after a geophysical inversion process in which its value is estimated based on the measured data. This is done by calculating a geophysical forward model, which simulates the data you would measure in the field or laboratory, given a certain value of the estimated property and then fitting the simulated data to the observed data.

Instead of describing the geophysical methods according Table 2.1, we discuss a number of main application areas for geophysics in hydrology [like in *Vereecken et al.*, 2007]. For this thesis we consider three of those applications areas, which are the vadose zone, landfills and contaminant transport and regional geology and coastal regions.

2.2.2 Vadose zone

The vadose zone, commonly referred to as unsaturated zone, plays an important role associated with environmental issues such as soil and groundwater contamination, ground stability and flood control. Monitoring the spatial and temporal variability of moisture content and the freezing/thawing of the subsurface can yield valuable information regarding these environmental concerns. Applications of geophysical techniques in frozen soils can be found in [*French and Binley*, 2004], which are commonly geo-electric methods to distinguish between the frozen and unfrozen part of the subsurface. To monitor moisture content θ [-], two groups of geophysical techniques are currently employed.

The first group of geophysical techniques comprises radar and geo-electric methods based on relating the electric permittivity and electrical resistivity of the subsurface with its water content. As pointed out in the previous paragraph, these geophysical techniques do not measure electric permittivity or resistivity directly, but estimate these values based on the measured data. For radar methods as Time Domain Reflectrometry (TDR) [*Michot et al.*, 2003] and Ground Penetrating Radar (GPR) [*Knight*, 2001], measured data comprise recorded electromagnetic wave velocities which are obtained by transmitting an electromagnetic wave after which their refracted and reflected waves are recorded.

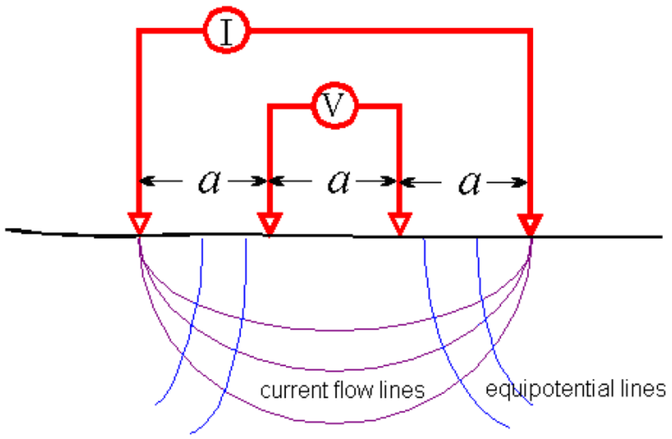

Figure 2.1 Measurement setup for Electric Resistivity Tomography [ERT]. a is the spacing between the electrodes (red arrows) where I indicates an electrical current [A] andV indicates the potential difference [V] that is measured during a survey

Figure 2.1 represents the setup of a geo-electric survey using Electric Resistivity Tomography (ERT), in which electrodes are placed in the subsurface after which potential differences (V) are measured by applying an electrical current (I) for different electrode combinations with a spacing a. Based on the potential differences [voltages] and the used electrode configuration (e.g. Wenner, Schlumberger), an apparent resistivity can be calculated. Apparent resistivities can be computed from subsurface resistivity distributions using the forward model for DC electric surveying. Matching measured and simulated apparent resistivities results in estimated subsurface resistivity distributions.

For radar methods the estimated electrical permittivity can be related to the soil moisture content by an empirical petrophysical relationship, called the Topp-equation [*Topp*, 1980]

$$\theta = -5.3 \cdot 10^{-2} + 2.92 \cdot 10^{-2} \varepsilon_r^2 + 4.3 \cdot 10^{-6} \varepsilon_r^3 \tag{2.5}$$

where ε_r is the electrical permittivity of the subsurface normalized over the permittivity of free space, also known as the relative permitivitty or dielectric constant. Examples of studies using this approach to estimate θ can be found in *Kowalsky et al.* [2004], *Lambot et al.* [2009] and *Huisman et al.* [2003]. A more general overview of environmental applications for GPR can be found in *Knight* [2001].

When using resistivity methods, often Archie's law is used to estimate the moisture content, given by [*Looms et al.*, 2008] as

$$\theta^n = r_w \frac{\theta_s^{n-m}}{r_b} \tag{2.6}$$

where r_w indicates the electrical resistivity of water and n and m are shape factors that are soil specific [*Looms et al.*, 2008]. r_b represents the resistivity of the bulk material. Note that r_b is the estimated parameter using a geo-electric method. To apply equation 2.6 for estimating moisture content a reasonable estimate is required for r_w.

The first group of techniques is not very attractive for clayey sediments, as radar methods suffer from a limited depth of penetration due to dielectric dispersion in sediments with a low electrical resistivity [*Knight*, 2001]. For geo-electric methods Archie's law does not apply anymore, as this empirical law does not include surface conductivity through the bulk material itself [*Lesmes and Friedman*, 2006]. This additional term is complicated to characterize and makes the estimation of soil moisture content less reliable.

The second group of methods does not require a relationship like Archie's law or the Topp-equation, but directly relate the measured geophysical signal with the moisture content of the subsurface in the geophysical forward model. Two of these methods are Nuclear Magnetic Resonance (NMR) or Magnetic Resonance Sounding (MRS) [*Legchenko and Valla*, 2002] and time-lapse gravity [*Montgomery*, 1971].

With relative gravimeters, the vertical component of the gravitational acceleration is measured. This reveals spatial differences in density which can be due to ore deposits, buried paleo-channels and changing depth to bedrock [*Carmichael and Henry*, 1977; *Zawila et al.*, 1997]. Time-lapse relative gravity (TL-RG) can be applied to monitor changes in mass, which can be used to monitor natural gas extraction [*van Gelderen et al.*, 1999] and quantify changes in water storage [e.g. *Christiansen et al., 2011*].

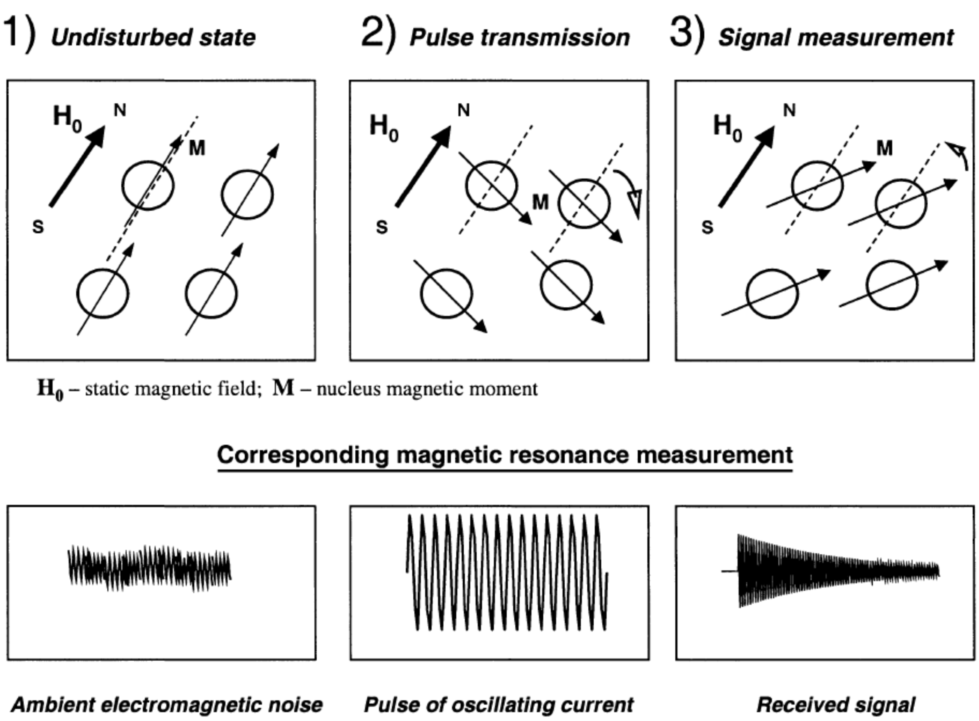

Figure 2.2 Observed data during a MRS sounding [picture from *Legchenko*, 2002]. 1) hydrogen protons in equilibrium state aligned along the Earth's magnetic field H_0, 2) hydrogen protons are excited with an external magnetic pulse and 3) hydrogen protons return to their equilibrium state yielding the received MRS signal shown on the bottom right side of the figure.

MRS is commonly known through its application in hospitals, where Magnetic Resonance Imaging (MRI) is used for imaging and diagnosis. With MRS the spins of the hydrogen protons of water molecules in the subsurface are excited with an external magnetic field, applied through a transmitter loop on the ground surface. After the external magnetic field is switched off, the spins of the hydrogen protons return to their original state generating a new magnetic field [*Legchenko et al.*, 2002], whose magnitude is measured by a receiver on the ground. Figure 2.2 [based on *Legchenko et al.*, 2002] shows the three stages of a MRS-sounding. The bottom-right panel of this figure shows the received MRS signal, which is oscillating with exponential decreasing amplitude. Typically two properties are extracted from this signal, which are the initial amplitude of this signal, depending on soil moisture content, and an exponential decrease rate of the amplitude (relaxation constant), which correlates with the pore characteristics of the subsurface and can be used to estimate hydraulic conductivity [*Mohnke and Yarmanci*, 2008; *Vouillamoz et al.*, 2008].

2.2.3 Landfills and contaminant transport

In the past low elevation areas, such as pits and wetlands were typically used for waste deposition [*Milosevic et al.*, 2011, *Lorah et al.*, 2009]. The waste deposition at these old landfills often lacked adequate control and documentation such that the boundaries of the landfill and the type of landfill material are unknown. Some of these landfills pose a significant environmental threat in polluting groundwater and surface water [*Christensen et al.*, 2001; *Lorah et al.*, 2009]. Such landfills usually contain household-, demolition- and chemical waste, where the main impact on surrounding water bodies is associated with inorganic macro-components (chloride, sodium, ammonium), dissolved organic carbon (DOC) and several different xenobiotic organic compounds [*Bjerg et al.*, 2011; *Kjeldsen et al.*, 2002]. The heterogeneous nature of an old landfill causes high spatial variability of the leachate compounds, and a large amount of work is required to accurately delineate the landfill, and detect leachate plumes.

Meju [2000] lists the geo-electric and electromagnetic methods as most popular geophysical techniques to characterize landfills due to their ability to detect changes in electrical resistivity, which correlates with moisture content and chemical composition of the pore water, and the relative low-costs to perform such surveys. Due to the presence of saline fluids in the landfill leachate, which is a good electrical conductor, it is possible to delineate the landfill and locate a contaminant plume by employing these geophysical techniques [*Naudet et al.*, 2004, *Chambers et al.*, 2004] One major limitation of using the electrical resistivity in landfill surveys is the fact that several factors influence the electrical resistivity of the subsurface, which makes it difficult to differentiate between one another. For example, clay and saline fluids both have a small electrical resistivity.

An upcoming technique for delineating landfills and detecting solute plumes is Induced Polarization (IP), which can be performed in combination with a geo-electric survey [*Dahlin et al.*, 2002; *Sogade et al.*, 2006]. IP is based on the fact that the subsurface is able to act as an electric capacitor and store electric charge. The same measurement setup as described in Figure 2.2 can be used, but instead of measuring the potential differences when an electrical current is applied, the decay of these potential differences is measured in time after terminating the applied electrical current. The decay rate of the potential difference can then be related to the chargeability of the subsurface. The signal that is retrieved with IP is mainly the result of the local redistribution of ionic charge in the electric double layer at the mineral-fluid interface [*Slater*, 2007]. Typically, the observed IP response is fitted by an empirical relationship named the Cole-Cole model [*Pelton et al.*, 1978], which parameters (chargeability, electrical resistivity, relaxation time and shape parameter) can be correlated with hydraulic conductivity and the presence of contaminant plumes. The Cole-Cole model, however, does not provide a mechanistic understanding of the retrieved IP-signal. A physical model is still lacking to explain the IP signature of contaminant plumes. [*Vaudelet et al.*, 2011], [*Revil and Florsch*, 2010] and [*Leroy and Revil*, 2009] are examples where the development of such a physical model is investigated.

2.2.4 Regional geology and coastal regions

To characterize regional geological properties and human structures, seismic and electromagnetic methods are often employed. With seismic methods, a seismic wave is generated by an explosion or vibrator, after which the wave is reflected and refracted at geological interfaces of materials with different seismic velocities. These reflected and refracted waves are recorded by receivers, called geophones or hydrophones (off-shore applications) to obtain a seismogram. Seismic velocity depends on the density of the rock, which makes the method attractive to determine the thickness of unconsolidated sediments overlying bedrock [*Miller et al.*, 1989].

Electromagnetic surveys can be performed using ground-based and airborne instruments. In Figure 2.3 a sketch is given of the measurement setup for a ground based electromagnetic survey using a Time-Domain Electromagnetic (TDEM) sounding. In this setup a square transmitter loop is used to generate an electrical current, which is switched off to generate a magnetic field in the subsurface whose strength decreases after the electrical current is turned off. A receiver coil, placed in the middle or outside the transmitter loop, is used to record this decrease in magnetic field strength, which can be translated to a series of apparent resistivities which, in turn, are inverted to obtain the subsurface resistivity distribution.

TDEM surveys are sensitive to estimate the depth of a layer with a low electrical resistivity, for example a clay layer or salt water saturated sediments. The depth of penetration can be up to 500 m [*Kearey et al.*, 2002], but this depends on the magnitude of the transmitted electrical pulse, the electrical resistivity of the subsurface and the frequency at which the electrical pulse is applied. In coastal regions this technique is very attractive as TDEM can potentially delineate the location of the freshwater/salt water interface, which is of major interest for supporting freshwater resources management in coastal aquifers. Examples of other applications of electromagnetic surveys are the mapping of buried channels [*Auken et al.*, 2008] and the mapping of a cave system in Mexico [*Supper et al.*, 2009].

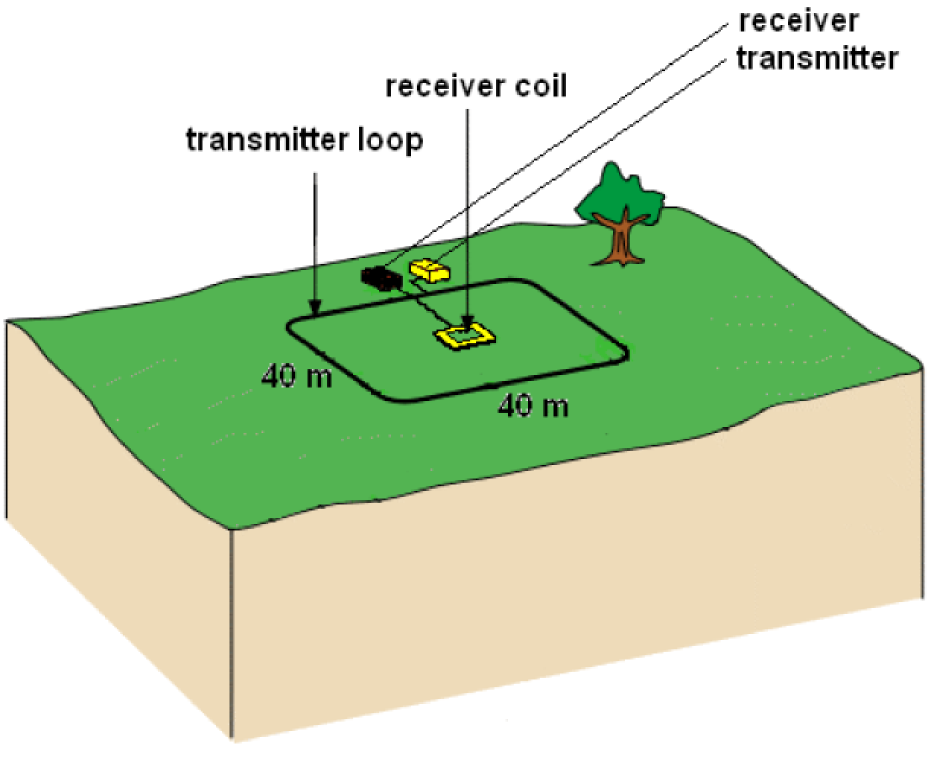

Figure 2.3 Measurement setup of a Time-Domain Electromagnetic (TDEM) sounding

Figure 3.1 Installing a benchmark point for a geodesy survey at Risby Landfill (upper left). Seepage meter measurements at Risby Landfill (upper right). Performing a Time Domain Electromagnetic (TDEM) sounding at Monterey Bay, California (bottom).

3 Field sites and data collection

3.1 Risby landfill

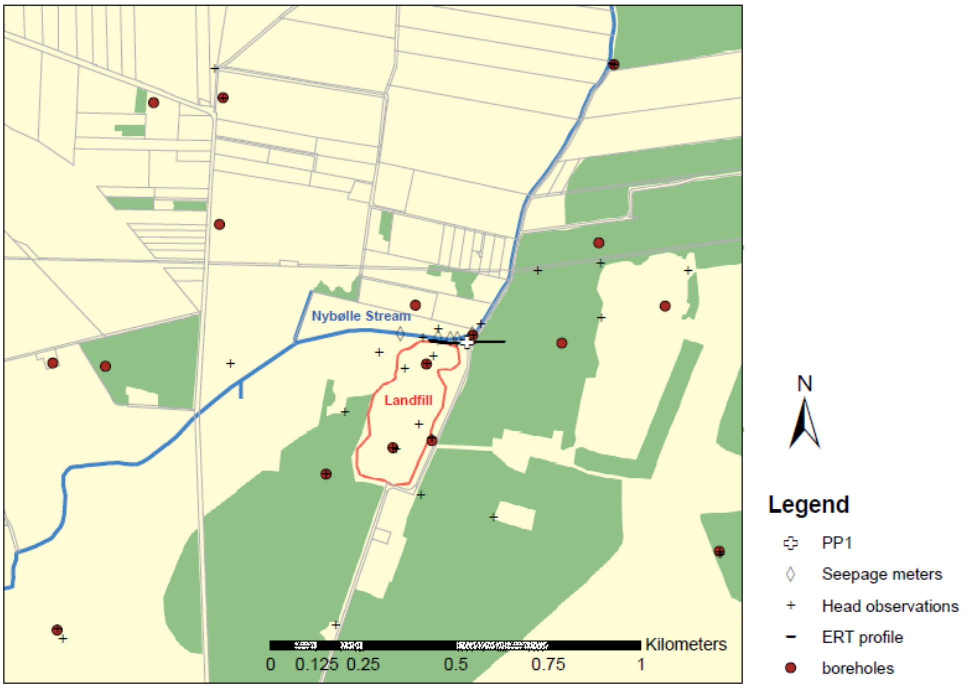

Figure 3.2 An overview of Risby Landfill and the collected measurement data that were used in paper **I**.

Risby landfill is located ca. 20 km west from Copenhagen, Denmark, and was chosen as a pilot-area in the RISKPOINT project to identify the dominant processes affecting the hydrogeological and geochemical interaction between the landfill, regional aquifer and the Nybølle stream. For this purpose boreholes have been drilled and leveled, together with the collection of indirect information using several geophysical methods. In Figure 3.2 a map is provided with the data that was used in paper **I**, comprising groundwater level measurements, seepage measurements in the Nybølle stream, borehole information and an ERT profile.

A detailed historical overview of Risby landfill was provided by [*Thomsen et al.*, 2011]. The geological setting of Risby landfill [*Gazoty et al.*, 2011, *Frederiksen et al.*, 2003; *Carl Bro A/S*, 1988] comprises pre-Quaternary limestone bedrock overlain by Quaternary glacial deposits. The pre-Quaternary limestone surface is located between -10 and +5 mamsl, corresponding to 20-30 m below the natural terrain surface. The Quaternary glacial deposits mainly consist of clay till, but intercalated sand lenses and sand layers are common. The sandy deposits range in thickness from a few centimeters to several meters.

In addition to the data that was used for paper **I**, water samples, ecological data and other geophysical data were collected in order to quantify contaminant fluxes from the landfill towards the stream and groundwater [*Milosevic et al.*, 2011, *Thomsen et al.,* 2011] and indentify which properties of a typical Danish landfill can be mapped using state-of-the-art geophysical techniques as magnetic methods, induced polarization and geo-electric methods [*Gazoty et al.*, 2011].

3.2 Monterey Bay, California

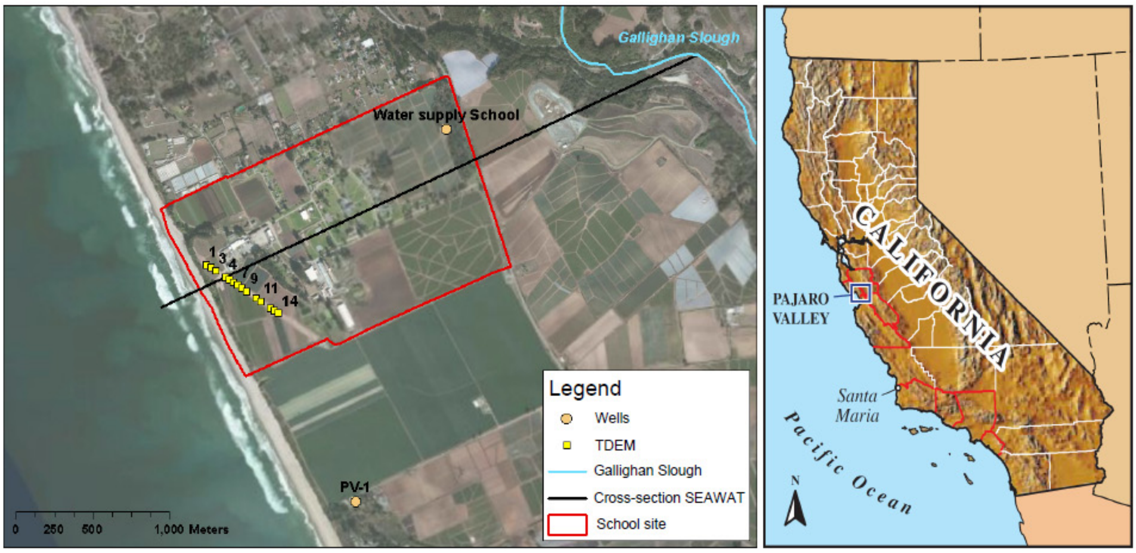

Figure 3.3 Right: Map of California, with a box highlighting Pajaro Valley, the water district where the School-site is located. Left: Overview of the School-site and the locations of the TDEM soundings.

At Monterey Bay, California, different electromagnetic (EM) methods were applied at two field sites, to evaluate the use of geophysical data for water managers in California. One of these field sites is called Monterey Bay Academy, to which we refer as the School-site. The other site is located 30 km south and is called Fort Ord. At Ford Ord there are plans to install a desalination plant that takes in salt water trough the upper aquifer system. [*Nenna et al.*, 2011] focus on the value of EM data at this site to inform local water managers about the current delineation of the salt water-fresh water interface and the presence of confining geological units that protect deep aquifers from induced salt water intrusion as a result of the placement of a desalination plant. Paper **II** is related to [*Nenna et al.*, 2011] and is focused on the TDEM data set collected at the School-site in relation to salt water intrusion at Monterey Bay. At the School-site 19 TDEM soundings were collected along an airstrip to obtain an electrical resistivity profile perpendicular to the coast that can be correlated to geological trends and changes in salt concentrations.

4 Inversion methodology

For the field sites in chapter 3, a hydrogeological model was employed to determine groundwater flow directions and quantify salt water intrusion, respectively. These hydrologic models require a significant amount of unknown input parameters, which have to be estimated based on prior knowledge or with an inversion approach using available measurement data. Measurement data include direct hydrologic observations but also indirect data such as geophysical measurements.

For both field sites in chapter 3 a CHI was applied, using a regional groundwater model in combination with TDEM or ERT data. When performing such a CHI a number of challenges were faced that are not taken in account in existing CHI-applications. The three most important challenges are:

- using the geophysical data to inform a hydrologic model about its input parameters
- allow for a separate estimation of essential geophysical parameters to achieve an acceptable geophysical data fit
- the large computational burden associated with the hydrologic model and the geophysical data sets

Ferré et al. [2009] provide a basic classification of hydrogeophysical inversion methods, which includes the division between CHI and SHI approaches. In addition to this classification, these CHI and SHI approaches can be divided into groups that couple geophysical models with a hydrologic model using the simulated hydrological state variables or the hydrologic input parameters. Paragraph 4.1 provides a short description of existing SHI and CHI approaches. Paragraph 4.2 describes the basics of performing a hydrogeophysical inversion using parameter and state coupling. In addition the differences are listed between existing CHI-applications and the CHI-frameworks that are developed in this thesis. Paragraph 4.3 concludes with a specification of the coupling constraints that can be used to inform hydrologic models with geophysical data, which we subdivide in geometric and petrophysical relationships.

4.1 Sequential and coupled hydrogeophysical inversion

Figure 4.1a and 4.1c show a Sequential Hydrogeophysical Inversion (SHI) approach. The first step in a SHI comprises a geophysical inversion in which a geophysical parameter is estimated (e.g. electrical resistivity). Subsequently, the estimated geophysical parameter distribution is translated to a number of hydrologic observations or hydrologic input parameters. This can be done directly or with the use of a petrophysical relationship (e.g. Archie's law, Topp-equation). The way a hydrologic model is informed with the inverted geophysical model depends on the geophysical technique and the hydrologic interpretation of the estimated geophysical model. The final step in the SHI is to perform a hydrologic inversion, in which the hydrologic model parameters are estimated using the estimated geophysical parameters as observation data.

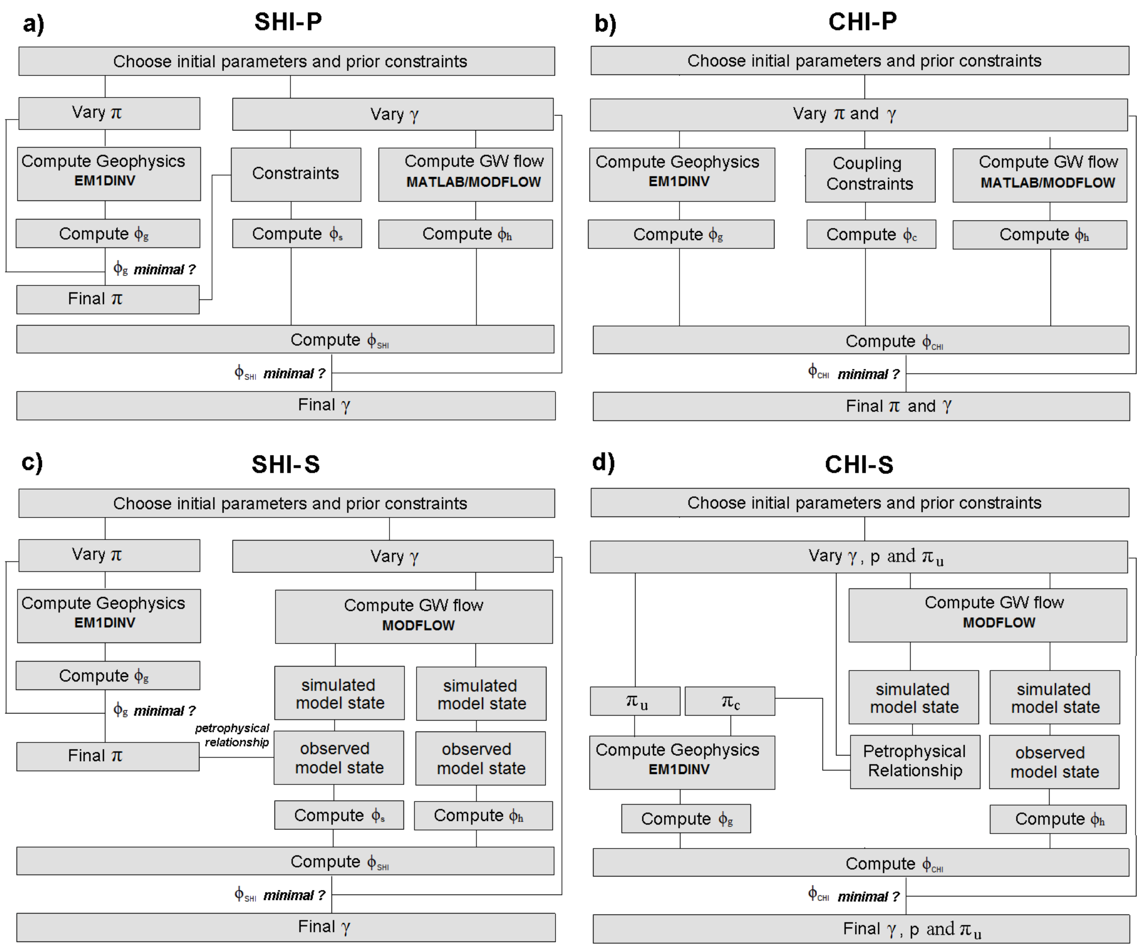

Figure 4.1 Inversion frameworks. Left: SHI, right: CHI. Up: Parameter coupling (P), down: State coupling (S). γ represents hydrologic parameters, π geophysical parameters and p petrophysical parameters. In Figure 4.1d π is divided into π_u and π_c, where π_u are uncoupled (u) geophysical parameters that are estimated independent from the hydrologic model.

In a SHI, the value of the geophysical data for informing the hydrologic models is not only influenced by the geophysical measurement errors, but also by the errors and assumptions associated with the geophysical forward model and the geophysical inversion. For example filter properties of a geophysical instrument might not be modeled correctly [*Effersø et al.*, 1999] and regularization constraints used for the geophysical inversion might bias the hydrologic parameter estimates [*Day-Lewis et al.*, 2005]. Another important error component is the relationship with which geophysical parameters are correlated with hydrologic properties, which might neglect processes or properties that are important for fitting the geophysical measurement data, e.g. heterogeneity in petrophysical properties [*Hinnell et al.*, 2010].

Instead of performing a hydrologic and geophysical inversion separately, a Coupled Hydrogeophysical Inversion (CHI) can be employed, in which the hydrologic model is included in the geophysical inversion (Figure 4.1b and 4.1d).

This has a number of advantages compared to an SHI:

- A geophysical inversion can be undertaken, which is consistent according to an a priori hydrologic interpretation of the geophysical data [*Hinnell et al.*, 2010]
- The geophysical model can be updated according to the hydrologic observations
- Subjective geophysical parameter constraints (i.e. regularization) are partly substituted by a hydrologic model
- As the hydrologic model provides an advanced type of regularization framework for the geophysical inversion, the resolution of the geophysical model can be improved

Disadvantages of a CHI are:

- Larger computational burden
- Propagating errors associated with the hydrologic model into the geophysical model
- Not taking into account processes or properties of the subsurface that are essential for fitting the geophysical measurement data due to a poor coupling strategy between the geophysical and hydrologic model

4.2 State and parameter coupling

Instead of separating hydrogeophysical inversion methods into SHI and CHI approaches, these methods can be subdivided in another way. Many studies have used geo-electric methods to estimate moisture content based on electrical resistivity [*Robinson et al.*, 2008]. *Slater* [2007], *Purvance and Andricevic* [2000] and *Niwas and de Lima* [2003] discuss the estimation of hydraulic conductivity based on electrical resistivity. In contrast to moisture content, hydraulic conductivity is not a simulated state variable of a hydrologic model, but a static hydrologic input parameter. In addition, *Vanderborght et al.* [2005], *Hubbard et al.* [1999] and *Hyndman and Gorelick* [1996] provide examples were geostatistical properties of hydrologic input parameters are estimated using geophysical models. For this purpose this study divides hydrogeophysical inversion methods into a group that uses geophysical models to inform hydrologic models about its input parameters and a group of methods that is focused on simulated hydrologic state variables. We refer to these approaches as parameter (P) and state coupling approaches (S).

Figures 4.1a and 4.1b show the implementation framework for estimating hydrologic model parameters with geophysical data using a parameter coupling approach (SHI-P and CHI-P), where figures 4.1c and 4.1d show the use of a state coupling approach (SHI-S and CHI-S). Paper **I** provides a thorough theoretical description of using a parameter coupling approach. Paper **II** includes the theory for state coupling approaches. For SHI applications parameter and state coupling approaches are straightforward, as a geophysical inversion is undertaken after which the estimated geophysical parameters can be used as additional observations to constrain the hydrologic model. For CHI applications these coupling approaches are more difficult to implement due to the three challenges mentioned at the start of this chapter.

Existing CHI-applications by *Pollock and Cirpka* [2010] *Kowalsky et al.* [2005], *Hinnel et al.* [2010] and *Lambot et al.* [2009] only consider state coupling approaches (CHI-S). In these studies hydrologic and petrophysical parameters are estimated, after which the hydrologic simulations are translated to geophysical parameters to generate a geophysical forward response.

This thesis introduces a small modification with respect to the traditional CHI-S approach applied in *Pollock and Cirpka* [2010], *Kowalsky et al.* [2005], *Hinnel et al.* [2010] and *Lambot et al.* [2009]. This modification comprises the separate estimation of some geophysical parameters (in Figure 4.1d represented by π_u)

that are not coupled with the hydrologic model in order to fit the geophysical measurement data satisfactorily as some geophysical parameters cannot be calculated from the hydrologic simulations. For example in paper **II**, the electrical resistivity of the unsaturated zone needed to be estimated for the geophysical model. The hydrologic model, however, did not provide any information about this geophysical parameter.

The most important development in this thesis is the introduction of CHI-P, which is to our knowledge a new CHI-method. CHI-P employs a parameter coupling between the geophysical and hydrologic model. In the CHI-P both hydrologic and geophysical parameters are estimated. Within these two parameter groups, parameters are constrained using standard regularization constraints. Across the two parameter groups, parameters are coupled using coupling constraints.

The strength of both the CHI-S and CHI-P is their flexibility with which the hydrologic interpretation of the geophysical models can be coupled to the structure, parameters and simulations of a hydrologic model. In principle CHI-S and CH-P can be performed simultaneously, but for clarity reasons this topic will not be further discussed in both the thesis and in papers **I**, **II** and **III**.

4.3 Petrophysical and geometric coupling constraints

Relationships between geophysical parameters and hydrologic models can generally be divided in two groups, petrophysical and geometric relationships. Petrophysical relationships can be specified by empirical laws that describe the correlation between a geophysical parameter value and a hydrologic state variable or parameter. Geometric relationships are different as they apply to the spatial characteristics of the subsurface.

The most widely used examples of petrophysical relationships are given by *Archie* [1942] and *Topp et al.* [1980], which were discussed in paragraph 2.2.2. These laws describe the dependence of, respectively, electrical resistivity and permittivity on soil moisture content. These properties represent the natural characteristics ('physics') of the subsurface or rock ('petro' in Latin). Examples of studies where such petrophysical relationships are used can be found in [*Kemna et al.*, 2002; *Singha and Gorelick*, 2006].

Slater [2007], *Purvance and Andricevic* [2000] and *Niwas and de Lima* [2003] discuss another important petrophysical relationship, which includes the estimation of hydraulic conductivity from geo-electric and IP-data. An important remark in these papers is the log-log relationship between electrical resistivity and hydraulic conductivity. In paper **I** we apply such a relationship in combination with a SHI-P and CHI-P using

$$\log10(K) - \log10(\rho_b) = P + e_s \tag{4.1}$$

In Equation 4.1, K represent the hydraulic conductivity [L/T] of a layer in the hydrologic model and ρ_b denotes the electrical resistivity in a TDEM or geo-electric model, where P is an expected value and e_s the assumed standard error associated with the petrophysical relationship. The assumption behind this relationship would be that the electrical resistivity is not influenced by another factor, e.g. the presence of a contaminant plume. The value for P and e_s depends on a priori knowledge and is site-specific.

In time-lapse applications of geophysical methods, petrophysical relationships can be employed differently. For example, ERT data can be used to monitor a salt tracer experiment. Salt tracer tests are commonly used to estimate the spatial distribution of hydraulic properties [e.g. *Kemna et al.*, 2002; *Vanderborght et al.*, 2005]. In such a setup concentration time series can be derived from the ERT data using a petrophysical relationship, which can be compared with simulated concentrations. Instead of comparing concentration time-series directly, temporal moments of the simulated and observed concentrations can be compared, which are a measure of the mean arrival time and the spread of a tracer [*Day-Lewis and Singha*, 2008]. For monitoring salt-tracer experiments with ERT data, *Singha and Gorelick* [2005] noted that only a fraction (25-50%) of the injected tracer was recovered from the inverted ERT model. To avoid such non-physical results, a CHI-S as in *Pollock and Cirpka* [2010] can be performed to consider the physics of the geophysical technique and the hydrologic process simultaneously.

The second type of coupling constraints between geophysical and hydrologic models comprises geometric constraints. Geometric constraints quantify spatial characteristics of hydrologic properties as the delineation of geological units and the spatial correlation structure of heterogeneous aquifer properties. Examples of studies which use such geometric constraints can be found in *Vanderborght et al.* [2005], *Hubbard et al.* [1999], *Hyndman and Gorelick* [1996] and many other papers. In paper **I** we use a geometric constraint to estimate the elevation of a geological layer in the groundwater model based on the thickness of a layer in the geophysical model.

5 Results

Each paragraph in this chapter successively addresses one of the three research objectives provided in paragraph 1.3 and the major findings in paper **I**, **II** and **III**.

5.1 Informing groundwater models with transient electromagnetic and geo-electric data

In paper **I** we present a CHI-P to inform a groundwater model with Time Domain Electromagnetic (TDEM) and Electrical Resistivity Tomography (ERT) data and compare the results with a SHI. The new aspect of the developed inversion strategy is the ability to constrain hydrologic model parameters with geophysical data. Previous studies about CHI have been applied using CHI-S only. As described in chapter 4 we developed a CHI-P approach. We tested our CHI-P approach for a synthetic groundwater model with TDEM measurements and a real-world groundwater model with ERT data.

For a synthetic study the CHI-P resulted in improved parameter estimates and a reduction in parameter uncertainty for both the groundwater model and the geophysical model compared with a SHI and a separate inversion. Figure 5.1 shows the estimates and confidence intervals for the synthetic groundwater and TDEM model parameters when performing a CHI-P. The x-axis of Figure 5.1 shows the strength of the coupling between the geophysical and groundwater model parameters, marked by e_c which denotes the standard deviation associated with the coupling constraint. When e_c is small, the coupling between the geophysical model and groundwater model is strong. In this analysis we generated 50 realizations of synthetic observation data which we used to estimate 3 groundwater model parameters and 3 geophysical model parameters. For smaller values for e_c, which again mark a stronger coupling between the geophysical and groundwater model, parameter estimates (dashed lines) approximate the truth (solid black line) more closely and parameter confidence intervals are reduced for all parameters. In Figure 5.1 the geophysical parameters are less impacted by the CHI-P.

For another study, considering a real-world groundwater model and an ERT section, a local sensitivity analysis for the groundwater model parameters showed that the use of petrophysical coupling constraints is likely to be of more importance compared to the use of geometric coupling constraints in order to improve groundwater model parameter estimates through a CHI-P. For this second study, parameter uncertainty could not be reduced as well compared to a SHI and the computational burden associated with the CHI-P increased with a factor of ca. 2-3. However, the CHI-P clearly impacted the parameter estimates in both the groundwater model and geophysical model, resulting in consistent parameter estimates between the groundwater model and the geophysical model according to the hydrogeological interpretation of the geophysical model.

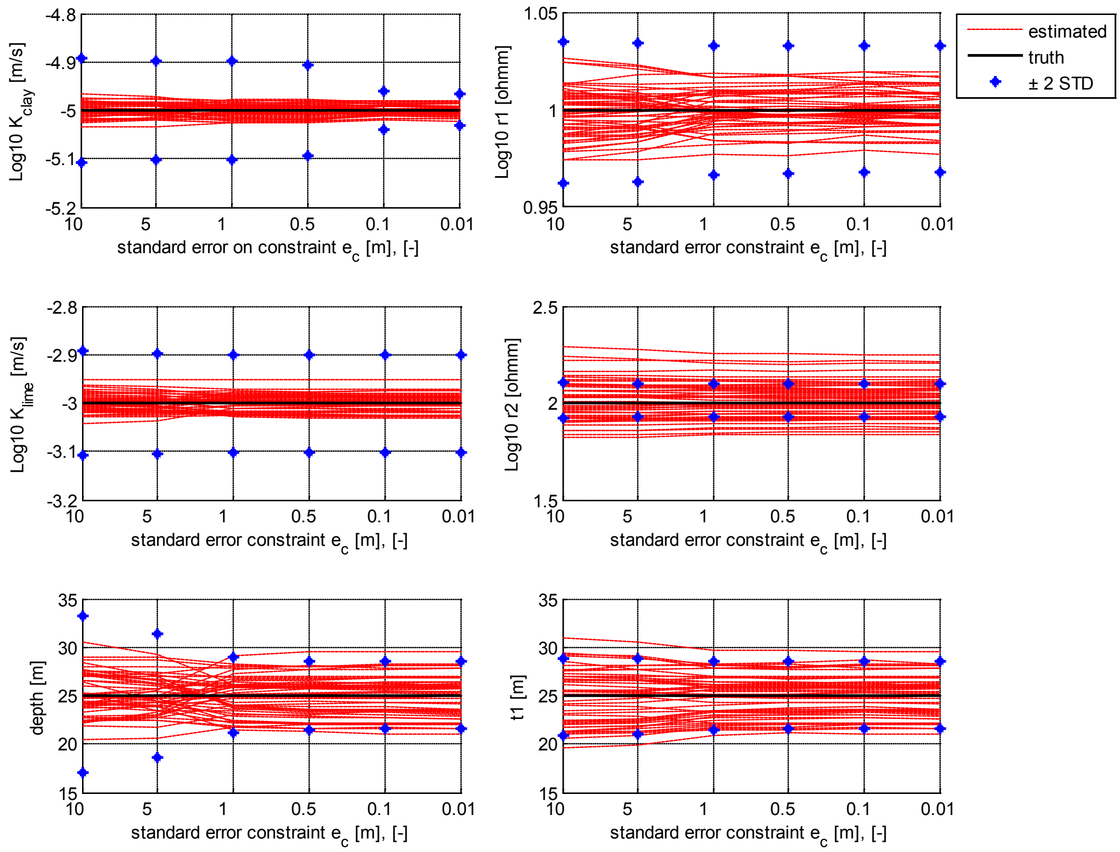

Figure 5.1 Parameter estimates (dashed red lines) for the synthetic example using a CHI with different e_c values for 50 realizations. Groundwater model parameters are shown in the left column of figures, geophysical parameters on the right. The straight black line marks the truth and the blued dots ± 2 standard deviations associated with the estimate. The x-axis shows the standard deviation of the two types of coupling constraints that were used, the geometrical constraint [m] between thickness clay and t1 and the petrophysical constraint between log10 K_{clay} and log10 r1 [-].

The impact by the CHI-P can be seen in Figure 5.2, which shows the inverted ERT model using a separate geophysical inversion and a CHI-P. Figure 5.2a shows a bottom layer of relatively resistive material of ca. 100 -150 Ωm, which dips down towards the east, which was interpreted as the regional limestone aquifer. The second layer at the right part of the profile with a resistivity of about

50 -80 Ωm was interpreted as a sandy deposit, while the first and second layer with a resistivity of ca. 10 Ωm in the left part of the profile were interpreted as clayey deposits. Figure 5.2c shows the uncertainty associated with the parameters that are estimated in the ERT model (layer resistivities: r1, r2, r3; layer thicknesses: t1, t2), expressed by their standard deviation as a percentage of the parameter estimate. This analysis included all the information provided by the data and parameter constraints. Note light colours in Figure 6c indicate relatively poorly resolved parameters, e.g. r1, r2 and t1 at the left part of the profile.

Figure 5.2b shows the inverted ERT model using a CHI-P with an e_c of 0.2. Compared with the result of a separate geophysical inversion in Figure 5.2a, the estimated resistivity of layer 2 decreased significantly from an average of 75 Ωm to ca. 30 Ωm for the first 10 resistivity models. Those were the models for which the electrical resistivity of layer 1 and 2 (r1 and r2) were coupled to the estimation of hydraulic conductivity of the clay in the groundwater model. In paper **I**, it can be seen in that the hydraulic conductivity of the clay was also impacted (Figure 8, paper **I**). Figure 5.2d shows the standard deviations associated with the estimated geophysical model obtained with the CHI-P. The parameter standard deviation of r2 indicates this parameter is not well-determined using the CHI-P as was the case in the separate geophysical inversion. r1 is determined with an approximate standard deviation of 10%. However, Figure 5.2d shows t1 is less well resolved for those model numbers where the petrophysical relationship was applied. The geometric coupling constraint does not show any effect on the estimated geophysical models in Figure 6.

With the results in paper **I** we show the main advantage of performing a CHI, a geophysical inversion that takes in account a hydrogeological interpretation of the geophysical data. *Hinnell et al.* [2010] point out that the formulation of a consistent framework for inference and solution between the geophysical model and hydrologic model is essential when performing a CHI. Our method would provide a very flexible framework to apply a CHI for hydrologic model parameters, which takes in account that 1) only part of a geophysical model can be coupled with a hydrologic model, 2) confidence associated with the hydrologic interpretation of a geophysical model can be altered using different weights for the employed coupling constraints and 3) scale issues can be overcome by coupling several geophysical parameters to hydrologic parameters and vice versa.

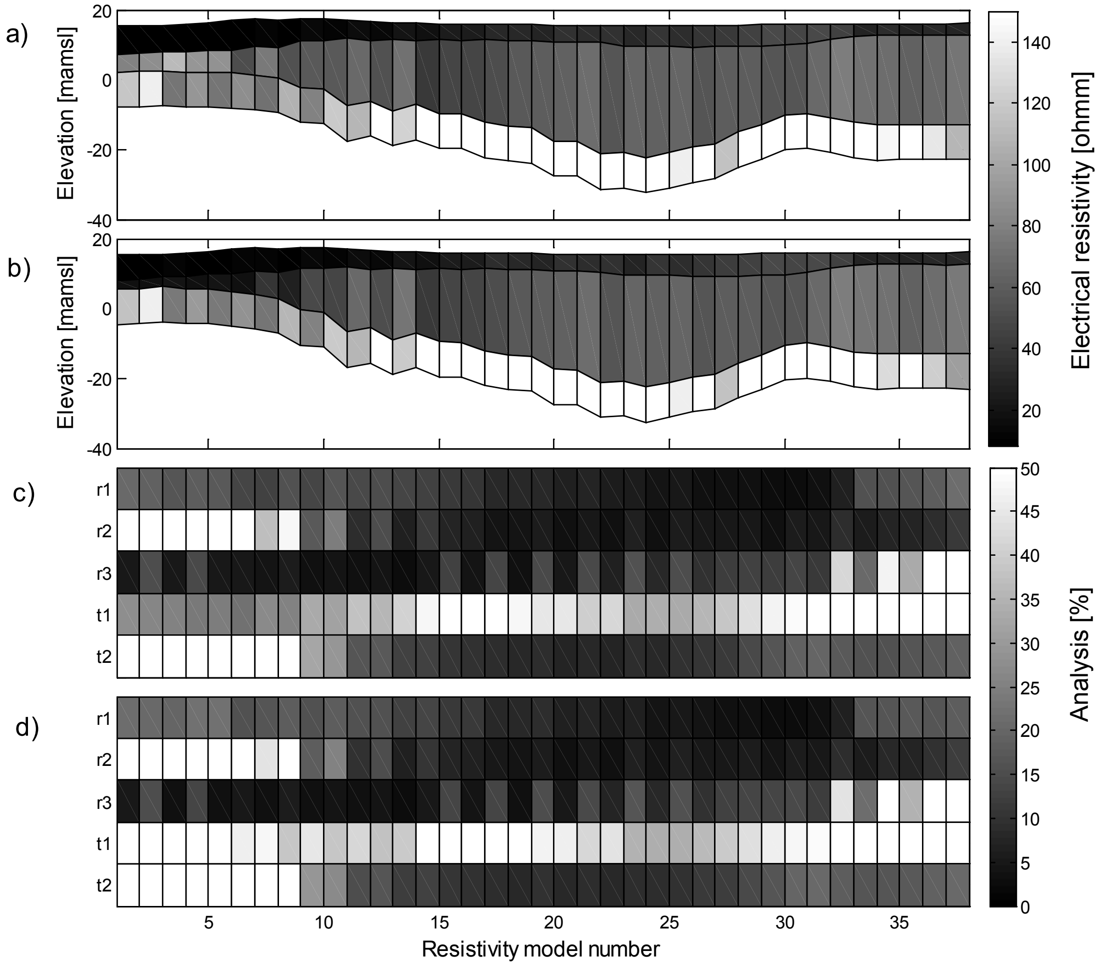

Figure 5.2 Inverted ERT model obtained after a separate geophysical inversion (a) and using the CHI with e_c=0.2 (b) together with a parameter uncertainty analysis expressed by their standard deviation relative to the parameter estimate. A gray scale marks well (dark coloured) and undetermined parameters (light coloured) for the separate geophysical inversion (c) and a CHI-P with e_c=0.2 (d).

5.2 Calibrating a saltwater intrusion model with time domain electromagnetic data

Attempts have been made to calibrate salt water intrusion models with different geophysical data [*Duque et al.*, 2008, *Langevin et al.*, 2003b, *Guérin et al.*, 2001], but all these approaches have been using a SHI (with the exception of *Bauer-Gottwein et al.*, 2010]. A SHI can induce a number of errors related to inconsistent scales between the geophysical and hydrologic models and the assumption behind the petrophysical relationship that converts the simulations of the hydrologic model to a geophysical parameter distribution. For this purpose we apply a CHI-S approach for a small pilot area in California in which we calibrate a salt water intrusion model with TDEM measurement data.

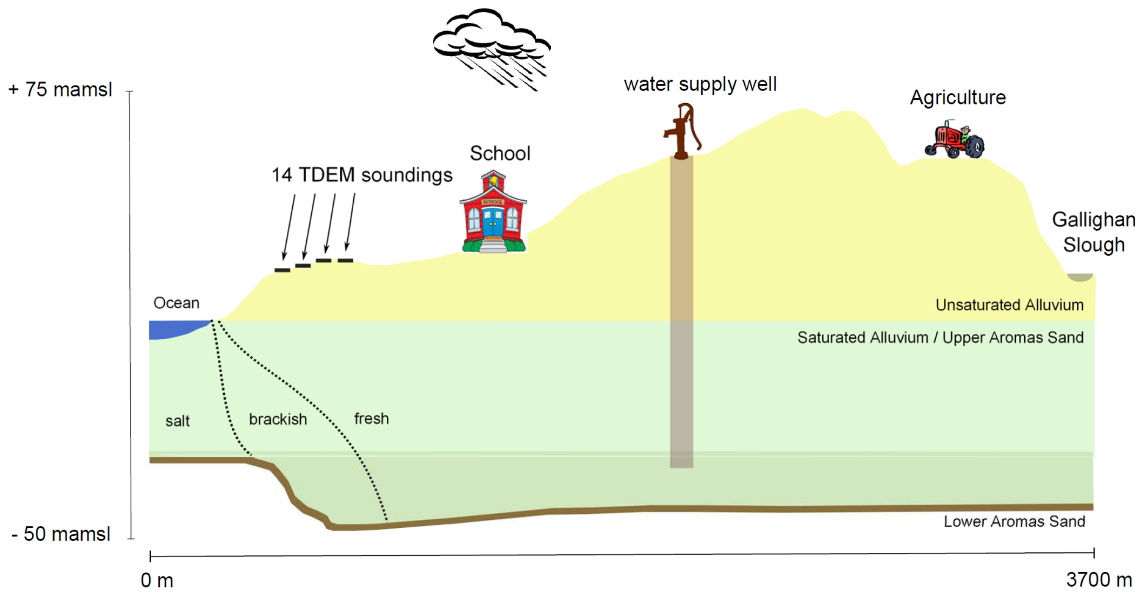

Figure 5.3 Hydrogeological schematization of the School site.

The CHI-P was applied for a semi-synthetic example, based on a real TDEM data set at a site in Monterey, California. For this site 14 TDEM soundings were available and we assumed a cross-sectional model with uniform aquifer properties. The geology and hydrologic processes that are represented by the salt water intrusion model are given by a conceptual hydrogeological cross-section in Figure 5.3, which only represents the water table aquifer that is found in this area, which is separated from the deep aquifer system by a clay unit marked by the Lower Aromas Sand formation. The current extent of the freshwater/salt water interface is the result of pumping activities at this site over a time period of 67 years. For the site no water level or salt concentration data were available and exact properties of the present and past water supply wells are unknown. For this aquifer we want to estimate five uniform aquifer properties (diffusion, dispersion, hydraulic conductivity, anisotropy and porosity) and one petrophysical shape parameter (m in Archie's law) by fitting the collected TDEM data (more than 300 apparent resistivities).

Except for the data at early time gates pertaining to three soundings all the TDEM data could be fitted with a RMSE close to 1 (Figure 6, paper **II**). Possible explanations for the poor data fit for these three soundings are the neglecting of spatial heterogeneity in the salt water intrusion model and not taking in account 3D effects for generating the TDEM forward responses.

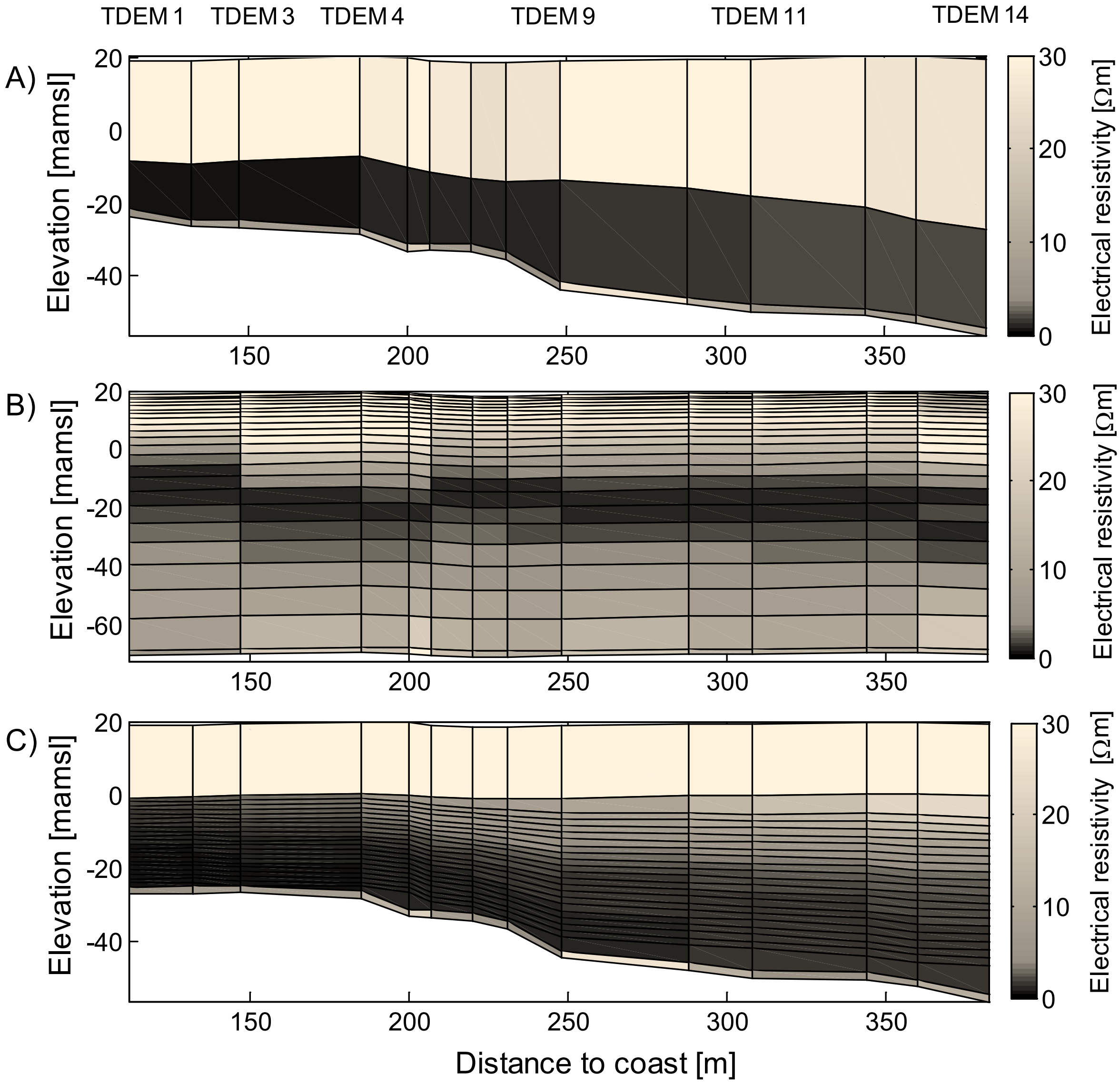

Figure 5.4 Inversion results of the 14 TDEM soundings using A) a 3-layer electrical resistivity model, B) 25-layer smooth inversion and C) CHI-S inversion.

Figure 5.4a presents the inverted 3-layer resistivity models for TDEM sounding 1-14 as a function of the distance with respect to the coast. All electrical resistivity models show a first layer with a high resistivity, a second layer with a very low electrical resistivity and a third layer with a higher resistivity compared to the second layer. The first TDEM-layer can be interpreted as a layer comprising both the dry deposits and the freshwater saturated aquifer, where the second layer with a very low electrical resistivity of less than 1 Ωm represents the salt water saturated sediments. The final third layer in Figure 5.4a is remarkable as it shows an increased electrical resistivity compared with the layer above. This layer has been interpreted as a freshwater saturated clay deposit. In

Figure 4a a dip can be seen associated with the clay layer. Figure 5.4b shows the inversion result for the 25-layer smooth model. The pattern is consistent with 5.4a, showing both the clay layer and the salt water saturated layer. The dip of the clay layer is not very obvious in Figure 5.4b, but provides more information about the distribution of fresh and salt water in the aquifer.

Figure 5.4c shows the resulting TDEM model using a CHI-S. The bottom layer is the same in both Figures 5.4a and 5.4c, representing the clay layer that is present at the site. We fixed the particular geophysical parameters for this clay layer when performing the CHI-S as the salt water intrusion model does not provide any information about this layer. The second commonality between 5.4c and the geophysical inversion results is the high electrical resistivity of the top layer. The difference, however, is the much higher amount of detail for the electrical resistivity in the aquifer. The electrical resistivity model resulting from the 25-layer smooth inversion has a similar resolution, but shows a much less consistent pattern about the distribution of salt and fresh water in the aquifer. Given the simple SEAWAT model, the data fit and the small amount of parameters which could be resolved well (Table 3, paper **II**), obviously the hydrologic model provided a well defined regularization or interpretation framework for inverting the TDEM data.

We think our CHI-S approach provides a great method to extract the huge amount of hydrogeological information that might be available within existing and future TDEM datasets with which salt water intrusion models can be constrained. This could improve the simulation of the past system state of a coastal aquifer, but also provides an opportunity to use TDEM data and salt water intrusion models together as a consistent real-time monitoring and simulation tool to support current coastal water management.

5.3 Monitoring aquifer pumping tests with time-lapse gravity and magnetic resonance sounding data

The previous two applications of applying a CHI were related to relative large scale hydrologic problems. To inform large scale simulation models aquifer pumping tests are conducted, to provide an indication of local aquifer properties as hydraulic conductivity and aquifer storage characteristics. *Blainey et al.* [2007] and *Damiata and Lee* [2004] provided a specific application of time-lapse signals retrieved with relative gravimetry (TL-RG) to estimate aquifer properties for aquifer pumping tests using a CHI-S.

Table 5.1 Properties of the different pumping test scenarios investigated in paper **III**.

Property	Scenario					
	Fully Penetrating	*High Noise*	*Partially Penetrating*	*Delayed Yield*	*Partially Penetrating & Delayed Yield & High Noise*	*Correlated Noise Gravity*
Thickness of aquifer (D), m	50					
Depth to initial water level (hi), m	25					
Hydraulic conductivity (Kh), m/s	10^{-4}					
Anisotropy Kh/Kz	1	1	10	1	10	1
Specific yield (Sy)	0.25					
Radius of borehole, m	0.1					
Well type	Fully Penetrating	Fully Penetrating	Partially Penetrating	Fully Penetrating	Partially Penetrating	Fully Penetrating
Screen interval, m below initial water level	0-50	0-50	40-50	0-50	40-50	0-50
Density of groundwater, kg/m3	1000					
Flow rate (Q), m3/s	0.06309					
Duration of pumping, d	7					
Locations observation wells, m from pumping well	5, 8.3, 13.9, 23.2, 38.7, 64.6, 107.8, 179.8, 300					
Locations RG observations, m from pumping well	5, 8.3, 13.9, 23.2, 38.7, 64.6, 107.8, 179.8, 300					
Locations MRS observations, m from pumping well	5, 179.8					
Measurement error drawdown, cm	5					
Measurement error TL-RG, μGal	2	4	2	2	4	4
Measurement error TL-MRS, nV	10	20	10	10	20	-
Delay index $1/\alpha_d$ [Boulton, 1970], d	0	0	0	2	2	0

In paper **III** we investigate this particular application of CHI-S, as these studies considered highly idealized conditions considering the configuration of the pumping test and accuracy of the geophysical methods. The aim of paper **III** is twofold: 1) major issues are investigated which likely limit the practical utility of TL-RG for pumping test monitoring and 2) we introduce TL-MRS data using a similar CHI-S framework and compare the performance of TL-MRS and TL-RG for pumping test monitoring.

The investigations were performed for a virtual aquifer pumping test, for which synthetic drawdown data was generated together with synthetic TL-MRS and TL-RG measurement data. Subsequently aquifer parameters were estimated using a CHI-S for 6 different scenarios listed in Table 5.1, which comprise respectively (1) a fully penetrating well with low-noise geophysical data, (2) a fully penetrating well with high-noise geophysical data, (3) a partially penetrating well in an anisotropic aquifer, (4) a fully penetrating well in an aquifer showing delayed drainage effects, (5) a real-world scenario of a partially penetrating well in an anisotropic aquifer showing delayed yield in combination with high-noise geophysical data and (6) TL-RG data with correlated measurement errors. Table 5.1 summarizes the assumed properties for the six pumping tests scenarios that were investigated, including the observation locations, the aquifer properties, the pumping test design variables and the standard deviation of the measurement errors that were assumed to generate synthetic observation data.

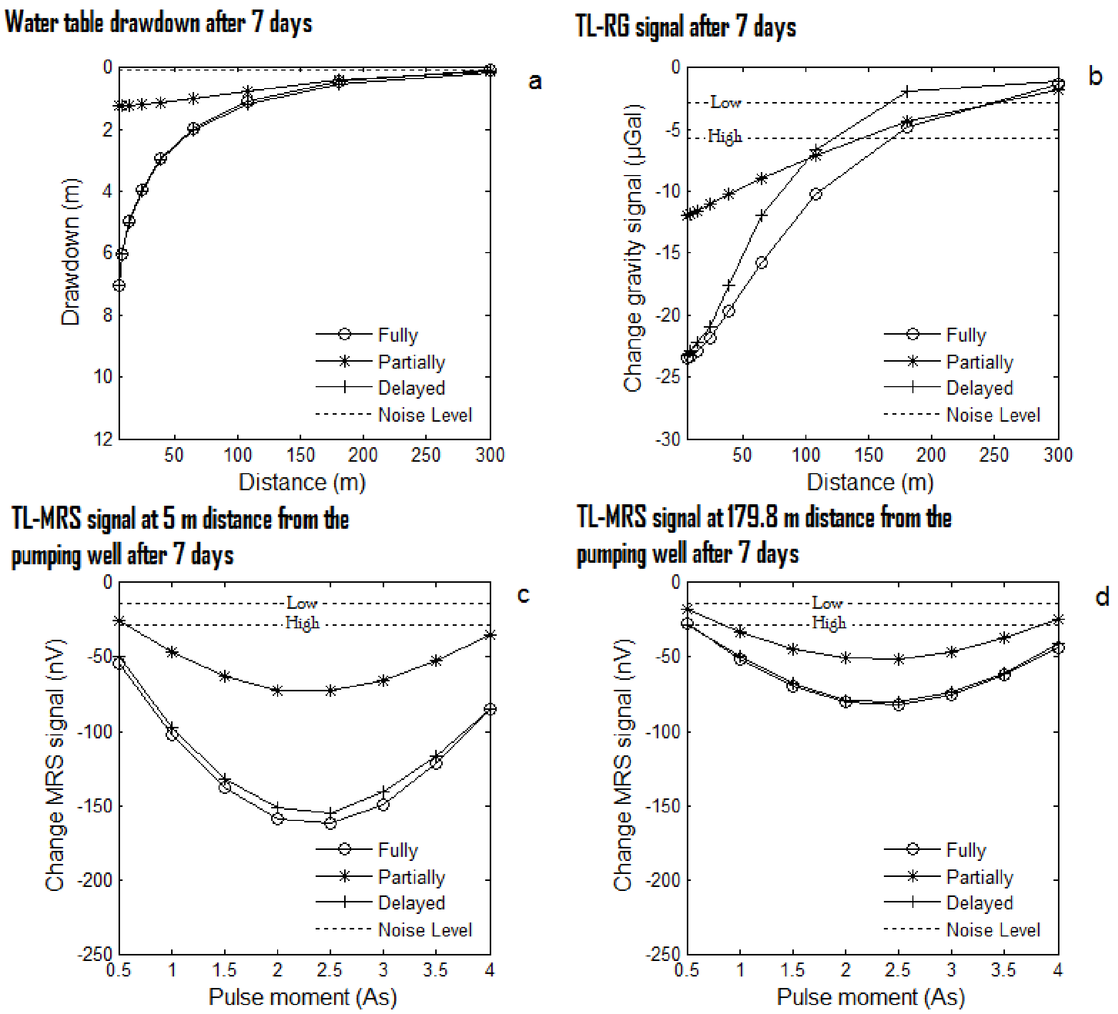

Figure 5.5 Water table drawdown (a) and simulated TL-RG data (b) after seven days of pumping for a fully and partially penetrating well and the inclusion of delayed yield. (c) and (d) show the TL-MRS signal at respectively 5.0 and 179.8 m from the extraction well. Note this figure shows the synthetic data without the added measurement errors. Indicated by the dashed lines are the standard deviations of the measurement errors ("Noise level") that were used to generate the synthetic TL-RG and TL-MRS observations.

In Figure 5.5 the synthetic drawdown, TL-RG and TL-MRS data are plotted without the added measurement errors, for scenrario "Fully Penetrating", "Partially Penetrating" and "Delayed Yield". Figure 5.5a shows the drawdown data of 9 different monitoring wells after 7 days of pumping, which marks an exponential decreasing water table drawdown when moving further away from the extraction well for scenario "Fully Penetrating" and "Delayed Yield". For scenario "Partially Penetrating" water table drawdown is much smaller closer to the pumping well compared with the other scenarios. Figure 5.5b shows the corresponding change in gravity signal together with the measurement errors we investigated for this data type. Figure 5.5c and d show the change in MRS signal (initial amplitude data only) for 8 pulse lengths at two locations with respect to the pumping well (5m and 179.8 m). Remarkable is the large size of the measurement error for the geophysical data compared to the actual signal (signal-to-noise ratio). This signal-to-noise ratio is one of the factors that might limit the sensitivity of TL-RG and TL-MRS to estimate aquifer parameters for a pumping test.

In Table 5.2 we listed the CHI-S results for the 6 different scenarios. Based on this table, we can conclude that more conservative TL-RG and TL-MRS data error estimates (according our own field experience) strongly limits the informative value of the TL-RG data; TL-MRS data was less affected by this. For a partially penetrating well under anisotropic conditions parameter uncertainty could be reduced more effectively compared to a fully penetrating well. Delayed drainage effects did not limit the ability of the TL-MRS and TL-RG data to reduce parameter uncertainty significantly. The incorporation of representative correlated measurement error in the TL-RG data neither affected its informative value.

A local sensitivity analysis showed that TL-RG and TL-MRS observations were most sensitive to the pumping rate and the thickness, specific yield and hydraulic conductivity of the aquifer. The inclusion of TL-MRS data proved to be more effective to constrain the aquifer parameters compared with TL-RG. The inclusion of both TL-RG and TL-MRS had a limited added value compared to TL-MRS only. We conclude that this particular application of CHI-S has a limited potential for TL-RG, while TL-MRS appears to be a more promising method.

Table 5.2 Inversion results showing data misfit, parameter cross-correlation, estimated values, uncertainty ranges and uncertainty reduction percentages for the hydraulic conductivity and specific yield for different observation data sets and each scenario described in Table 5.1.

Calibration dataset	RMSE[a]	Cr-Corr[b] Sy-Kh	Kh[c] (m/s)	Parameter uncertainty (%)[d]	Uncertainty reduction [%][e]	Sy[c] (-)	Parameter uncertainty (%)[d]	Uncertainty reduction [%][e]	Scenario
Truth	-	-	$1 \cdot 10^{-4}$	-	-	0.25	-	-	Truth
Heads	0.82	-0.86	$9.99 \cdot 10^{-5} \pm 2.35 \cdot 10^{-6}$	2%	-	0.251 ± 0.022	9%	-	Fully Penetrating
Gravity	0.77	1.00	$1.07 \cdot 10^{-4} \pm 2.60 \cdot 10^{2}$	>> 100 %	-	0.259 ± 2.248	>> 100 %	-	
MRS	0.86	0.99	$1.07 \cdot 10^{-4} \pm 1.96 \cdot 10^{-4}$	>> 100 %	-	0.278 ± 0.339	>> 100 %	-	
Heads & Gravity	0.86	-0.80	$1.00 \cdot 10^{-4} \pm 1.79 \cdot 10^{-6}$	2%	24%	0.250 ± 0.016	6%	27%	
Heads & MRS	0.92	-0.82	$9.98 \cdot 10^{-5} \pm 1.58 \cdot 10^{-6}$	2%	33%	0.252 ± 0.014	6%	34%	
Heads & Gravity & MRS	0.92	-0.77	$1.00 \cdot 10^{-4} \pm 1.45 \cdot 10^{-6}$	1%	38%	0.251 ± 0.013	5%	42%	
Heads	0.82	-0.86	$9.99 \cdot 10^{-5} \pm 2.35 \cdot 10^{-6}$	2%	-	0.251 ± 0.022	9%	-	High Noise
Heads & Gravity	0.93	-0.84	$9.99 \cdot 10^{-5} \pm 2.08 \cdot 10^{-6}$	2%	11%	0.252 ± 0.019	8%	12%	
Heads & MRS	0.95	-0.85	$1.00 \cdot 10^{-4} \pm 1.73 \cdot 10^{-6}$	2%	26%	0.250 ± 0.016	6%	28%	
Heads & Gravity & MRS	0.92	-0.84	$1.00 \cdot 10^{-4} \pm 1.74 \cdot 10^{-6}$	2%	26%	0.251 ± 0.016	6%	27%	
Heads	0.83	-0.87	$9.99 \cdot 10^{-5} \pm 2.43 \cdot 10^{-6}$	2%	-	0.251 ± 0.023	9%	-	Delayed yield
Heads & Gravity	0.86	-0.83	$1.00 \cdot 10^{-4} \pm 1.89 \cdot 10^{-6}$	2%	22%	0.250 ± 0.018	7%	24%	
Heads & MRS	0.93	-0.83	$9.98 \cdot 10^{-5} \pm 1.60 \cdot 10^{-6}$	2%	34%	0.252 ± 0.015	6%	35%	
Heads & Gravity & MRS	0.92	-0.79	$1.00 \cdot 10^{-4} \pm 1.49 \cdot 10^{-6}$	1%	39%	0.251 ± 0.014	5%	41%	
Heads	0.76	-0.97	$1.01 \cdot 10^{-4} \pm 5.91 \cdot 10^{-5}$	58%	-	0.250 ± 0.057	23%	-	Partially Penetrating
Heads & Gravity	0.83	-0.96	$1.04 \cdot 10^{-4} \pm 4.97 \cdot 10^{-5}$	33%	42%	0.247 ± 0.036	14%	38%	
Heads & MRS	0.90	-0.93	$9.74 \cdot 10^{-5} \pm 3.02 \cdot 10^{-5}$	31%	49%	0.254 ± 0.033	13%	43%	
Heads & Gravity & MRS	0.83	-0.92	$9.94 \cdot 10^{-5} \pm 2.91 \cdot 10^{-5}$	29%	51%	0.251 ± 0.032	13%	44%	
Heads	0.77	-0.98	$1.02 \cdot 10^{-4} \pm 4.46 \cdot 10^{-5}$	44%	-	0.250 ± 0.061	25%	-	Partially Penetrating & High Noise & Delayed yield
Heads & Gravity	0.92	-0.97	$1.00 \cdot 10^{-4} \pm 3.61 \cdot 10^{-5}$	36%	19%	0.250 ± 0.052	21%	15%	
Heads & MRS	0.92	-0.97	$1.00 \cdot 10^{-4} \pm 2.81 \cdot 10^{-5}$	27%	37%	0.249 ± 0.041	16%	34%	
Heads & Gravity & MRS	0.96	-0.97	$1.00 \cdot 10^{-4} \pm 2.76 \cdot 10^{-5}$	27%	38%	0.251 ± 0.040	16%	34%	
Heads & Gravity	0.84	-0.84	$1.00 \cdot 10^{-4} \pm 1.97 \cdot 10^{-6}$	2%	16%	0.250 ± 0.018	7%	17%	Correlated Noise Gravity

[a] Root Mean Square Error, [b] Cross-correlation, [c] Mean ± 2 standard deviations, [d] relative to the estimated parameter value, [e] percentual decrease of parameter ucertainty

6 Conclusions

The combination of hydrologic models and geophysical datasets is powerful as a united characterization tool. Where geophysical techniques are able to provide high resolution datasets that can be correlated with hydrogeological properties, hydrologic models can provide a method to understand and identify the relevant physical processes underlying the geophysical parameter distributions.

This study focused on development of new and the application of existing methods to inform groundwater models with near-surface geophysical data in a consistent way. In paper **I**, **II** and **III** the following key-findings and developments have been made:

- A new Coupled Hydrogeophysical Inversion (CHI) approach has been developed, which is called CHI-P. CHI-P uses a parameter coupling approach, which can be used to estimate hydrologic input parameters with geophysical data by coupling the estimation process of geophysical and hydrologic parameters directly. To our knowledge, existing CHI methods are only focused on CHI-S, in which hydrologic model simulations are transformed to a geophysical model, not on parameter coupling. We believe our CHI-P method increases the flexibility of performing a CHI greatly, especially for the estimation of hydraulic conductivity in groundwater models.

- A minor change was made with respect to the existing CHI-S approaches [*Pollock and Cirpka*, 2010; *Kowalsky et al.*, 2005; *Hinnel et al.*, 2010; *Lambot et al.*, 2009], in order to allow for the separate estimation of geophysical parameters that cannot be computed from simulated hydrological state variables.

- Compared with a Sequential Hydrogeophysical Inversion (SHI), the CHI-P resulted in improved parameter estimates and a reduction in parameter uncertainty for a synthetic groundwater and a Time Domain Electromagnetic (TDEM) model. For a real-world groundwater model and a geo-electric profile, the CHI-P resulted in significant parameter changes in both the geophysical as the groundwater model, which were consistent with the coupling constraints that represented the hydrogeological interpretation of the geophysical model. Parameter uncertainty was not reduced significantly. The computational burden associated with the CHI-P increased with a factor of ca. 2-3 compared with a SHI.

- We successfully applied a CHI-S to estimate an acceptable range of parameter values for the main hydraulic properties of an aquifer, using the data of 14 TDEM soundings in combination with a salt water intrusion model. Given the simple parameterization of the saltwater intrusion model, the data fit and narrow parameter confidence intervals, we think the saltwater intrusion model provided an excellent spatial correlation structure for the geophysical model, yielding a superior resolution which could never be obtained with a separate geophysical inversion and standard regularization constraints.

- We successfully applied a CHI-S to evaluate the potential for time-lapse relative gravimetry (TL-RG) and magnetic resonance sounding (TL-MRS) to estimate aquifer properties during a pumping test. We investigated four practical issues that might limit the sensitivity of these techniques which are (1) a partially penetrating well in an anisotropic aquifer, (2) typical environmental noise properties for TL-RG, (3) delayed yield and (4) correlated measurement error. The findings of this thesis suggest a limited applicability of a CHI-S with TL-RG data for practical pumping tests, but inversion results proved to be more optimistic than we expected beforehand, especially for the partially penetrating well. The inclusion of TL-MRS data appeared more promising compared to the TL-RG data, as parameter uncertainty could be reduced with ca. 30 % for most of the investigated scenarios in this paper.

7 Perspectives

A CHI offers a great opportunity to integrate geophysical information into groundwater models, but like all methods it should fit a clear purpose. Factors determining the suitability of a CHI will depend on whether the targeted prediction is sensitive with respect to the geophysical data, whether the geophysical model will be significantly impacted by the CHI and whether there is enough data to support the assumption behind the coupling relationships between the geophysical and hydrologic model.

Based on this research, we like to address some future challenges and opportunities:

- In Denmark, Australia and the United States large airborne electromagnetic data sets have been collected to map salt water intrusion and delineate groundwater protection zones. At the same time, large regional models are available to simulate salt water intrusion and groundwater flow. According to the results in this thesis, the computational time and the CHI-approach are no practical limitations to perform a CHI on this scale. However, the main question is whether the improvement in groundwater and geophysical models will outweigh the additional effort of performing a CHI.

- In general, large-scale hydrologic models are supported by less data compared to geophysical models. This means the hydrologic model can incorporate large conceptual errors which should not be propagated to the geophysical model by using a CHI. Additional research could focus on the transfer of such conceptual errors and a set of general guidelines about when to use a SHI instead.

- A real aquifer pumping test should be performed in combination with time-lapse magnetic resonance sounding (TL-MRS) and relative gravimetry. For selecting a potential site, aquifer properties and environmental noise properties should be assessed. At three sites in Denmark the environmental noise properties for MRS seem acceptable, which are Skive [paper **I**], Dalby and Bredal [*Chalikakis et al.*, 2008]. To assess the suitability of these field sites, synthetic simulations as in paper **I** need to be performed, in which a rough estimate of the local aquifer characteristics and the intended pumping test design are taken in account.

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9 Papers

I. Herckenrath, D., Legaz-Gazoty, A., Fiandaca, G., Auken, E., Christensen, M., Balicki, M. and P. Bauer-Gottwein, Sequential and Coupled Hydrogeophysical Inversion of a Groundwater Model using Geoelectric and Transient Electromagnetic Data, *Journal of Hydrology*, submitted.

II. Herckenrath, D., Odlum, N., Nenna, V., Auken, E., and P. Bauer-Gottwein, Calibrating salt water intrusion models with Time-Domain Electromagnetic Data, *Groundwater*, submitted. Herckenrath, D., Behroozmand, A., Christiansen, L., Auken, E., and P. Bauer-Gottwein, *Groundwater*, submitted.

III. Coupled hydrogeophysical inversion using time-lapse magnetic resonance sounding and time-lapse gravity data for hydraulic aquifer testing: potential and limitations, *Water Resources Research*, in review.

The papers are not included in this online-version, but can be obtained from the library at DTU Environment. Contact library@env.dtu.dk or
Department of Environmental Engineering
Technical University of Denmark,
Miljøvej, Building 113
DK-2800 Kgs. Lyngby
Denmark

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DTU Environment
Department of Environmental Engineering
Technical University of Denmark

Miljoevej, building 113
DK-2800 Kgs. Lyngby
Denmark

Phone: +45 4525 1600
Fax: +45 4593 2850
e-mail: reception@env.dtu.dk
www.env.dtu.dk

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