WP5 D5.1 D12

Validated algorithms for fully coupled 3-D inversion

ITN Enigma

ENIGMA ITN - This project has received funding from European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie Grant Agreement N°722028.

WP5 - Design inverse modelling strategies for dynamic processes in complex subsurface structures

D5.1/D12: Validated algorithms for fully coupled 3-D inversion

December 2018

Lead Beneficiary:

EKUT Tübingen: Olaf A. Cirpka (Senior manager of this deliverable)

Contributors for this report:

EKUT Tübingen: Olaf A. Cirpka, Veronika Rieckh, Carsten Leven
UL Liège: Jorge Lopez Alvis

ENIGMA ITN - This project has received funding from European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie Grant Agreement N°722028.

Objectives of the Work Package

The challenges addressed in WP 5 are

(1) to enhance our capability to represent complex sedimentary and fractured structures that determine the spatial distribution of preferential flow paths, the dispersion of dissolved chemical species, and the related fluxes and reaction rates,
(2) to infer groundwater flow transport and reaction processes from geophysical measurements in a consistent, fully coupled framework rather than relying on decoupled geophysical inversion and hydrological interpretation of the tomograms.

Description of work

The identified activities are

(i) to define new strategies for representing complex architectures of sedimentary and fractured media, based on training images, multi-point geostatistics, and genetic approaches,
(ii) to develop inversion frameworks that integrate data of diverse nature, and address model uncertainty,
(iii) to establish novel tomographic inversion approaches for 3-D imaging based on fully coupled inversion of time lapse ERT and GPR of tracer motion, hydraulic tomography and heat tracer tests.

ENIGMA ITN - This project has received funding from European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie Grant Agreement N°722028.

Introduction

The transport of fluids and their constituents in the subsurface causes a change in the physical properties of the medium. The aim of hydrogeophysical investigations is to study these changes by geophysical surveying techniques in order to infer the groundwater flow and solute transport behavior in the investigated domain, estimate hydraulic, geophysical and other material properties, and predict the system behavior under changing boundary conditions. Hydrogeological data such as hydraulic heads, tracer concentrations, or derived variables such as solute travel times provide additional information to the geophysical data. While combining data of such disparate nature should theoretically improve the accuracy of the subsurface description, it also adds complexity, introduces additional properties to be considered (which are non-uniform and uncertain by themselves) and can cause inconsistent interpretations. Therefore, the joint analysis of geophysical and hydrogeological data is an active area of research (Binley et al. 2015; Rubin and Hubbard 2005; Vereecken et al. 2006).

The aim of this report is to give an overview of existing algorithms to jointly use hydrological and geophysical data in a single problem set. We have divided available methods into four groups of inverse modeling approaches and summarize these in a paragraph each.

Inverse modelling

The most important parameter in hydrogeology, the hydraulic conductivity, cannot directly be measured in-situ. Instead, it must be inferred from measurements of dependent state variables, such as hydraulic heads. The usual procedure of fitting analytical solutions to the observations (e.g., in pumping-test analysis) is based on the assumption that the subsurface properties are spatially uniform, which is in contrast to the observation that subsurface environments are highly heterogeneous. Thus, the aim of hydrogeological inverse modeling is to infer the spatial distribution of hydraulic parameters from a few measurements of dependent quantities. As the number of observations is always finite, whereas a continuous parameter field is theoretically infinite-dimensional, regularization is needed, in which either the domain is discretized into a fixed set of zones, or deviations from smoothness are penalized, or the parameter field is assumed to be autocorrelated with known correlation function.

If more information is included in the inversion, typically also more parameter fields need to be estimated: storativity in case of transient hydraulic-head information, porosities and dispersivities in case of concentration measurements, and petrophysical parameters in case of geophysical measurements. At the same time, the measurements are prone to measurement error and potential bias, and the models suffer from numerical errors and conceptual deficiencies. In inverse modeling, the task is thus to find effective parameter distributions so that the models fit the observations within their observational error, while avoiding overfitting to spurious oscillations in the data. A review on inverse methods for in subsurface hydrology is given by Zhou et al. (2014), among others.

ITN Enigma

ENIGMA ITN - This project has received funding from European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie Grant Agreement N°722028.

Standard techniques often divide the subsurface into distinct zones and estimate a finite set of zone-related parameters. This procedure predefines the structure of the solution. In an alternative approach, each grid cell of a numerical model is allowed to have its own parameter set, which facilitates high flexibility. However, the number of model grid cells is typically much larger than the number of observations, thus requiring regularization as mentioned above. In problems that are underdetermined without regularization, many parameter distributions can explain the data equally well. Stochastic approaches aim at exploring the ensemble of all parameter fields that can explain the observations, called the conditional parameter fields, with respect to mean parameters, remaining uncertainty, and correlation among the conditional parameter sets. Some approaches, such as the Quasi-Linear Geostatistical Approach (Kitanidis 1995) explore the uncertainty bounds by linearized uncertainty propagation, which requires that the dependence of the observations on the parameters is only weakly nonlinear, while other methods generate multiple parameter sets of equal probability. Geostatistical approaches targeting the maximum a-posteriori likelihood of the parameter sets are mathematically equivalent to Tikhonov regularization, commonly applied in geophysical inversion, in which deviations from a given mean value or derivatives are penalized (Tarantola, 2005). Targeting the mean parameter values, the approaches do not yield the fine-scale variations of parameters that exist in the unknown reality. While it is impossible to perfectly resolve the heterogeneity on all scales, neglecting fine-scale variability altogether can lead to erroneous macroscopic behavior (e.g., solute plumes remain too compact in the model prediction), requiring parameterizations of the unresolved variability (e.g., the introduction of resolution-dependent dispersion coefficients). Thus, conditional realizations of parameter fields have the advantage that the fine-scale variability is simulated rather than accounted for by parameterization. Conversely, they typically require a higher computational effort than the estimation of the smooth best estimate.

The competing objectives of an inverse method for hydrogeophysics are thus:

(i) The approach should in principle be capable of including as many types of data sets as possible without redeveloping the entire code.

(ii) The approach should allow maximum flexibility with respect to spatial representation of the parameter fields.

(iii) The approach should reflect the coupled physical behavior of flow, transport, and geophysical surveying in the subsurface

(iv) The approach should be based on conditional realizations rather than aiming at a single best estimate to address uncertainty and avoid parameterization of the effects of unresolved heterogeneity on flow and transport.

(v) The approach should not introduce inversion artifacts (bias caused by the inversion itself).

(vi) The approach should be computationally efficient, easy to implement, and easy to extend.

Obviously, the last requirement stands in contrast to the preceding ones so that compromises have to be found.

ITN Enigma

ENIGMA ITN - This project has received funding from European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie Grant Agreement N°722028.

The most common approach in hydrogeophysics is to decouple the inverse geophysical problem from the inverse hydrogeological problems (e.g., Day-Lewis et al. 2006; Day-Lewis et al. 2003; Johnson et al. 2012; Muller et al. 2010; Perri et al. 2018; Vanderborght et al. 2005). That is, the geophysical measurements are inverted to obtain presumed distributions of real or complex electric resistivity, seismic velocity, or other typical target properties of geophysics. These are then transformed either directly to hydraulic parameter estimates by assuming petrophysical relationships, or to hydraulic state variables such as concentrations that are inverted in a second step. The key difficulty of this approach is that the geophysical inversion is not constrained to geophysical parameter fields that meet hydraulic conservation laws. A classic example is that the inversion of electrical-resistivity tomography (ERT) data gathered during a salt-tracer test leads to tomograms that – after being transferred to concentration distributions – don't conserve solute mass (Singha and Gorelick 2005). This can be avoided in fully coupled hydrogeophysical inversion, in which the geophysical surveying data are directly inverted to the hydraulic parameters.

Geophysical methods for hydrological applications

Applying geophysical surveying techniques has a long-standing tradition in hydrogeology (Butler 2005; Kirsch 2006). The most classic applications aim at revealing subsurface structural information, such as the base of a gravel aquifer and the extent of features within the aquifer. Also the detection of the groundwater table by geoelectrical methods has been used already decades ago. Exerting a hydraulic stress onto the groundwater body does not only change hydraulic state variables but also geophysical properties which can be detected by geophysical surveying. As example, lowering the groundwater table in a pumping test can be observed by gravimetric measurements (e.g., Gehman et al. 2009), or via the change of electrical properties with changing water saturation by geoelectrical and/or electromagnetic surveying (Rizzo et al. 2004; Straface et al. 2007). The clearest response with respect to electrical properties is gained by changing the concentration of dissolved solids in salt-tracer tests or in the monitoring of seawater intrusion. Changes in geophysical properties can be monitored by geophysical surveying techniques. Because of their non-invasive nature, their speed and cost effectiveness, geophysical methods are considered "smart" observation techniques. Combining them with hydraulic tests, in which the cause of changes in geophysical properties is perfectly known, helps overcoming problems of ambiguity.

ITN Enigma

ENIGMA ITN - This project has received funding from European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie Grant Agreement N°722028.

Geophysical Methods

Excellent introductions to the field of shallow subsurface geophysics are given by Rubin and Hubbard (2005) and Hubbard and Linde (2010). Knödel et al. (2007) and Kirsch (2006) focus on the application of geophysical methods and give practical advice for planning surveys and interpreting the results. In the following, we briefly review the four most important techniques.

Electrical Resistivity Tomography

Electrical Resistivity Tomography (ERT) is a geoelectrical method to determine the distribution of electric conductivity in the subsurface. An electrical current is injected into two electrodes and the occurring voltage difference is measured at two other electrodes. Parallel instruments are able to measure various voltage differences simultaneously and provide fully automated monitoring procedures. Due to its speed, flexibility and simplicity, ERT is widely used in many applications.

Various lab studies (Bing and Greenhalgh, 1997; Pollock and Cirpka, 2010; Lekmine et al., 2017) have shown that Electrical Resistivity Tomography is suitable for tracking a moving fluid parcel which differs in electrical conductivity from the background solution. ERT has also been used in field applications, either for the monitoring of salt-tracer tests (Singha and Gorelick, 2005; Perri et al., 2012; Doro, 2015), or for the monitoring of electrical-conductivity fluctuations in the subsurface (e.g., Doetsch et al., 2012; Auken et al., 2014; Wagner et al., 2015; Coscia et al. 2011; Rosales et al. 2012). Monitoring seawater intrusion (e.g., Nguyen et al. 2009) as well as landslide monitoring (e.g., Perrone et al. 2014; Loke et al., 2013; Friedel et al., 2006; Travelletti et al. 2012) are other possible fields.

Most of the cited studies applied a decoupled approach of interpreting the ERT data. They typically image the distribution of dissolved salts (from tracer tests or seawater intrusion). These images are then used to interpret the flow field. Examples are given in de Franco et al. (2009); Martinez et al. (2009); Zarroca et al. (2011) who investigated dynamics of the saltwater intrusion. An exception is Pollock and Cirpka (2010), who determined the temporal moments of the ERT response in a salt-tracer test and applied a fully coupled inversion method based on the Quasi-Linear Geostatistical Approach of Kitanidis (1995). Bouzaglou et al. (2018) interpreted ERT signals obtained in laboratory tests on sea water intrusion applying a fully coupled approach using SUTRA as flow-and-transport simulator and the Ensemble Kalman Filter as inverse kernel.

A key problem of ERT is that the underlying Poisson equation is an elliptic diffusion equation. Like all other potential methods, ERT is incapable of detecting sharp contrasts, both in the geological structure and the salt-concentration of the tracer solution. The smoothing constraints commonly applied for regularization in the inversion prevents the recovery of sharp contrasts even further. Another inherent problem of the method is its inability to detect more resistive zones embedded in a higher conductive environment as the current flows primarily in the more conductive zones. Even if these zones are large enough to be detected, the ability to resolve the specific value of electrical conductivity is very limited. To overcome the mentioned shortcoming of the methods, many studies have coupled ERT with other

ITN Enigma
ENIGMA ITN - This project has received funding from European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie Grant Agreement N°722028.

geophysical methods (Doetsch et al., 2010; Linde et al., 2008; Linde et al., 2006; Gallardo and Meju, 2004; Binley et al. 2002). Synthetic studies (Jardani et al., 2013; Irving and Singha, 2010) demonstrate the potential of fully-coupled ERT with the transport problem in salt tracer tests. Pollock and Cirpka (2010) and Camporese et al. (2015) have used it in a laboratory experiment.

A major problem in field studies is that the petrophysical relationship for converting bulk electrical conductivity to salt-tracer concentrations (or mixing ratios of seawater) is uncertain. Attempts have been made to couple ERT, Ground Penetrating Radar (GPR) and hydrological data based on structural similarity constraints (Lochbühler et al., 2013). A cross-gradient regularization ensures structural similarity of the obtained parameter fields.

For the vadose zone, Binley et al. (2002) have shown that electrical resistivity as well as cross-borehole radar data bears information on the soil moisture dynamics, that can be integrated into soil-hydrological modeling. In the mentioned study only a trial-and-error approach was used to fit the geophysical to the hydrological data.

Electromagnetic Induction

This method uses electromagnetic induction of the soil to study electrical conductivity and magnetic susceptibility distributions in the shallow subsurface. It usually consists of a single transmitter and several receiver coils in a fixed distance. Unlike ERT, the measurement device does not require direct coupling to the ground, making it feasible to be mounted on small vehicles for rapid data collection. The investigations depth depends on the coil separation.

Electromagnetic induction is often applied for soil moisture mapping (Lavoué et al., 2010; Robinson et al., 2009) as well as studying the distribution of contaminants in soils (Yoder et al., 2001). Studies for the saturated zone are rare. In general, electromagnetic induction is primarily used as a mapping tool. Data sets from devices with several receiver coils also permit inferring the vertical electric-conductivity profile (Mester et al., 2011). Often a local 1-D assumption, where the conductivity variations only occur in the vertical axis, is taken. Gradient-based inversion approaches work well as the number of model parameters is small. Depending on the prior knowledge, the data can be inverted for the value of electrical conductivity in a given number of layers. The thickness of these layers may be known a-priori or also included as parameters. With limited prior information an Occam inversion (Constable et al. 1987) in 1-D is used. The model parameters are the electrical conductivity of predefined fixed layers and regularized with a smoothing constraints.

Electromagnetic methods are used in hydrological application, e.g., for the monitoring of spatiotemporal moisture variations and the estimation of saturated and unsaturated hydraulic conductivity (e.g., Farzamian et al. 2015; Farzamian et al. 2017; Huang et al. 2016; Huang et al. 2017).

ITN Enigma
ENIGMA ITN - This project has received funding from European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie Grant Agreement N°722028.

Ground Penetrating Radar

In Ground Penetrating Radar (GPR), high frequency electromagnetic waves are used to investigate the subsurface. The propagation of these waves is sensitive to the dielectric permittivity and the electric conductivity of the subsurface. These waves are also reflected at interfaces exhibiting sharp contrasts of these properties. The method is either used with surface measurements or in a tomographic setup in boreholes. Depending on the objectives of the study and the survey design, imaging as well as parameter estimations is possible. The latter is more suitable for fully-coupled hydrogeophysical inversion. An inherent problem of GPR in practical applications is that it becomes unsuitable at sites with high clay contents. Clay attenuates the electromagnetic wave severely and thus leads to insufficient signal strength. In many fluvial settings, alluvial fines prohibit the use of surface GPR for the investigation of the underlying sandy gravel aquifers. In these situations, however, cross-borehole GPR is suitable. In several studies (e.g, Doetsch et al. (2010) for sedimentary aquifers, Looms et al. (2008) for the unsaturated zone, and Dorn et al. (2012) for fractured aquifers) GPR was used for monitoring flow and transport in the subsurface.

Attenuation of the electromagnetic waves has been traditionally disregarded as a source of information about the subsurface, including its hydrologic state (e.g., Linde et al. 2006). However, recent advances in full-waveform forward modeling and full-waveform inversion for GPR (Meles et al. 2010) have made feasible to quantify attenuation (in addition to travel time) and relate it to changes in electric conductivity. As a result, recent studies have proposed to use attenuation data from full-waveform inversion to monitor changes in hydrologic states (Jadoon et al. 2012; Haruzi et al. 2018).

The underlying principle for fully-coupled analysis is provided by the possibility to relate changes in hydrologic states to changes in both travel time and attenuation (phase and amplitude) of the electromagnetic waves, which are mainly dependent on dielectric permittivity and electric conductivity, respectively. Kowalsky et al. (2005) give an early example where fully-coupled inversion of cross-hole GPR was applied to estimate soil hydraulic parameters during infiltration experiments by relating changes in water content to changes in travel time (i.e. changes in dielectric permittivity). Most of the studies using a fully-coupled inversion for GPR data have focused on changes in water content and simple parameterizations of the subsurface (Slob et al., 2008; Jadoon et al., 2012; Busch et al. 2013).

Seismics

For a seismic survey a sound wave, travelling through the subsurface, is triggered at a defined source location and recorded by various geophones distributed over various distances or boreholes. The travel-time of such a wave is affected by various physical properties of the material, specifically the density and the Young’s modulus. Also the wave is reflected on interfaces where these parameters change abruptly. In hydrogeophysical surveys, the fact that increasing fluid pressure will decrease the effective stress and hence the speed of the sound wave is exploited. Especially studies using the occurring differences between primary and secondary waves, which correspond to compressional waves and shear waves, give promising results for tracking flow in the subsurface (e.g. Pasquet et al. 2015).

Principles of the Joint Analysis of Geophysical and Hydraulic Data

A key challenge in coupling the analysis of hydraulic and geophysical data in a hydrogeophysical framework is that the datasets used are disparate at first, and a unique relationship is difficult to establish. The joint analysis of hydrogeological and geophysical data can be based on (1) assumed petrophysical relationships, (2) assumed structural similarity of parameter fields, (3) targeted triggering of changes in geophysical properties during hydraulic tests.

(1) Petrophysical relationships

Petrophysical relationships are laws connecting two or more physical properties of a rock. They are typically based on a conceptual model of the pore geometry and properties of the grain surfaces. Some petrophysical laws involve hydraulic state variables, such as the water saturation or the concentration of salt, while others predict both hydraulic properties, such as the hydraulic conductivity, and geophysical properties, such as the electrical resistivity, the spectral complex resistivity, or the electromagnetic permittivity. In petroleum engineering, empirical relationships between porosity (which is well accessible by geophysical borehole logging) and intrinsic permeability are popular. Unfortunately, establishing these relationships is often site-specific, so that without site-specific calibration the spatial distribution of, e.g., electric conductivity, cannot directly be transferred to that of hydraulic conductivity.

(2) Structural similarity

The key idea of joint inversion within geophysics is that the distribution of geophysical properties is related to structural features of the subsurface. The assumption is that different facies are distinct from each other with respect to several geophysical properties, such as electrical resistivity and seismic velocity. Even without a clear petrophysical relationship among those properties, the inference of one property can be enhanced by considering the estimated spatial distribution of the other property. Cross-gradient approaches, in which gradients of the different properties are forced to correlate, have been widely used in near-surface geophysical inversion with promising results regarding the identification of different geophysical facies (e.g., Doetsch, 2010; Lochbühler, 2013). Some attempts have been made to interpret the identified facies also as units with distinct hydraulic parameters, so called hydrofacies. In this framework, geophysical methods are used to identify the distribution of a few distinct materials, the hydraulic properties of which need to be identified by calibrating flow-and-transport models using the structural zonation from geophysics.

ITN Enigma
ENIGMA ITN - This project has received funding from European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie Grant Agreement N°722028.

(3) Geophysical monitoring of hydraulic tests

The two approaches listed above are based on a static view onto the subsurface, in which geophysics is used to identify the fixed spatial distribution of electric, magnetic, electromagnetic, seismic, or gravimetric properties of the subsurface. This is very much in line with classic geophysical surveying, performed once to obtain structural information that does not change in time. A key difficulty in relating these properties to hydraulic properties lies in the ambiguity of the relationships. To overcome at least some of the ambiguity, geophysics may be used to monitor changes of subsurface properties induced by hydraulic tests. This could be pumping tests, in which the water table and thus all water-saturation related geophysical properties change, or salt-tracer tests, in which the electric conductivity is altered by the tracer injection. If sufficient hydraulic data exists, also natural signals (both water-table fluctuations and changes in salinity) can be monitored by geophysical methods and well interpreted by hydrological models.

The key difference to the static analysis is that the cause of the induced change is known. If time series are considered, the laws describing the transient behavior of hydraulic state variables are well known, and even without exactly knowing the hydrogeological parameters, the timing of the geophysical response is constrained. In classic time-lapse geophysical inversion, regularization in time is applied by penalizing major changes from one time step to the next. This regularization in time is reasonable because the properties only gradually change. However, a physically more consistent regularization is to enforce that the hydraulic state variables (hydraulic head, tracer concentration) meet the well-known conservation laws of groundwater flow and solute transport. As the coefficient of the flow and transport equations are not known, the inverse problem now involves jointly estimating the evolution of the hydraulic state variables, the hydraulic parameters, and parameters related to the petrophysical relationships between the hydraulic and geophysical properties. This problem can be seen as a data assimilation application when the full time series is exploited. The latter strategy is followed by Camporese et al. (2015) who used the Ensemble Kalman Filter to analyze the monitoring of a laboratory-scale seawater-intrusion experiment monitored by ERT. The coupled model of Pflotran for groundwater flow and transport (Lichtner et al. 2017) and E4D for geolectrics (Johnson et al. 2010) is set up as the forward model for the same purpose.

A key difficulty of coupled data assimilation with updating the parameters is that many different quantities are simultaneously updated: the observed states at locations without observations and parameters of the system, which are supposed to be static. A misfit between model prediction and observations can be compensated by updating the states only (which is the main objective of classical data assimilation). While this does not improve the insight about the functioning of the system under investigation, it does at least improve the prediction of the immediate future. This would be the main purpose of classical real-time modeling (e.g. numerical weather forecast). Here, a model with wrong parameters is not considered to be too problematic, as the forecast is pulled towards the observations in each data assimilation cycle. Without data assimilation, however, the model would continuously

ENIGMA ITN - This project has received funding from European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie Grant Agreement N°722028.

deviate from the real system. Data assimilation has been used in hydrogeology only recently (e.g., Hendricks-Franssen and Kinzelbach, 2008). In hydrogeophysics it is an attractive way of using geophysical measurements for pure monitoring purposes, e.g., in the observation of seawater intrusion. The only extension to purely hydraulic models needed is the geophysical measurement operator.

If the target quantities are parameters rather than states, the data assimilation framework is somewhat more critical. Now, a misfit between model predictions and observations can be attributed to a wrong approximation of the states or to wrong parameters. Adding parameters of petrophysical relationships introduces even more degrees of freedom. In a purely hydrogeological application, Hendricks-Franssen and Kinzelbach (2008) augmented the state vector by the parameters, and performed a parameter update less frequently than the state update. However, changes of hydraulic conductivity over time, which are inferred by the data assimilation method, are in contradiction to the expectation that hydraulic conductivity is a constant material property. Erdal and Cirpka (2016) showed that it is impossible to jointly infer hydraulic conductivity and recharge without strong prior knowledge. The same authors also discussed that environmental tracers react to hydraulic forcings on completely different time scales than hydraulic heads which makes their use in data assimilation difficult (Erdal and Cirpka 2017). While the hope in the joint assimilation of states and parameters is that the parameter fields stabilize, it is questionable whether this can be guaranteed if a sequence of models with associated parameters are jointly estimated, which is the case in fully couple hydrogeophysical data assimilation.

The Validated Fully Coupled Hydrogeophysical Inversion Method of Pollock and Cirpka

Pollock and Cirpka (2008; 2010; 2012) followed a different approach of fully coupled analysis of hydrogeophysical data. Their base setting was geoelectrical monitoring of artificial salt-tracer tests. That is, unlike to many field monitoring applications, the boundary conditions were well controlled. They related the timing of the response in geophysical surveying to the timing of the hydraulic response in the hydraulic test. Towards this end, they developed temporal-moment generating equations for the resistance perturbation of a geoelectrical configuration based on the temporal moments of salt-tracer concentrations and extended the quasi-linear geostatistical inversion method for temporal concentration moments (Cirpka and Kitanidis 2000) to the temporal moments of the resistance perturbations. With this, they could directly infer the hydraulic-conductivity distribution from the ERT signals without performing an intermediate purely geophysical inversion. The advantage of using temporal moments of concentration and electrical-resistance time series are threefold:

(1) The large dataset of time-dependent observations is compressed in a physically meaningful way (zeroth moment: total response; first normalized moment: mean time of the response).

ENIGMA ITN - This project has received funding from European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie Grant Agreement N°722028.

(2) The timing of the geophysical response is less sensitive to the petrophysical parameters (here the formation factor) than the measured electrical resistance itself. In essence the impact of the formation factor cancels almost out by taking the ratio of the first over the zeroth moment.
(3) The dependence of the tracer arrival time (and thus of the mean arrival time in the geoelectrical monitoring) on hydraulic conductivity is monotonic, which dramatically increases the convergence radius of the inverse method. Even when starting with an initial parameter distribution that differs significantly from the final estimate, the search direction is clear.

The method of Pollock and Cirpka (2010) uses a Gauß-Newton method with geostatistical regularization as inverse kernel. The sensitivity of all measurements with respect to all parameters is evaluated by adjoint equations, which are all steady-state equations. The steps in inverting the temporal moments of resistance perturbations are:

(1) Solve the forward problem by:
    a. Solving the steady-state groundwater flow equation
    b. Solving the moment-generating equations of the zeroth and first moment of concentration
    c. Solving the moment-generating equations of the zeroth and first moment of resistance perturbation for each current-electrode configuration
(2) Solve the sensitivity for each potential-electrode configuration with respect to log-hydraulic conductivity by:
    a. Solving the adjoint equations for the first moment and zeroth moment of resistance perturbation
    b. Solving the adjoint equation for the first and zeroth moment of concentration
    c. Solving the adjoint equation for hydraulic head
    d. Postprocessing of state variables and adjoint states to obtain the sensitivity
(3) Perform a stabilized Gauß-Newton step to update the log-hydraulic conductivity field and return to step 1 until convergence is reached

The scheme has been tested by 2-D laboratory experiments (Pollock and Cirpka, 2012). A parallelized 3-D code for high-performance computing clusters has been developed and tested by virtual experiments (Schwede et al. 2012). The latter code version jointly inverts the temporal moments of resistance perturbations from ERT monitoring of tracer tests, temporal moments of solute concentrations, temporal moments of heat signals in heat-tracer tests, and hydraulic heads.

A key difficulty of the temporal-moment generating equations is that they require a steady-state flow field, which is not easy to guarantee under field conditions. Also, the evaluation of temporal moments from signal time series requires that the series are complete. Truncated moments cannot be simulated by moment-generating equations.

Based on a Gauß-Newton method, the code requires the evaluation of the sensitivity of all measurements with respect to all parameters, which is computationally very demanding and requires

ITN Enigma
ENIGMA ITN - This project has received funding from European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie Grant Agreement N°722028.

the formulation and solution of at least as many adjoint partial differential equations as there are measurement configurations.

While the underlying quasi-linear geostatistical approach can be used in a mode that infers conditional realizations rather than a single best estimate, the computational effort per realization is as high as the inference of the best estimate. This means that conditional realizations are computationally too expensive to be used in practice, implying the necessity to parameterize the effects of unresolved heterogeneity, e.g., by jointly estimating effective dispersion parameters (Nowak and Cirpka 2006). Also, the method is not set up to account for non-local parameterizations on the scale of unresolved heterogeneity (e.g., mobile-immobile transport), even though discrepancies between solute-concentration observations and geoelectrical monitoring have been identified as signature of mobile-immobile transport (e.g., Day-Lewis and Singha 2008; Singha et al. 2011; Swanson et al. 2012). Indications of anomalous transport also exist at the highly instrumented field site used by ESR 13 (Sanchez-León et al. 2016).

While the method of Pollock and Cirpka has been validated, we see the need to advance the approach in the following aspects:

(1) Changing the inverse kernel from the Gauß-Newton method to an ensemble-based approach that directly generates conditional realizations.
(2) Implementing a Jacobian-free inverse approach so that new measurement types can be easily integrated without developing the associated adjoint operator.
(3) Performing transient calculations of flow, transport and associated ERT monitoring so that flow fluctuations in time and truncation of temporal-moments evaluations can be simulated in the forward operator.
(4) Extending the temporal-moment based approach to address dual-domain (a.k.a. mobile-immobile, anomalous, nonlocal) transport, either by extending the moment-generating equations or by performing transient simulations the results of which are characterized by their temporal moments.

The development of such an improved approach and its application to field data sets is the objective of ESR 13.

ITN Enigma

ENIGMA ITN - This project has received funding from European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie Grant Agreement N°722028.

Inversion Algorithms

All inversion approaches have in common that they reduce the difference between the measured data and their prediction by the model, which is an optimization problem. If Gaussian errors are assumed, the misfit is expressed in terms of an L2-norm (Menke 2012). If $f(m)$ is a non-linear forward operator of the parameters m, and the measured data is contained by the data vector d_{obs}, the objective function becomes, interpreted as the negative log-likelihood of the data in Bayesian inference:

$$\Phi_d = (f(m) - d_{obs})^T C_{dd}^{-1} (f(m) - d_{obs}) \tag{1}$$

If the number of independent measurements is considerably larger than the number of parameters, this objective function defines a well posed problem. A fine spatial resolution of the parameter fields, however, causes the problem to be underdetermined, requiring regularization (Tarantola, 2005; Menke, 2012). This can be achieved by adding a second term Φ_m to the objective function with a relative weight λ_m, expressing the relative importance of fitting the data versus meeting the additional constraints on the model parameters. Typical expressions for Φ_m are the squared deviations from a prior mean value (damping) and the squared gradient of model parameters:

$$\Phi_m^{(0)} = (m - \mu)^T (m - \mu) \tag{2}$$

$$\Phi_m^{(1)} = (Gm)^T (Gm) \tag{3}$$

in which $\Phi_m^{(0)}$ is the zeroth-order Tikhonov regularization term with vector of expected mean values μ, and $\Phi_m^{(1)}$ is the first-order Tikhonov regularization term with the numerical gradient operator G. Both expressions are quadratic with respect to the parameter vector m and thus resemble the kernel of a Gaussian distribution. The latter is assumed in geostatistical regularization, in which the model parameters are assumed to be a second-order stationary random space function:

$$\Phi_m^{(geostat)} = (m - \mu)^T C_{mm}^{-1} (m - \mu) \tag{4}$$

in which C_{mm} is the prior covariance matrix of the parameters resulting from the spatial discretization of the covariance function.

The combined objective function now reads as:

$$\Phi = \Phi_d + \lambda_m \Phi_m \tag{5}$$

Note that the relative weight λ_m of the regularization is not needed in the geostatistical approach where this weight is part of the prior covariance function. Also, the model of the prior mean can be more complex than assuming a uniform value, and regularizations across known discontinuities can be broken to prevent smoothing across such interfaces.

The inverse approaches listed below differ in the way of obtaining the minimum of the objective function.

ITN Enigma

ENIGMA ITN - This project has received funding from European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie Grant Agreement N°722028.

Gauß-Newton and Conjugate-Gradient Type Approaches

In gradient-based approaches, the model response to a parameter change is linearized:

$$f(m + \Delta m) \approx f(m) + J\Delta m \tag{6}$$

in which J is the Jacobian matrix containing the partial derivative of all model-predicted measurements with respect to all model parameters

$$J_{i,j} = \frac{\partial f_i}{\partial m_j} \tag{7}$$

Then, the objective function is minimized by setting its derivative to zero, leading to the following expression for the step size Δm in each iteration (here formulated for geostatistical regularization):

$$\left(J^T C_{dd}^{-1} J + C_{mm}^{-1}\right)\Delta m = J^T C_{dd}^{-1}\left(d_{obs} - f(m)\right) + C_{mm}^{-1}(\mu - m) \tag{8}$$

After each iteration, the model-parameter set is updated, $m_{new} = m_{old} + \Delta m$**,** and the scheme is repeated until a convergence criterion is met.

The scheme can be reformulated such that the order of the system of equations to be solved equals the number of measurements rather than the number of model parameters:

$$m_{new} = \mu + C_{mm} J^T \left(C_{dd} + J C_{mm} J^T\right)^{-1} \left(d_{obs} - f(m_{old}) + J(m_{old} - \mu)\right) \tag{9}$$

The given expression is the original Gauß-Newton method for which variants regarding stabilization and improvement of efficiency exist. Examples of the approach are the Quasi-Linear Geostatistical Approach of Kitanidis (1995), or the open-source package pyGIMLi (Rucker et al. 2017).

Due to the computationally demanding calculation of the Jacobian, the Gauß-Newton method becomes inefficient for problems with many measurements and many observations. In the conjugate-gradient method, which also exists in many variants, the full Jacobian is not needed, as here only the derivative of the objective function Φ with respect to all parameters rather than the derivative of all simulated measurements with respect to all parameters is needed. While the Gauß-Newton method requires evaluating as many adjoint equations as measurements, the conjugate gradient method works with a single combined adjoint equation. For an efficient application using geostatistical regularization, see Klein et al. (2017).

The Gauß-Newton and conjugate gradient methods aim at finding the single best estimate minimizing the objective function. If the regularization is formulated as Tikhonov regularization, aiming at a single estimate is consistent. In a geostatistical framework this is not fully the case. Here, the prior information states that variability exists on all scales, including small ones, but the best estimate is much smoother than any single conditional realization that would meet the measurements. The geostatistical approach gives a linearized estimate of the conditional covariance $C_{mm,c}$:

ITN Enigma
ENIGMA ITN - This project has received funding from European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie Grant Agreement N°722028.

$$C_{mm,c} \approx \left(J^T C_{dd}^{-1} J + C_{mm}^{-1}\right)^{-1} = C_{mm} - C_{mm} J^T \left(C_{dd}^{-1} + J C_{mm} J^T\right)^{-1} J C_{mm} \tag{10}$$

However, generating conditional realizations from the best estimate and the conditional covariance matrix is computationally very demanding if many model parameters are to be considered, and the linearization of the uncertainty propagation causes a bias in the uncertainty estimate if the model $f(m)$ is too nonlinear.

In contrast to geostatistical regularization, the Tikhonov regularization does not provide a direct uncertainty estimate, as the problem is not posed as a Bayesian inference problem.

Ensemble Kalman Methods

In data assimilation, Equation (9) is known as the extended Kalman filter. The original Kalman filter was developed for the strictly linear problem $f(m) = Jm$. Then equation 9 simplifies to:

$$m = \mu + C_{mm} J^T \left(C_{dd} + J C_{mm} J^T\right)^{-1} \left(d_{obs} - f(\mu)\right) \tag{11}$$

This variant is often used in weakly nonlinear problems. It solves the linearized problem by a single update step.

In data assimilation, the states at unobserved locations rather than model parameters are estimated. Here, the mean μ is the propagated state vector originating from the predictive model and $f(\mu)$ is the measurement operator, relating the state vector to the observed quantities. If the state vector at a given time is updated and subsequently propagated further in time by the predictive model, the method is denoted Kalman Filter. By contrast, if the initial state of a forward model is updated to better meet the observations at the end of the time step, the method is denoted Kalman Smoother. In nonlinear subsurface-flow applications, such as in petroleum engineering, smoothers are preferred over filters as they produce physically more consistent model results. The Kalman filters and smoothers can be adapted to update for states and model parameters (Hendricks-Franssen and Kinzelbach, 2008), or parameters only (Nowak 2009; Schoniger et al. 2012). For brevity, we restrict the further discussion to pure model-parameter estimation.

The matrix products in Equation (11) have clear statistical meanings:

- $C_{mm} J^T = C_{mf}$ is the linearly propagated cross-covariance of model parameters m and predicted observations $f(m)$ evaluated before updating the parameters, at $m = \mu$,
- $J C_{mm} J^T = C_{ff}$ is the linearly propagated covariance matrix of the predicted observations. In the update step it is added to the covariance matrix C_{dd} expressing the measurement error of the data. The sum $C_{ff} + C_{dd}$ thus expresses the total uncertainty of the measurements.

The Kalman filter/smoother using the Jacobian J is computationally very expensive for larger problems if the Jacobian cannot be computed analytically. Evensen (1994) suggested to replace the linearized uncertainty propagation by ensemble evaluations (see also Burgers et al. 1998; Evensen 2003). The starting point is an ensemble of prior model parameter sets m_i^{prior} drawn from the prior Gaussian distribution with mean μ and covariance matrix C_{mm}. With each ensemble member, a forward run is performed, resulting in an ensemble of measurement predictions f_i. Then the cross-covariance matrix C_{mf} and the covariance matrix of model predictions C_{ff} can be evaluated from the ensemble:

$$C_{mf} = M^{prior} F^T \tag{12}$$

$$C_{ff} = FF^T \tag{13}$$

in which M^{prior} and F are matrices the columns of which are the deviations of the individual parameter vectors m_i^{prior} and corresponding model predictions f_i from their ensemble mean. Now, for each ensemble member also a random measurement error-vector ε_i drawn from the Gaussian distribution with zero mean and covariance matrix C_{dd} is added to the true observations d_{obs}, and each individual ensemble member is updated by:

$$m_i^{post} = m_i^{prior} + C_{mf}\left(C_{dd} + C_{ff}\right)^{-1}(d_{obs} + \varepsilon_i - f_i) \tag{14}$$

The key advantages of the Ensemble Kalman filters and smoothers over the original variants is that

- no costly Jacobian needs to be evaluated,
- the scheme directly results in an ensemble of possible parameter sets exhibiting variability on all scales,
- the ensemble-based propagated (cross-)covariance matrices are more representative for the entire parameter distribution than their Jacobian based counterparts, which are evaluated at the prior mean only.

The Ensemble Kalaman Filter (EnKF) and Ensemble Kalman Smoother (EnKS) are easy to implement as they only require a forward model and a method to generate an initial ensemble. However, the methods are single linear update steps, which may lead to severe errors in strongly nonlinear applications. In the iterative Ensemble Kalman Smoother (IEnKS), the Gauß-Newton method of Equation (9) is transferred to the ensemble-based approach, circumventing the evaluation of the Jacobian (e.g., Evensen 2018). Even simpler is the Ensemble-Kalman Smoother with Multiple-Data Assimilation (EnKS-MDA), in which the same data are assimilated several times, but in each update step a considerably larger covariance matrix of the measurement error is applied than the original C_{dd} (Evenson, 2018). In The Ensemble Kalman Generator (Nowak, 2009; Schöniger et al., 2012), the same data are used multiple times too, but here individual ensemble members are eliminated from the update step as soon as the likelihood term has reached a threshold value so that overfitting is prevented.

A large number of variants exists for Ensemble Kalman filters and smoothers. Among the common techniques are the restriction to correlations to predefined zones of influence (denoted localization)

ENIGMA ITN - This project has received funding from European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie Grant Agreement N°722028.

to avoid artifacts introduced by small ensemble sizes, the rescaling of the predicted model outcomes to standard normal distributions (normal-score transformation), and the artificial increase of the ensemble spread after application of a few update cycles (variance inflation) to counteract so-called filter-inbreeding, that is, the reduction of the ensemble spread to unrealistically small values centered about the wrong mean.

Within ENIGMA, ESR13 will use the Ensemble-Kalman Smoother with Multiple Data Assimilation for the inversion of steady-state drawdown from pumping tests, mean arrival times of solute tracers in tracer tests, and mean arrival times in electrical-potential perturbations for multiple electrode configuration obtained during salt-tracer tests.

Markov Chain Monte Carlo Methods (MCMC)

The geostatistics-based inversion introduced above is a special application of Bayes theorem:

$$p(m \vee d) = \frac{p(d \vee m)p(m)}{p(d)} \tag{15}$$

in which $p(m \vee d)$ is the conditional probability density function of the model parameters, given the data, $p(d \vee m)$ is the likelihood of the data provided that the model parameters are correct, $p(m)$ is the prior probability density function of the model parameters before considering the data of the dependent quantities, and $p(d)$ is the so-called Bayesian model evidence, which is a mere scaling factor if the objective of the inversion is to estimate the model parameters. A comparison between the objective function of Equation (5) and Bayes theorem reveals that assuming multi-Gaussian distributions of the likelihood and the prior parameter distribution leads to the combined Equations (1), (4), and (5) as maximum the a-posteriori likelihood of Equation (15) is identical to minimizing is negative logarithm.

Both the Gauß-Newton and conjugate-gradient method and the Ensemble Kalman methods strictly require multi-Gaussianity of the underlying distributions, because otherwise the Bayesian inference problem cannot be converted to a weighted least-square optimization. The latter property is the very reason why the mentioned methods are comparably effective, because setting the derivative of a quadratic function to zero (in order to find the minimum) results in a system of linear equations.

A second restriction of the methods discussed above is that they are all based on linearized uncertainty propagation, in case of the standard EnKF/EnKS about the prior ensemble, in case of the iterative EnKF/EnKS about the posterior ensemble, and in case of the Gauß-Newton method about the single best estimate. If the underlying model $f(m)$ is strongly nonlinear, the posterior distribution $p(m|d)$ severely differs from a multi-Gaussian distribution even if the prior and likehood are multi-Gaussian.

The aim of the Markov-Chain Monte-Carlo (MCMC) method is to explore the true conditional probability density function of the model parameters, regardless of multi-Gaussianity and linearized uncertainty propagation. As the name suggests, this is done by a Markov chain. The MCMC scheme generates one proposal parameter set after the other and computes the logarithm of the posterior

ITN Enigma
ENIGMA ITN - This project has received funding from European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie Grant Agreement N°722028.

likelihood $p(m|d)$ for this specific proposal. The log-posterior likelihood is then compared to the log-posterior likelihood of the last accepted proposal, and depending on this comparison and a randomly drawn probability of acceptance, the new proposal is accepted or rejected. After the so-called burn-in period, the Markov chain becomes independent from the start and will sample the entire posterior probability density space, with the sampling density according to their posterior probability of the occurrence. To avoid undersampling of the pdf, the chains have to be rather long. Also, evaluating the posterior probability density of a proposal requires solving the full forward model. This implies that the method of proposing new realizations is crucial for the efficiency of the approach, because a low acceptance rate means solving many forward problems in vain.

The large number of forward runs needed in MCMC is the reason why most applications are restricted to a small number of model parameters and forward models that can quickly be evaluated. Irving and Singha (2010) presented a synthetic study performing a fully coupled hydrogeophysical inversion of a 2-D salt-tracer test monitored by ERT, in which they estimated the spatial distribution of two distinct facies by an MCMC approach. In the latter application, the hydraulic-conductivity value of each facies was uniform and known, but the spatial arrangement of the two facies was not. For the generation of proposal distributions, the authors kept 90% of the model cells constant, and generated new indicator values for the remaining 10% conditioned on the fixed 90%. In each proposal step, they randomly selected a different set of cells to be perturbed. In the virtual truth, they added auto-correlated variability in log-hydraulic conductivity to the indicator fields and also used a slightly different cementation factor in Archie's law for the conversion of concentrations to electrical conductivities. The authors also considered direct observations of concentrations. While the study is very promising with respect to the applicability of MCMC to fully coupled hydrogeophysical inversion, it was restricted to a grid of 20×30 cells, facilitating forward runs within a few seconds. In realistic 3-D applications, the number of grid cells is more than three orders of magnitude larger

Bayesian Evidential Learning

The preceding methods aimed at determining hydraulic parameter values of the subsurface using hydraulic and geophysical data. The underlying hypothesis is that the inversion leads to conditional parameter fields that can be used for all hydrogeological predictions thinkable. The experience in practice, however, is often that tests performed in the field are sensitive to parameters in specific subdomains (e.g., hydraulic conductivities close to pumping and observation wells), whereas specific predictions, such as the breakthrough of a solute in a control plane, are sensitive to other parameters at other locations (e.g., the unresolved heterogeneity of hydraulic conductivity at points far away from the wells). Thus, the high effort of inferring parameter fields from measurements of dependent quantities may not be justified by the limited improvement of the predictive skills of the calibrated models.

If the final application of the model is well defined (such as predicting solute breakthrough curves or drawdown according to not-yet-installed well), the estimation of the underlying parameter fields may

ITN Enigma
ENIGMA ITN - This project has received funding from European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie Grant Agreement N°722028.

not be necessary at all. Instead, a large ensemble of unconditional parameter fields can be used to generate corresponding ensembles of simulated field-survey measurements and of the well-defined prediction metrics. Then, machine-learning tools can be used to relate the observations of the field surveys to the management-related predictions without explicitly addressing the parameter fields that generated the relationship. Such methods are referred to as prediction-focused approaches (Scheidt et al., 2015; Hermans, 2017) or goal-oriented approaches (Sun and Sun, 2015). A Bayesian framework is particularly useful to solve such problems since relations between all variables involved may be expressed through conditional probabilities. Also, it is possible to add realistic structural information by means of non-multi-Gaussian prior distribution.

Bayesian Evidential Learning (Scheidt and Caers, 2018) is a method proposed to find a direct probabilistic link from the observations to the predictions. It is based on Monte Carlo sampling of the whole joint probability distribution of the observations and predictions. Samples are generated by considering many realizations of the subsurface model parameters (expressed through the prior distribution) and then used to simulate the dynamic process to be predicted and the observations used to inform this process. The samples define the marginal distribution of the predictions and observations and the statistical dependence.

Predictions and observations are usually lower-dimensional than the number of subsurface parameters (typically equaling an integer multiple of the number of computational grid cells), they are typically still too high-dimensional to be directly used (e.g., number of electrode configurations times number of times an ERT survey is performed as the dimension of the measurements, and number of times at which concentrations are to be considered times the number of target points as the dimension of predictions). Therefore, methods for dimension reduction have been applied to make Bayesian Evidential Learning computationally feasible. For instance, Scheidt et al. (2015) used a nonlinear principal component analysis (NLPCA) to reduce the dimensions of observations (concentration measurements in one borehole) and predictions (contaminant breakthrough in another borehole) and then applied kernel smoothing in the new low-dimensional space to approximate the posterior probability distribution of the prediction of interest. Similarly, Hermans et al. (2016) used a combination of principal component analysis (PCA) and canonical correlation analysis (CCA) to predict change in temperature due to transport of a heat tracer using borehole electrical resistivity tomography data.

ENIGMA ITN - This project has received funding from European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie Grant Agreement N°722028.

Choosing the method of jointly analyzing geophysical and hydrogeological data most appropriate for the application

The methods mentioned above differ in their computation effort, data requirement, and predictive skill. Typically, higher accuracy and larger generality of the analysis requires a higher experimental, computational (and conceptual) effort. Which type of effort pays of depends on the exact purpose of the analysis. We see four general fields of using geophysical methods in hydrogeological applications:

(i) Using geophysical methods to identify structural features of the subsurface (geometry of major geological units, facies) without assigning hydrogeological properties to these features. ⇨ Structure identification

(ii) Using geophysical surveying as a monitoring method to observe hydrogeological states (water saturation, groundwater table, salt concentration) without inferring hydrogeological parameter fields. ⇨ Geophysical monitoring

(iii) Using geophysical methods as a tool to support hydrogeophysical inversion with the main target of identifying hydrogeological parameter fields. ⇨ Joint hydrogeophysical inversion

(iv) Using geophysical methods to improve well defined hydrogeological predictions without requesting the underlying hydrogeological parameter fields. ⇨ Hydrogeophysical prediction

Geophysical structure identification for hydrogeological purposes can rely on purely geophysical joint inversion methods, such as the cross-gradient regularization of disparate geophysical tests with subsequent cluster analysis (e.g., Paasche et al. 2006). Even though the geophysical facies will not be fully identical to hydrofacies, a sufficient agreement between the different facies can be used to define zones in hydrogeological models with distinct mean hydraulic parameters. The objective of structure identification does not require a fully coupled inversion framework.

In geophysical monitoring a clear relationship between the hydrogeological state of interest (e.g., seawater concentration) and a geophysical property (e.g., electric conductivity) is needed. However, the geophysical observation can be used for a pure state update of the hydrogeological model. Particularly in the monitoring of dynamic systems, this is a classical data assimilation problem, in which the geophysical measurements prevent the hydrogeological model to deviate from the true system behavior. The geophysical measurements need not be used to update the hydrogeological model parameters. It may even be counterproductive if the deviation between measured and predicted geophysical observations stem from erroneous boundary conditions rather than hydraulic parameters. Most likely, a classical Ensemble Kalman Filter or Ensemble Kalman Smoother without parameter update is the appropriate method for such an application.

Fully coupled hydrogeophysical inversion is more demanding as the target is to obtain the hydraulic parameters from geophysical data. Now the geophysical data must not only be sensitive to a

ENIGMA ITN - This project has received funding from European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie Grant Agreement N°722028.

hydrogeological state, but also a clear dependence on the underlying hydraulic parameters is needed. To reduce ambiguity, this should be attempted only when geophysical surveying techniques are used in the monitoring of hydraulic tests in which hydraulic boundary conditions are well defined and a specific hydraulic stress is applied to the system. As mentioned above, it also pays off to consider which metrics in the geophysical response monotonically depend on the hydraulic property of interest and which metrics are the least affected by the uncertainty of petrophysical relationships. That is, while the original data could be a time series of electrical resistances, the mean time of the measured response may be a better indicator of hydraulic conductivity than the resistance time series itself. Successful applications include the Gauß-Newton method (Pollock and Cirpka, 2010, 2012) and the Markov-Chain Monte Carlo method (Irving and Singha, 2010), but the Iterative Ensemble-Kalman Smoother or the Ensemble-Kalman Smoother with Multiple Data Assimilation (Evenson, 2018) applied to the appropriate data metric appear promising, too.

If the target of hydrogeophysical prediction is well defined, there is no need to infer the underlying hydrogeological parameter fields and machine learning techniques that directly relate the geophysical observations to the hydrogeological prediction may be the method of choice. We suggested Bayesian Evidential Learning for this purpose. However, many numerical tests need to be performed to choose appropriate dimension reduction techniques and to analyze which set of geophysical observations is most informative for a specific prediction task.

In summary, it is important to clarify the purpose of a study before selecting the appropriate geophysical surveying technique and setup, the type of dynamic process model, and the method of joint data analysis. Unfortunately, in many practical applications the purpose of a model is not clearly enough defined in beforehand. Because the experimental and computational effort of joint/coupled hydrogeophysical site assessment is very high, unclear objectives can lead to suboptimal measurement designs and choice of data-analysis tools.

ITN Enigma

ENIGMA ITN - This project has received funding from European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie Grant Agreement N°722028.

References

Auken, E., Doetsch, J., Fiandaca, G., Christiansen, A. V., Gazoty, A., Cahill, A. G., and Jakobsen, R. (2014). Imaging subsurface migration of dissolved CO2 in a shallow aquifer using 3-D time-lapse electrical resistivity tomography. *Journal of Applied Geophysics*, *101*, 31-41.

Beven, K. (2016). Facets of Uncertainty: Epistemic Uncertainty, Non-Stationarity, Likelihood, Hypothesis Testing, and Communication. *Hydrological Sciences Journal*, 61 (9), 1652–65.

Bing, Z., and Greenhalgh, S. A. (1997). A synthetic study on crosshole resistivity imaging using different electrode arrays. *Exploration Geophysics*, *28*(1/2), 1-5.

Binley A, Hubbard SS, Huisman JA, Revil A, Robinson DA, Singha K, Slater LD (2015). The emergence of hydrogeophysics for improved understanding of subsurface processes over multiple scales. *Water Resources Research* 51:3837-3866 doi:10.1002/2015wr017016

Binley, A., Cassiani, G., Middleton, R., and Winship, P. (2002). Vadose zone flow model parameterisation using cross-borehole radar and resistivity imaging. *Journal of Hydrology*, *267*(3-4), 147-159.

Bouzaglou V, Crestani E, Salandin P, Gloaguen E, Camporese M (2018). Ensemble Kalman Filter Assimilation of ERT Data for Numerical Modeling of Seawater Intrusion in a Laboratory Experiment. *Water* 10:26 doi:10.3390/w10040397

Burgers G, van Leeuwen PJ, Evensen G (1998) Analysis scheme in the ensemble Kalman filter. *Monthly Weather Review* 126:1719-1724 doi:10.1175/1520-0493

Busch, S., Weihermüller L., Huisman J. A., Steelman C.M., Endres A. L., Vereecken H., and van der Kruk J. (2013), Coupled hydrogeophysical inversion of time-lapse surface GPR data to estimate hydraulic properties of a layered subsurface, Water Resour. Res., 49, 8480–8494, doi:10.1002/2013WR013992.

Butler DK (2005) Near-Surface Geophysics. Society of Exploration Geophysicists, Tulsa, OK. doi:10.1190/1.9781560801719

Camporese M, Cassiani G, Deiana R, Salandin P, Binley A (2015) Coupled and uncoupled hydrogeophysical inversions using ensemble Kalman filter assimilation of ERT-monitored tracer test data. *Water Resources Research* 51:3277-3291 doi:10.1002/2014wr016017

Cirpka OA, Kitanidis PK (2000) Sensitivities of temporal moments calculated by the adjoint-state method and joint inversing of head and tracer data. *Advances Water Resour*ces 24:89-103

Constable SC, Parker RL, Constable CG (1987) Occams Inversion - A practical algorithm for generating smooth models from electromagnetic sounding data. *Geophysics* 52:289-300 doi:10.1190/1.1442303

ENIGMA ITN - This project has received funding from European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie Grant Agreement N°722028.

Coscia, I., Greenhalgh, S. A., Linde, N., Doetsch, J., Marescot, L., Günther, T., ... and Green, A. G. (2011). 3D crosshole ERT for aquifer characterization and monitoring of infiltrating river water. *Geophysics*, *76*(2), G49-G59.

Crestani, E., Camporese, M., and Salandin, P. (2015). Assessment of hydraulic conductivity distributions through assimilation of travel time data from ERT-monitored tracer tests. *Advances in water resources*, *84*, 23-36.

Crestani, E., Camporese, M., Baú, D., and Salandin, P. (2013). Ensemble Kalman filter versus ensemble smoother for assessing hydraulic conductivity via tracer test data assimilation. *Hydrology and Earth System Sciences*, *17*(4), 1517.

Day-Lewis FD, Lane JW, Gorelick SM (2006) Combined interpretation of radar, hydraulic, and tracer data from a fractured-rock aquifer near Mirror Lake, New Hampshire, USA. *Hydrogeology Journal* 14:1-14 doi:10.1007/s10040-004-0372-y

Day-Lewis FD, Lane JW, Harris JM, Gorelick SM (2003). Time-lapse imaging of saline-tracer transport in fractured rock using difference-attenuation radar tomography. *Water Resources Research* 39 doi:10.1029/2002wr001722

Day-Lewis FD, Singha K (2008). Geoelectrical inference of mass transfer parameters using temporal moments. *Water Resources Research* 44 doi:10.1029/2007wr006750

de Franco R et al. (2009). Monitoring the saltwater intrusion by time lapse electrical resistivity tomography: The Chioggia test site (Venice Lagoon, Italy). *Journal of Applied Geophysics*, 69:117-130 doi:10.1016/j.jappgeo.2009.08.004

Doetsch, J., Linde, N., and Binley, A. (2010). Structural joint inversion of time-lapse crosshole ERT and GPR traveltime data. *Geophysical Research Letters*, *37*(24).

Doetsch, J., Linde, N., Coscia, I., Greenhalgh, S. A., and Green, A. G. (2010). Zonation for 3D aquifer characterization based on joint inversions of multimethod crosshole geophysical data. *Geophysics*, *75*(6), G53-G64.

Doetsch, J., Linde, N., Vogt, T., Binley, A., and Green, A. G. (2012). Imaging and quantifying salt-tracer transport in a riparian groundwater system by means of 3D ERT monitoring. *Geophysics*, *77*(5), B207-B218.

Dorn, C., Linde, N., Le Borgne, T., Bour, O., and Klepikova, M. (2012). Inferring transport characteristics in a fractured rock aquifer by combining single-hole ground-penetrating radar reflection monitoring and tracer test data. *Water Resources Research*, *48*(11).

Doro, K. O. (2015). *Developing Tracer Tomography as a Field Technique for Aquifer Characterization* (Doctoral dissertation, Eberhard-Karls-Universität Tübingen).

ITN Enigma

ENIGMA ITN - This project has received funding from European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie Grant Agreement N°722028.

Erdal D, Cirpka OA (2016). Joint inference of groundwater-recharge and hydraulic-conductivity fields from head data using the ensemble Kalman filter. *Hydrology and Earth System Sciences* 20:555-569 doi:10.5194/hess-20-555-2016

Erdal D, Cirpka OA (2017). Preconditioning an ensemble Kalman filter for groundwater flow using environmental-tracer observations. *Journal of Hydrology* 545:42-54 doi:10.1016/j.jhydrol.2016.11.064

Evensen G (1994). Sequential data assimilation with a nonlinear quasi-geostrophic model using Monte-Carlo methods to forecast error statistics. *Journal of Geophysical Research-Oceans,* 99:10143-10162 doi:10.1029/94jc00572

Evensen G (2003). The Ensemble Kalman Filter: theoretical formulation and practical implementation. *Ocean Dynamics* 53:343-367 doi:10.1007/s10236-003-0036-9

Evensen G (2018). Analysis of iterative ensemble smoothers for solving inverse problems. *Computational Geosciences* 22:885-908 doi:10.1007/s10596-018-9731-y

Farzamian M, Santos FAM, Khalil MA (2015). Application of EM38 and ERT methods in estimation of saturated hydraulic conductivity in unsaturated soil. *Journal of Applied Geophysics* 112:175-189 doi:10.1016/j.jappgeo.2014.11.016

Farzamian M, Santos FAM, Khalil MA (2017). Constraining Unsaturated Hydraulic Parameters Using the Latin Hypercube Sampling Method and Coupled Hydrogeophysical Approach. *Pure and Applied Geophysics* 174:4471-4487 doi:10.1007/s00024-017-1656-1

Friedel, S., Thielen, A., and Springman, S. M. (2006). Investigation of a slope endangered by rainfall-induced landslides using 3D resistivity tomography and geotechnical testing. *Journal of Applied Geophysics*, *60*(2), 100-114.

Gallardo, L. A., and Meju, M. A. (2004). Joint two-dimensional DC resistivity and seismic travel time inversion with cross-gradients constraints. *Journal of Geophysical Research: Solid Earth*, *109*(B3).

Gehman CL, Harry DL, Sanford WE, Stednick JD, Beckman NA (2009). Estimating specific yield and storage change in an unconfined aquifer using temporal gravity surveys. *Water Resources Research* 45 doi:10.1029/2007wr006096

Haruzi, P., Gueting, N., Klotzsche, A., Vanderborght, J., Vereecken, H., van der Kruk, J. (2018). Time-lapse ground-penetrating radar full-waveform inversion to detect tracer plumes: A numerical study. 2486-2490. 10.1190/segam2018-2996599.1.

Hendricks Franssen, H. J., and Kinzelbach, W. (2008). Real-time groundwater flow modeling with the ensemble Kalman filter: Joint estimation of states and parameters and the filter inbreeding problem. *Water Resources Research*, *44*(9).

ENIGMA ITN - This project has received funding from European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie Grant Agreement N°722028.

Hermans, T. (2017). Prediction-Focused Approaches: An Opportunity for Hydrology. *Groundwater*, 55(5), 683–687.

Hermans, T., Oware, E., and Caers, J. (2016). Direct prediction of spatially and temporally varying physical properties from time-lapse electrical resistance data. *Water Resources Research*, 52(9), 7262–7283.

Huang J, Santos FAM, Triantafilis J (2016). Mapping soil water dynamics and a moving wetting front by spatiotemporal inversion of electromagnetic induction data. *Water Resources Research* 52:9131-9145 doi:10.1002/2016wr019330

Huang JY, McBratney AB, Minasny B, Triantafilis J (2017). 3D soil water nowcasting using electromagnetic conductivity imaging and the ensemble Kalman filter. *Journal of Hydrology* 549:62-78 doi:10.1016/j.jhydrol.2017.03.067

Hubbard, S. S., and Linde, N. (2010). *Hydrogeophysics* (No. LBNL-3341E). Lawrence Berkeley National Lab.(LBNL), Berkeley, CA (United States).

Irving J, Singha K (2010). Stochastic inversion of tracer test and electrical geophysical data to estimate hydraulic conductivities. *Water Resources Research* 46 doi:10.1029/2009wr008340

Jadoon, K. Z., Weihermüller L., Scharnagl B., Kowalsky M. B., Bechtold M., Hubbard S. S., Vereecken H., and Lambot S. (2012). Estimation of Soil Hydraulic Parameters in the Field by Integrated Hydrogeophysical Inversion of Time-Lapse Ground-Penetrating Radar Data. Vadose Zone J. 11. doi:10.2136/vzj2011.0177

Jardani, A., Revil, A., and Dupont, J. P. (2013). Stochastic joint inversion of hydrogeophysical data for salt tracer test monitoring and hydraulic conductivity imaging. *Advances in Water Resources*, *52*, 62-77.

Johnson TC, Slater LD, Ntarlagiannis D, Day-Lewis FD, Elwaseif M (2012). Monitoring groundwater-surface water interaction using time-series and time-frequency analysis of transient three-dimensional electrical resistivity changes. *Water Resources Research* 48 doi:10.1029/2012wr011893

Johnson TC, Versteeg RJ, Ward A, Day-Lewis FD, Revil A (2010). Improved hydrogeophysical characterization and monitoring through parallel modeling and inversion of time-domain resistivity and induced-polarization data. *Geophysics* 75:WA27-WA41 doi:10.1190/1.3475513

Johnson, T. C., Hammond, G. E., and Chen, X. (2017). PFLOTRAN-E4D: A parallel open source PFLOTRAN module for simulating time-lapse electrical resistivity data. *Computers and Geosciences*, *99*, 72-80.

Kirsch R (ed). (2006). Groundwater Geophysics - a tool for hydrogeology. Springer, Berlin

ENIGMA ITN - This project has received funding from European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie Grant Agreement N°722028.

Kitanidis PK (1995). Quasi-linear geostatistical theory for inversing. *Water Resources Research,* 31:2411-2419

Klein O, Cirpka OA, Bastian P, Ippisch O (2017). Efficient geostatistical inversion of transient groundwater flow using preconditioned nonlinear conjugate gradients. *Advances in Water Resources* 102:161-177 doi:10.1016/jadvwatres.2016.12.006

Knödel, K., Lange, G., and Voigt, H. J. (2007). Environmental geology: handbook of field methods and case studies. *Springer Science and Business Media*.

Kowalsky, M. B., Finsterle S., Peterson J., Hubbard S., Rubin Y., Majer E., Ward A., and Gee G. (2005), Estimation of field-scale soil hydraulic and dielectric parameters through joint inversion of GPR and hydrological data, Water Resour. Res., 41, W11425, doi:10.1029/2005WR004237.

Lavoué, F., Van Der Kruk, J., Rings, J., André, F., Moghadas, D., Huisman, J. A., and Vereecken, H. (2010). Electromagnetic induction calibration using apparent electrical conductivity modelling based on electrical resistivity tomography. *Near surface geophysics*, *8*(6), 553-561.

Lekmine, G., Auradou, H., Pessel, M., and Rayner, J. L. (2017). Quantification of tracer plume transport parameters in 2D saturated porous media by cross-borehole ERT imaging. *Journal of Applied Geophysics*, *139*, 291-305.

Lichtner PC et al. (2017). *PFLOTRAN*. http://wwwpflotran.org

Linde, N., Binley, A., Tryggvason, A., Pedersen, L. B., and Revil, A. (2006). Improved hydrogeophysical characterization using joint inversion of cross-hole electrical resistance and ground-penetrating radar traveltime data. *Water Resources Research*, *42*(12).

Linde, N., Tryggvason, A., Peterson, J. E., and Hubbard, S. S. (2008). Joint inversion of crosshole radar and seismic traveltimes acquired at the South Oyster Bacterial Transport Site. *Geophysics*, *73*(4), G29-G37.

Lochbühler, T., Doetsch, J., Brauchler, R., and Linde, N. (2013). Structure-coupled joint inversion of geophysical and hydrological data. *Geophysics*, *78*(3), ID1-ID14.

Loke, M. H., Chambers, J. E., Rucker, D. F., Kuras, O., and Wilkinson, P. B. (2013). Recent developments in the direct-current geoelectrical imaging method. *Journal of Applied Geophysics*, *95*, 135-156.

Looms, M. C., Jensen, K. H., Binley, A., and Nielsen, L. (2008). Monitoring unsaturated flow and transport using cross-borehole geophysical methods. *Vadose Zone Journal*, 7(1), 227-237.

Martinez J, Benavente J, Garcia-Arostegui JL, Hidalgo MC, Rey J (2009). Contribution of electrical resistivity tomography to the study of detrital aquifers affected by seawater intrusion-extrusion effects: The river Velez delta (Velez-Malaga, southern Spain). *Engineering Geology* 108:161-168 doi:10.1016/j.enggeo.2009.07.004

ENIGMA ITN - This project has received funding from European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie Grant Agreement N°722028.

Meles G. A., Van der Kruk J., Greenhalg S. A., Ernst J. R., Maurer H., Green A. G. (2010). A New Vector Waveform Inversion Algorithm for Simultaneous Updating of Conductivity and Permittivity Parameters From Combination Crosshole/Borehole-to-Surface GPR Data. IEEE Transactions on Geoscience and Remote Sensing 48(9), 3391-3407. doi: 10.1109/TGRS.2010.2046670

Menke W (2012). Geophysical Data Analysis: Discrete Inverse Theory, 3rd Edition. Geophysical Data Analysis: Discrete Inverse Theory, 3rd Edition. Elsevier Academic Press Inc, San Diego

Mester, A., van der Kruk, J., Zimmermann, E., and Vereecken, H. (2011). Quantitative two-layer conductivity inversion of multi-configuration electromagnetic induction measurements. *Vadose Zone Journal*, *10*(4), 1319-1330.

Muller K, Vanderborght J, Englert A, Kemna A, Huisman JA, Rings J, Vereecken H (2010). Imaging and characterization of solute transport during two tracer tests in a shallow aquifer using electrical resistivity tomography and multilevel groundwater samplers. *Water Resources Research* 46 doi:10.1029/2008wr007595

Nguyen, F., Kemna, A., Antonsson, A., Engesgaard, P., Kuras, O., Ogilvy, R., ... and Pulido-Bosch, A. (2009). Characterization of seawater intrusion using 2D electrical imaging. *Near Surface Geophysics*, *7*(5-6), 377-390.

Nowak W (2009). Best unbiased ensemble linearization and the quasi-linear Kalman ensemble generator. *Water Resources Research* 45 doi:10.1029/2008wr007328

Nowak W, Cirpka OA (2006). Geostatistical inference of hydraulic conductivity and dispersivities from hydraulic heads and tracer data. *Water Resources Research* 42 doi:10.1029/2005wr004832

Paasche H, Tronicke J, Holliger K, Green AG, Maurer H (2006). Integration of diverse physical-property models: Subsurface zonation and petrophysical parameter estimation based on fuzzy c-means cluster analyses. *Geophysics* 71:H33-H44 doi:10.1190/1.2192927

Pasquet S., Bodet L., Dhemaied A., Mouhri A., Vitale Q., Rejiba F., Flipo N., Guérin R. (2015) Detecting different water table levels in a shallow aquifer with combined P-, surface and SH-wave surveys: Insights from VP/VS or Poisson's ratios, Journal of Applied Geophysics, 113, pp. 38-50,

Perri MT, De Vita P, Masciale R, Portoghese I, Chirico GB, Cassiani G (2018). Time-lapse Mise-a-la-Masse measurements and modeling for tracer test monitoring in a shallow aquifer. *Journal of Hydrology* 561:461-477 doi:10.1016/j.jhydrol.2017.11.013

Perri, M. T., Cassiani, G., Gervasio, I., Deiana, R., and Binley, A. (2012). A saline tracer test monitored via both surface and cross-borehole electrical resistivity tomography: Comparison of time-lapse results. *Journal of Applied Geophysics*, *79*, 6-16.

Perrone, A., Lapenna, V., and Piscitelli, S. (2014). Electrical resistivity tomography technique for landslide investigation: A review. *Earth-Science Reviews*, *135*, 65-82.

ENIGMA ITN - This project has received funding from European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie Grant Agreement N°722028.

Pollock D, Cirpka OA (2008). Temporal moments in geoelectrical monitoring of salt tracer experiments. *Water Resources Research* 44 doi:10.1029/2008wr007014

Pollock D, Cirpka OA (2010). Fully coupled hydrogeophysical inversion of synthetic salt tracer experiments. *Water Resources Research* 46 doi:10.1029/2009wr008575

Pollock D, Cirpka OA (2012). Fully coupled hydrogeophysical inversion of a laboratory salt tracer experiment monitored by electrical resistivity tomography *Water Resources Research.* 48 doi:10.1029/2011wr010779

Pollock, D., and Cirpka, O. A. (2010). Fully coupled hydrogeophysical inversion of synthetic salt tracer experiments. *Water Resources Research*, *46*(7).

Renard, P. (2007). Stochastic hydrogeology: what professionals really need? *Groundwater*, *45*(5), 531-541.

Rizzo E, Suski B, Revil A, Straface S, Troisi S (2004). Self-potential signals associated with pumping tests experiments. *Journal of Geophysical Research-Solid Earth* 109 doi:10.1029/2004jb003049

Robinson, D. A., Lebron, I., Kocar, B., Phan, K., Sampson, M., Crook, N., and Fendorf, S. (2009). Time-lapse geophysical imaging of soil moisture dynamics in tropical deltaic soils: An aid to interpreting hydrological and geochemical processes. *Water Resources Research*, *45*(4).

Rosales, R. M., Martínez-Pagan, P., Faz, A., and Moreno-Cornejo, J. (2012). Environmental monitoring using electrical resistivity tomography (ERT). in the subsoil of three former petrol stations in SE of Spain. *Water, Air, and Soil Pollution*, *223*(7), 3757-3773.

Rubin Y, Hubbard SS (eds). (2005). Hydrogeophysics. Vol 50. Water Science and Technology Library. Springer, Dordrecht

Rucker C, Gunther T, Wagner FM (2017). pyGIMLi: An open-source library for modelling and inversion in geophysics. *Computers & Geosciences* 109:106-123 doi:10.1016/j.cageo.2017.07.011

Sanchez-León E, Leven C, Haslauer CP, Cirpka OA (2016). Combining 3D Hydraulic Tomography with Tracer Tests for Improved Transport Characterization. *Groundwater* 54:498-507 doi:10.1111/gwat.12381

Scheidt, C., Li, L., and Caers, J. (2018). Quantifying Uncertainty in Subsurface Systems. Hoboken, NJ and Washington D.C.: John Wiley and Sons and American Geophysical Union.

Scheidt, C., Renard, P., and Caers, J. (2015). Prediction-Focused Subsurface Modeling: Investigating the Need for Accuracy in Flow-Based Inverse Modeling. *Mathematical Geosciences*, 47(2), 173–191.

Schöniger, A., Nowak, W., and Hendricks Franssen, H. J. (2012). Parameter estimation by ensemble Kalman filters with transformed data: Approach and application to hydraulic tomography. *Water Resources Research*, *48*(4). doi:10.1029/2011wr010462

ENIGMA ITN - This project has received funding from European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie Grant Agreement N°722028.

Schwede RL, Ngo A, Bastian P, Ippisch O, Li W, Cirpka OA (2012). Efficient parallelization of geostatistical inversion using the quasi-linear approach Computers & Geosciences 44:78-85 doi:10.1016/j.cageo.2012.03.014

Singha K, Gorelick SM (2005). Saline Tracer Visualized with Three-Dimensional Electrical Resistivity Tomography: Field-Scale Spatial Moment Analysis. *Water Resources Research*4 1:W05023

Singha K, Li L, Day-Lewis FD, Regberg AB (2011). Quantifying solute transport processes: Are chemically "conservative" tracers electrically conservative? *Geophysics* 76:F53-F63 doi:10.1190/1.3511356

Singha, K., and Gorelick, S. M. (2005). Saline tracer visualized with three-dimensional electrical resistivity tomography: Field-scale spatial moment analysis. *Water Resources Research*, *41*(5).

Slob E., Lambot S., Rhebergen J., Lopera O., and Vereecken H. (2008) Closed loop hydrogeophysical inversion of time-lapse GPR data to determine hydraulic properties of a sandy soil. SEG Technical Program Expanded Abstracts 2008. pp. 1183-1187.

Straface S, Fallico C, Troisi S, Rizzo E, Revil A (2007). An inverse procedure to estimate transmissivity from heads and SP signals. *Ground Water* 45:420-428 doi:10.1111/j.1745-6584.2007.00310.x

Sun, N.-Z., and Sun, A. (2015). Model calibration and parameter estimation: for environmental and water resource systems. New York: Springer.

Swanson RD, Singha K, Day-Lewis FD, Binley A, Keating K, Haggerty R (2012). Direct geoelectrical evidence of mass transfer at the laboratory scale. *Water Resources Research* 48 doi:10.1029/2012wr012431

Tarantola, A. (2005). *Inverse problem theory and methods for model parameter estimation* (Vol. 89). SIAM.

Travelletti, J., Sailhac, P., Malet, J. P., Grandjean, G., and Ponton, J. (2012). Hydrological response of weathered clay-shale slopes: water infiltration monitoring with time-lapse electrical resistivity tomography. *Hydrological processes*, *26*(14), 2106-2119.

Vanderborght J, Kemna A, Hardelauf H, Vereecken H (2005). Potential of electrical resistivity tomography to infer aquifer transport characteristics from tracer studies: A synthetic case study. *Water Resources Research* 41 doi:10.1029/2004wr003774

Vereecken H, Binley A, Cassiani G, Revil A, Titov K (eds). (2006). Applied Hydrogeophysics. Vol 71. NATO Science Series. Springer Netherlands, Dordrecht

Wagner, F. M., Bergmann, P., Rücker, C., Wiese, B., Labitzke, T., Schmidt-Hattenberger, C., and Maurer, H. (2015). Impact and mitigation of borehole related effects in permanent crosshole resistivity imaging: An example from the Ketzin CO2 storage site. *Journal of Applied Geophysics*, *123*, 102-111.

ENIGMA ITN - This project has received funding from European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie Grant Agreement N°722028.

Yoder, R. E., Freeland, R. S., Ammons, J. T., and Leonard, L. L. (2001). Mapping agricultural fields with GPR and EMI to identify offsite movement of agrochemicals. *Journal of Applied Geophysics*, *47*(3-4), 251-259.

Zarroca M, Bach J, Linares R, Pellicer XM (2011). Electrical methods (VES and ERT). for identifying, mapping and monitoring different saline domains in a coastal plain region (Alt Emporda, Northern Spain). *Journal of Hydrology* 409:407-422 doi:10.1016/j.jhydrol.2011.08.052

Zhou, H., Gómez-Hernández, J. J., and Li, L. (2014). Inverse methods in hydrogeology: Evolution and recent trends. *Advances in Water Resources*, *63*, 22-37.

ENIGMA ITN - This project has received funding from European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie Grant Agreement N°722028.

End of deliverable WP5 D5.1 D12

ENIGMA ITN - This project has received funding from European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie Grant Agreement N°722028.