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Dynamic Inversion for Hydrological Process Monitoring with Electrical Resistance Tomography Under Model Uncertainties

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Abstract. We propose an approach for imaging the dynamics of complex hydrological processes. The evolution of electrically conductive fluids in porous media is imaged using time-lapse electrical resistance tomography. The related dynamic inversion problem is solved using Bayesian filtering techniques, that is, it is formulated as a sequential state estimation problem in which the target is an evolving posterior probability density of the system state. The dynamical inversion framework is based on the state space representation of the system, which involves the construction of a stochastic evolution model and an observation model. The observation model used in this paper consists of the complete electrode model for ERT, with Archie's law relating saturations to electrical conductivity. The evolution model is an approximate model for simulating flow through partially saturated porous media. Unavoidable modeling and approximation errors in both the observation and evolution models are considered by computing approximate statistics for these errors. These models are then included in the construction of the posterior probability density of the estimated system state. This approximation error method allows the use of approximate—and therefore computationally efficient—observation and evolution models in the Bayesian filtering. We consider a synthetic example and show that the incorporation of an explicit model for the model uncertainties in the state space representation can yield better estimates than a frame-by-frame imaging approach.

1. Introduction

Monitoring subsurface systems and their temporal changes is essential to improve understanding of hydrological processes in the unsaturated zone. Electrical resistance tomography (ERT) has been used to monitor time- and space-varying targets such as water content distributions and solute concentrations [Daily *et al.*, 1992; Park, 1998; Binley *et al.*, 2002; French *et al.*, 2002; Yeh *et al.*, 2002], hydrological barriers [Daily and Ramirez, 2000], tracer transport [Slater *et al.*, 2000; Kemna *et al.*, 2002], underground tank leakage [Ramirez *et al.*, 1996], remediation processes [Ramirez *et al.*, 1993], and resistivity changes caused by rainfall [Zhou *et al.*, 2001]. ERT and ground penetrating radar (GPR) have been combined to perform joint inversion to yield significantly enhanced water content estimates [Linde *et al.*, 2006b].

The value of constraining ERT models with hydrological process modeling is increasingly recognized [Ferre *et al.*, 2006]. Hydrogeophysical data fusion approaches within a stochastic framework that combines primary and secondary data of different types and iteratively updates state estimates, unsaturated hydraulic properties, and the related covariance structures, have been used in sequential inversion of ERT data [Yeh and Simunek, 2002; Zhang and Yeh, 1997; Hughson and Yeh, 2000; Yeh *et al.*, 2002].

As a comment on stationary techniques, classical ERT inversion algorithms tend to provide spatially smooth reconstructions. It is, however, possible to obtain reconstructions with sharp edges and recover

small inclusions when more elaborate explicit prior models are used, e.g., see Dobson and Santosa [1996]; Kaipio *et al.* [1999, 2000].

We consider a dynamic imaging technique that includes an evolution model describing the transient system behavior. In addition, an observation model is used to relate the calculated system state (saturation) to indirectly observable variables (here: electrical resistivity or conductivity). As a crucial part of inversion, we account for random and systematic errors in the underlying evolution and observation models, significantly decreasing estimation errors and bias.

1.1. Dynamical inversion framework

The traditionally used reconstruction approach in which the data at different times are used to compute snapshot type estimates, may not yield images of sufficient accuracy and resolution to serve as a basis for understanding complex hydrogeological processes. Inversion artifacts can be significantly reduced by including an explicit evolution model for the system. Numerical and practical studies in process tomography, for example, show how the use of an approach that incorporates a temporal model of the imaged target in the data processing (which we refer to as the dynamic inversion method) significantly improves the quality of the estimated system state [Kaipio and Somersalo, 1999; Seppänen *et al.*, 2001; Kaipio and Somersalo, 2004]. Lehtikoinen *et al.* [2009] have adapted the dynamic inversion method for imaging the distribution of water content in porous media based

on time-lapse ERT data. The traditional frame-by-frame inverse problem is recast as a state estimation problem, where measurement sets at different times are combined by means of a stochastic evolution model of unsaturated flow.

We refer to the conventional, frame-by-frame imaging method (possibly using the previous estimate as a center point), where each image and its supporting data define a frame, as the stationary technique. The main and foremost difference of the stationary frame-by-frame techniques and the (full) dynamical inversion approach is that in the latter the uncertainties of the models are incorporated in a systematic manner and thus i) the estimate errors are more realistic and ii) the resulting weighting of the model predictions and the new data more closely corresponds to the statistically optimal weighting.

State estimation approaches are based on the state space representation, which consists of an evolution and an observation model. The evolution model predicts the system state; the observation model is a mapping between system state and measurements. The state estimation problem can be solved using recursive Bayesian filtering techniques.

For example, the ensemble Kalman filter [Evensen, 1994] has been used for hydrogeological inverse problems [Vrugt *et al.*, 2005], the extended Kalman filter (EKF) [Anderson and Moore, 1979] has been used for solving the non-stationary inverse problem in process tomography [Kaipio and Somersalo, 1999; Seppänen *et al.*, 2001] and in hydrogeophysics [Lehikoinen *et al.*, 2009]; finally, the iterated extended Kalman filter (IEKF) [Kaipio and Somersalo, 2004] has been applied to estimate lake water constituents [Voutilainen *et al.*, 2007]. Note that, as opposed to the term commonly used in geostatistics, in this paper the term non-stationary refers to dynamic or time-varying. Furthermore, Eppstein and Dougherty [1998] tested approximative Extended Kalman filter type algorithm to map the location of the controlled time varying salt water plume with GPR.

We do not consider the estimation of the source parameters and take these to be known. The estimation of the inputs to the evolution model is based on the formulation and computational approach described in this paper and is basically a straightforward task, see [Voutilainen and Kaipio, 2009] for a related source estimation problem.

The ensemble Kalman filter (as well as other sampling based methods) is inefficient for solving high-dimensional inverse problems, because exploring the entire state-space by sampling is computationally very demanding. Our approach is based on approximating all statistics with Gaussian models which makes it possible to use the more computationally efficient extended Kalman filter approach.

1.2. Stochastic Richards' model

In Lehikoinen *et al.* [2009], we considered a method for imaging the evolution of electrically conductive fluids in porous media. The state evolution was modeled with the stochastic Richards equation. In this method, the non-stationary inversion problem was solved using extended Kalman filtering. The method was validated using a synthetically generated test case in which a time-varying water plume in an unsaturated porous medium with homogeneous or slightly heterogeneous permeability fields was monitored based on ERT measurements. The evolution model used in the inversion was close to but not identical to the model used to generate the synthetic data. Under these near-ideal conditions, the dynamic inversion approach yielded accurate or at least acceptable results. It was apparent that the approach could not tolerate significant errors in the Richards model. The reconstructions using the similar frame-by-frame imaging technique were too smooth even in this simple test case.

In this paper, we extend the approach to the estimation of unsaturated flows in highly heterogeneous porous media using a simplified (homogeneous) evolution model. The basic idea of the extension is to construct a statistical model for the difference between i) the flow through a fixed homogeneous and ii) the actual random heterogeneous permeability fields, and to use this information in the inversion scheme.

In this study, we use the stochastic Richards equation [Richards, 1931] for unsaturated flow as the evolution model, and the complete electrode model [Cheng *et al.*, 1989] as the observation model for ERT. The traditional construction of the evolution and observation models relies either on the assumption that modeling inaccuracies are insignificant, or that the errors can be taken into account by using a white noise process, i.e., an ad hoc adaptation of the measurement error model by employing larger variances than the analysis of the (electronic) measurement system suggests.

1.3. Model uncertainties

In geophysical and hydrological applications, however, the models are generally simplified representations of the underlying complex systems. In addition, the parameters of the models are uncertain or unknown. These approximation and modeling errors are often more significant than the measurement and evolution noise processes, and they may make the solution of the inverse problem highly misleading. For example, in most practical situations with slow evolution, the available measurement times can be made so long that the errors in the measurement models are almost completely due to modeling and approximation errors rather than the (electronic) measurement noise.

In the classical least-squares inversion approach, modeling, discretization and parameter errors are sometimes combined and treated as a single white noise term. Vrugt *et al.* [2005] claim that combining errors into a single term results in parameter estimates that reflect a compromise between input, output, and model structure errors. This trade-off (affected by the estimation approach) leads to an inconsistency when estimating parameter uncertainty, which is supposed to reflect the sensitivity of the least-squares criterion to parameter deviations (not modeling and discretization errors). There are some attempts to represent the modeling and approximation errors using stochastic forcing terms [Evensen, 1994; Vrugt *et al.*, 2005].

1.4. Approximation error approach

In this paper, we use the approximation error theory [Kaipio and Somersalo, 2004, 2007] which is a Bayesian approach based on explicit modeling of all uncertainties. This is a computationally efficient and flexible framework for including different types of modeling errors into inverse problem formulations. The approximation error theory for errors related to model reduction has been applied to stationary inverse problems, such as electrical impedance tomography [Kaipio and Somersalo, 2004], deconvolution problems [Kaipio and Somersalo, 2007], and optical tomography [Arridge *et al.*, 2006]. Furthermore, treatment of errors in the modeling of unknown boundary data has been considered in Lehikoinen *et al.* [2007]. Although the approximation error approach would technically facilitate the treatment of all uncertainties, we only consider the uncertainties related to the Richards' equation in this paper.

In approximation error theory, errors (which are due to discretization errors, uncertainties in fixed model parameters, and model structure errors) in the evolution and observation models are represented as stochastic processes. Sampling methods are used to estimate the statistics of these processes, although in linear problems the relevant statistics can sometimes be computed explicitly. The estimated

statistics are then included in the state estimation procedure. The nonstationary extension of the approximation error approach for linear state estimation problems has been carried out in *Huttunen and Kaipio* [2007a]. They demonstrated that the approximation error method allows for the use of highly reduced state models and long time steps to invert one-dimensional heat flow data. The nonlinear extension to nonstationary inverse problems has been derived in *Huttunen and Kaipio* [2007b].

In this study, we apply the approximation error method to nonlinear evolution and observation models as part of a dynamic inversion approach. In the solution of the inverse problem, we aim to use a highly simplified evolution model and a very coarse discretization of the observation model, which significantly reduces the computational load. As an extension to *Huttunen and Kaipio* [2007b], we investigate the applicability of importance sampling in the refinement of the approximation error model during the data accumulation.

The proposed approach is not restricted to ERT; it can in principle be applied to different data types and a variety of geophysical, medical, and process imaging problems. GPR is an alternative geophysical method to estimate water content distribution in the vadose zone. While generally having a higher resolution than ERT, GPR's range of applicability is limited to the near surface due to its small penetration depth in conductive media. A combination of ERT with GPR or other geophysical data is a potentially useful approach to obtain quality images of the subsurface and its fluid distribution. The joint inversion concept and related uncertainty considerations can be adapted to accommodate different types of geophysical data, including GPR.

The structure of this paper is as follows: the evolution (Richards) and observation (ERT) models are explained in Sections 2.1 and 2.2, respectively. The modeling of the dynamic approximation errors is given in Section 2.3. The approximation error approach provides us with the stochastic completion of the evolution model and the modification to the ERT observation model. The dynamic filtering approach is described in Section 3. Here the general sequential Bayesian filtering concept is reviewed briefly and an importance sampling type extension to the dynamic approximation error approach is introduced. This approach enables us to refine and update the initial uncertainty models during the data accumulation. A synthetic test case is examined in Section 4 to give a feasibility assessment, and conclusions are given in Section 5.

2. Evolution and Observation Models

2.1. Evolution model

The evolution of water saturation in unsaturated porous media can be modeled by solving the Richards equation [*Richards*, 1931]:

$$\phi \frac{\partial S}{\partial t} - \nabla \left[\frac{K(S)}{\rho_w g} \nabla P_c(S) + K(S) \hat{z} \right] = 0. \quad (1)$$

Here, S is the water saturation, ϕ is the porosity, K and P_c are the unsaturated hydraulic conductivity and the capillary pressure, respectively (both nonlinear functions of water saturation), ρ_w is the density of water, g is the gravitational constant, and $\hat{z}$ is the unit vector, positive upward.

The unsaturated hydraulic conductivity is given by

$$K = k \frac{k_{rel}(S) \rho_w g}{\mu_w}, \quad (2)$$

where k is the absolute permeability, k_{rel} is the relative permeability (a nonlinear function of water saturation), and μ_w is the dynamic viscosity of water.

For the present study we assume that the relative permeability k_{rel} and the capillary pressure P_c can be modeled

appropriately with the parametric representation given by *van Genuchten* [1980]:

$$P_c = -\alpha^{-1} (S_e^{-1/m} - 1)^{1-m} \quad (3)$$

$$k_{rel} = \sqrt{S_e} (1 - (1 - S_e^{m-1})^m)^2 \quad (4)$$

$$S_e = \frac{S - S_{wr}}{1 - S_{wr}}, \quad (5)$$

where m and α are soil-specific parameters, S_e is the effective water saturation, and S_{wr} is the residual water saturation.

Generally, all the hydrological coefficients are heterogeneous and unknown. Handling these uncertainties is the main target in this paper. Specifically, in Section 4, we consider a case in which the absolute permeability field is heterogeneous and anisotropic, whereas all the other hydraulic parameters (ϕ , α , m , and S_{wr}) are homogeneous. In contrast, the evolution model used in the inversion employs the approximate model in which permeability is homogeneous and isotropic. This introduces a substantial structural modeling error, which will be addressed by the dynamic approximation error method that is discussed in Section 2.3.

We use the modified finite volume numerical simulator TOUGH2 [*Pruess et al.*, 1999] with an implicit Euler scheme for time discretization to solve the Richards' equation (1) for given initial and boundary conditions, source terms, and hydraulic parameters. The TOUGH2 code was modified to compute the Jacobian matrices that correspond to the integration of the evolution over the time steps, that is, the mapping $S_t \mapsto S_{t+1}$.

The numerical solution at time $t+1$ when all parameters are known, can be written as

$$S_{t+1} = f_t(S_t), \quad (6)$$

where S_t is the vector of the discretized temporally varying saturation values at the element centers at time t , and f_t is a nonlinear function that can depend explicitly on time. This is the evolution model for the water saturation.

There are various sources of errors associated with the simulation of unsaturated flow. For example, hydraulic parameters of the soil (i.e., the absolute permeability and the parameters describing the capillary pressure and relative permeability functions) are not known a priori. Other approximations (such as the assumption of constant viscosity) and uncertainties (for example regarding the location and size of the injection point) as well as discretization errors lead to additional errors in the solution. Thus, it is necessary to write the numerical solution of the unsaturated flow model in the more general form

$$S_{t+1} = f_t(S_t) + \omega_t \quad (7)$$

where ω_t is a stochastic process representing modeling errors. In the terminology of system theory the process ω_t is called the state noise process. Equation (7) is referred to as the state evolution model for water saturation.

The specification of the statistics of the state noise process and the initial state S_0 are discussed in Sections 2.3 and 4, respectively.

2.2. Observation model

We consider the geophysical method ERT, which is useful for tracking electrically conductive targets. In ERT, electric currents are injected into the target zone through electrodes placed in boreholes, at the ground surface, or both, and

the resulting voltages between (typically adjacent) electrode pairs are measured. Assume that there are N electrodes. First electrodes 1 and 2 are used for injection and the data are obtained as potential differences between the electrode pairs 3 – 4, 4 – 5, ... Then the current is injected between electrodes 1 and 4, and the potential differences are measured between 2 – 3, 5 – 6, ... In total per a fixed time, $N - 1$ electrode pairs are used to inject the current and all electrode pair measurements are employed. Thus, all measurements are carried out according to the so-called 4 electrode system. Traditionally, potential differences are not measured using current injection electrodes, but the adoption of the complete electrode model [Cheng *et al.*, 1989] in principle would facilitate also such measurements. In geophysics, such measurements have not been employed.

The observation model consists of the forward model that relates voltages for a given measurement setup to the distribution of (saturation-dependent) electrical conductivities, as well as the related errors. We employ the complete electrode model [Cheng *et al.*, 1989] as the ERT observation model, as it simulates the applied current density on the electrodes and the contact impedance between the electrode and the porous medium accurately. We will not, however, employ measurements using the current carrying electrodes.

The complete electrode model is given by the following boundary value problem:

$$\nabla \cdot (\sigma \nabla u) = 0, \quad \text{in } \Omega_{\text{ert}} \quad (8)$$

$$u + z_\ell \sigma \frac{\partial u}{\partial \bar{n}} = U_\ell, \quad \text{on } e_\ell, \ell = 1, \dots, L \quad (9)$$

$$\int_{e_\ell} \sigma \frac{\partial u}{\partial \bar{n}} dA = I_\ell, \quad \ell = 1, \dots, L \quad (10)$$

$$\sigma \frac{\partial u}{\partial \bar{n}} = 0, \quad \text{on } \partial\Omega_{\text{ert}} \setminus \cup_{\ell=1}^L e_\ell \quad (11)$$

where $\sigma = \sigma(x)$ is the electrical conductivity distribution, $u = u(x)$ is the electric potential, $\partial\Omega_{\text{ert}}$ is the boundary of the monitored closed system Ω_{ert} , L is the number of electrodes, e_ℓ is the ℓ^{th} electrode, U_ℓ is the potential on the ℓ^{th} electrode, z_ℓ is the contact impedance at electrode e_ℓ , dA is an infinitesimal boundary element, and $\bar{n}$ is the outward unit normal vector.

The equation (8) is the Poisson equation in the domain Ω_{ert} without internal current sources. The electrodes are modelled as surface patches with equation (9) and it takes into account the contact impedance between the (metallic) electrode and the soil. The equation (10) describes how the injected current is related to the current density on the electrodes. Finally, equation (11) sets the normal current density to vanish on the soil surface.

It is to be noted that when the computational domain is fixed and truncated, we do not know the boundary data on the truncation boundaries. If the computational domain is made extensive, that is, the boundaries are located approximately 3 times further from all electrodes than the maximum electrode separation, we can use the boundary model (11) also on the truncation boundaries. If this is not the case, the approximation error approach can also be used to handle the associated uncertainty [Lehikoinen *et al.*, 2007]. In this paper, we assume that the modelling error due to the unknown boundary data is insignificant when compared to other errors and uncertainties.

Usually, when the complete electrode model is used, the contact impedances are not exactly known and experimental nominal values are used. It is, however, possible to estimate the contact impedances simultaneously with the conductivity distribution. The relevant protocol includes also measurements on the current carrying electrodes. In the example in Section 4, we do not employ these measurements or

estimate the contact impedances, and we assume that these are known.

The monitored target is the time-varying water saturation distribution S . Archie's law [Archie, 1942] is used to convert the water saturation distribution calculated by the evolution model to the electrical conductivity distribution used by the observation model. Archie's law is given by

$$\sigma(S) = \sigma_w \phi^b S^n, \quad (12)$$

where σ_w is the electrical conductivity of the liquid phase, ϕ is porosity of the porous medium, b is the so-called cementation index, and n is the saturation index. While Archie's law is the most widely used model, the uncertainties related to the parameters are significant and they should be taken into account in field applications.

Multiple voltage measurements are needed using different patterns of current injections to sufficiently constrain the estimation of water saturation distribution. A set of voltage measurements (potentially involving multiple current patterns) collected at a given time is referred to as one frame. The target is assumed to be stationary during the measurement of a frame, which is usually justified given that hydrological processes are relatively slow, i.e., the water saturation distribution S_t does not change significantly while data are collected. Should geophysical data acquisition be relatively slow compared to the dynamics of the process to be imaged, the proposed framework can be extended to address such highly dynamic systems, as shown in Kaipio and Somersalo [1999]; Seppänen *et al.* [2001]. The assumption that the target is stationary during data collection for a frame allows one to combine all data of a given frame into a single voltage measurement vector V_t .

The ERT observation model, which relates the system state S to the voltage observations V , can be written in the following form [Vauhkonen *et al.*, 1999]:

$$V = R(\sigma(S))I, \quad (13)$$

where $R(\sigma(S))$ is the resistance matrix and I is the injected current. Here the electrical conductivity σ depends on water saturation S . By combining the ERT observational model (13) and Archie's law (12), the model for the errorless observations can be written in the following form:

$$V_t = g_t(S_t). \quad (14)$$

Here, g_t is a nonlinear mapping from $\mathbb{R}^N$ to $\mathbb{R}^{N_I N_V}$, where N_I is the number of current injections in the injection pattern, N_V is the number of voltage measurements per current injection, and the vector $V_t \in \mathbb{R}^{N_I N_V}$ contains all voltage measurements of the frame at time t .

In this study, we assume that the data are corrupted by additive Gaussian noise, $\epsilon \sim \mathcal{N}(0, \Gamma_\epsilon)$. Hence the observation model is written as

$$V_t = g_t(S_t) + \epsilon_t. \quad (15)$$

In this paper, we assume that the measurement noise process is Gaussian. The observation error model needed to describe the distribution of the estimates must account for random measurement noise, approximation errors due to model simplifications, and the impact of other potentially systematic errors (such as electrode mislocations).

2.3. Dynamic approximation error method

This section describes how approximation errors are handled in the proposed ERT inversion approach. Specifically, we account for uncertainties in the evolution model caused by uncertainty in the permeability distribution, and uncertainties in the observation model caused by numerical discretization errors. The approach can also be used to analyze

a variety of other modeling errors, for example, those caused by the truncation of the computational domain [Lehikoinen et al., 2007], or the impact of unknown borehole deviations [Linde et al., 2006a]. Structural error and uncertainties in the flow model, petrophysical model (Archie’s law), and the ERT forward model (complete electrode model) are significant but could also be addressed with this approach. They are, however, not considered in this paper.

First, we consider the uncertainty in the evolution model. The true, heterogeneous permeability distribution used to generate synthetic water saturation distributions is denoted by k , and the corresponding discretized flow model is denoted by $f_t(\cdot, k)$. Hence, the evolution model evaluated with the true permeability field can be written as

$$S_{t+1} = f_t(S_t, k) + \omega_t. \quad (16)$$

Note that in the inversion the details of the true heterogeneous permeability distribution are unknown. To account for the resulting uncertainty in the structure of the observation model, there are several options. One approach would be to directly estimate the spatial distribution of the permeability in the inversion problem. However, the estimation of the heterogeneous permeability increases ill-posedness of the problem and increases computation time. In addition, the parametrization of a heterogeneous field is a simplification of the true field which introduces additional uncertainty, which is not modeled here.

We propose an alternative approach which involves the use of geostatistical simulation techniques to generate multiple permeability realizations which are then used to characterize the uncertainty with respect to the assumed model structure. We note that such information on stratifications and soil types may not be readily available. In such a case a maximally uncertain structural model should be used.

Specifically, we use the dynamic approximation error method, which allows us to use simplified models in the inversion step and to approximate the heterogeneous model structure by a highly simplified model with homogeneous permeability k^* . Substituting the heterogeneous permeability with one that is homogeneous leads to an evolution model equation (16) that can be rewritten as follows:

$$\begin{aligned} S_{t+1} &= f_t(S_t, k) + \omega_t \\ &= f_t(S_t, k^*) + (f_t(S_t, k) - f_t(S_t, k^*)) + \omega_t \\ &= f_t(S_t, k^*) + \omega_t^* + \omega_t, \end{aligned} \quad (17)$$

where

$$\omega_t^* = f_t(S_t, k) - f_t(S_t, k^*) \quad (18)$$

is the stochastic process that represents the modeling errors due to uncertainties in the permeability field, provided that statistical information about the process ω_t^* can be given.

In addition to errors in the evolution model, we also have to consider the associated errors in the observation model, which are due to the discretization error of the ERT forward model and the contribution of the uncertain permittivity. The approach presented in Kaipio and Somersalo [2004] has been verified with real ERT data in Nissinen et al. [2008]. A similar approach can also be used to take into account the errors due to truncation of the computational domain [Lehikoinen et al., 2007].

The mesh used to solve the complete electrode model (8)–(11) during the inversion is denoted by $\mathcal{M}$. Let $\mathcal{M}^d$ be a fine mesh with a high resolution such that discretization errors are negligible compared to other errors (e.g., measurement noise). Then the accurate observation model can be written as

$$V_t = g_t^d(S_t) + \epsilon_t, \quad (19)$$

where the superscript d in function g_t^d indicates that the observation model (15) is constructed with the fine mesh $\mathcal{M}^d$. Then, the statistical model of the observations including discretization errors is given by

$$\begin{aligned} V_t &= g_t(S_t) + [g_t^d(S_t) - g_t(S_t)] + \epsilon_t \\ &= g_t(S_t) + \epsilon_t^d + \epsilon_t, \end{aligned} \quad (20)$$

where

$$\epsilon_t^d = g_t^d(S_t) - g_t(S_t) \quad (21)$$

represents approximation errors due to spatial discretization.

The statistics of the approximation error that is related to the uncertainty in the permeability field in the evolution model and the discretization in the observation model can be computed based on sampling techniques. The extension of EKF to accommodate error models and the procedure to compute the statistics of the error model are presented below.

3. Dynamic filtering

The objective of Bayesian filtering is to determine the posterior distribution of the state S_t conditioned on the observations, obtained up to time t , denoted as $D_t = \{V_1, V_2, \dots, V_t\}$. Bayesian filtering can be understood as a sequential process in which we update our knowledge of the system each time a new observation is made. The updating process is a recursive scheme in which an evolution updating step and observation updating step alternate. The posterior densities are then obtained recursively with the following updating formulas [Kalman, 1960], see also [Kaipio and Somersalo, 2004]:

1. Evolution (time) update:

$$p(S_{t+1}|D_t) = \int p(S_{t+1}|S_t)p(S_t|D_t)dS_t. \quad (22)$$

2. Observation (measurement) update:

$$p(S_{t+1}|D_{t+1}) = \frac{p(V_{t+1}|S_{t+1})p(S_{t+1}|D_t)}{p(V_{t+1}|D_t)}, \quad (23)$$

where

$$p(V_{t+1}|D_t) = \int p(V_{t+1}|S_{t+1})p(S_{t+1}|D_t)dS_{t+1}. \quad (24)$$

The evolution density (22) can be interpreted as a sequentially updated prior model for the system state S_{t+1} . The conditional probability densities $p(S_{t+1}|S_t)$ and $p(V_{t+1}|S_{t+1})$ are related to the evolution and the observation models, and are called the evolution (or prediction) density and the likelihood density, respectively. In addition, the distribution for the initial state, $p(S_0|D_0) = p(S_0)$, reflects the uncertainty in the state before any measurements are carried out. With stable state evolution models, the effect of the initial distribution commonly disappears soon during the process [Anderson and Moore, 1979]. If this is not the case, Kalman smoother algorithms can be used. The smoother algorithms provide an estimate for the state variable at each time using *all* available data, that is, also the data after the considered time. Naturally, smoother algorithms are off-line algorithms, see [Anderson and Moore,

1979] for different types of smoothers. The main requirement for the initial state model is that the uncertainty is not underestimated, that is, an adequately large covariance (high uncertainty) is posed for the initial state.

The sequential posterior densities are the solution of the dynamic inverse problem. The posterior density distribution is usually reported by point estimates, such as the conditional mean. For a linear Gaussian system, the conditional mean can be computed using the standard Kalman filter algorithm [Kalman, 1960].

In nonlinear problems, approximate estimates can be obtained using one of the extended Kalman filter algorithms [Anderson and Moore, 1979]. In this study, the extended Kalman filter (sequential linearization at the currently best available estimate) and the iterated extended Kalman filter are used to compute point estimates for the dynamic nonlinear system.

3.1. Extended Kalman Filter (EKF)

The extended Kalman filter (EKF) algorithm is based on the Kalman filter recursion. The basic idea is to linearize the observation and evolution models around the current state estimate available at each time step. Then the Kalman filter recursion is used with this linearized model. For details, see Anderson and Moore [1979].

The error terms in the evolution and observation models, in (17) and (20), respectively, depend on the state S_t . Therefore, EKF in its standard form is not applicable. The modification of the EKF to accommodate approximation error models was derived in Huttunen and Kaipio [2007b]. This modification is also used in this paper. The filter estimate for S_t based on data D_k is denoted by $S_{t|k}$, and the corresponding covariance estimate is denoted by $\Gamma_{t|k}$. The filter is summarized by the following equations:

$$S_{t+1|t} = f_t(S_{t|t}) + \mu_{t|t}^* \quad (25)$$

$$\Gamma_{t+1|t} = J_{f_t} \Gamma_{t|t} J_{f_t}^T + \Gamma_{\omega_t} + \Gamma_{t|t}^* \quad (26)$$

$$K_{t+1} = \Gamma_{t+1|t} J_{g_{t+1}}^T \times (J_{g_{t+1}} \Gamma_{t+1|t} J_{g_{t+1}}^T + \Gamma_{\epsilon_{t+1}} + \Gamma_{t+1|t}^d)^{-1} \quad (27)$$

$$\Gamma_{t+1|t+1} = (I - K_{t+1} J_{g_{t+1}}) \Gamma_{t+1|t} \quad (28)$$

$$S_{t+1|t+1} = S_{t+1|t} + K_{t+1} (V_{t+1} - g_{t+1}(S_{t+1|t}) - \mu_{t+1|t}^d), \quad (29)$$

where J_{f_t} is the Jacobian matrix of f_t evaluated at $S_{t|t}$, $J_{g_{t+1}}$ is the Jacobian matrix of g_{t+1} evaluated at $S_{t+1|t}$, Γ_{ω_t} is the covariance of ω_t and $\Gamma_{\epsilon_{t+1}}$ is the covariance of ϵ_{t+1} . In addition, $\mu_{t|t}^*$ and $\Gamma_{t|t}^*$ are the conditional expectation and covariance of ω_t^* given D_t , and $\mu_{t+1|t}^d$ and $\Gamma_{t+1|t}^d$ are the conditional expectation and covariance of ϵ_{t+1}^d given D_t . The matrix K_t is called the Kalman gain.

The Jacobian matrix associated with the observation model (15) is $J_{g_{t+1}} = J_R(\sigma(S)) \cdot J_\sigma(S)$, where the Jacobian matrix J_σ associated with Archie's law is

$$J_\sigma(S) = \sigma_w \phi^b n \cdot \text{diag}(S_1^{n-1}, S_2^{n-1}, \dots, S_N^{n-1}). \quad (30)$$

The computation of the Jacobian matrix J_R is described in Vauhkonen [2004]. The computation of the Jacobian J_{f_t} is done numerically by the perturbation method within a modified version of iTOUGH2 [Finsterle, 2004], where the modification involves the returning of the sequence of the Jacobians from the program.

3.2. Iterated Extended Kalman Filter (IEKF)

In the EKF, the observation model is linearized in the predicted state $S_{t+1|t}$. However, in the case of highly nonlinear observation models, this linearization approach may lead to large errors if the true state is far from the predicted

state. In the iterated extended Kalman filter (IEKF) the observation update step is solved using the following iterative approach.

The measurement update step (23) can be written as

$$p(S_{t+1}|D_{t+1}) \propto p(V_{t+1}|S_{t+1})p(S_{t+1}|D_t) \quad (31)$$

The density $p(S_{t+1}|D_t)$ is approximated with a Gaussian density with mean $S_{t+1|t}$ and covariance $\Gamma_{t+1|t}$ which are given by Equations (25)–(26). If the error terms in an observation model of the form (20) were independent of the state, the likelihood density could be written as

$$p(S_{t+1}|D_{t+1}) \quad (32)$$

$$\propto \exp\left(-\frac{1}{2}(V_{t+1} - g_{t+1}(S_{t+1}) - \mu_{t+1}^d)^T \quad (33)$$

$$\times (\Gamma_{\epsilon_{t+1}} + \Gamma_{t+1}^d)^{-1}(V_{t+1} - g_{t+1}(S_{t+1}) - \mu_{\epsilon_{t+1}^d}^d)), \quad (34)$$

where μ_{t+1}^d and Σ_{t+1}^d are the expectation and covariance of ϵ_{t+1}^d . Evidently, this assumption is not valid in our case. However, in the general case there is no explicit form for the likelihood density corresponding to the model (20). Hence, to overcome this problem, the likelihood density is approximated with the above formula. Then the filtering density $p(S_{t+1}|D_{t+1})$ can be written as

$$p(S_{t+1}|D_{t+1}) \propto \exp\left(-\frac{1}{2}f(S_{t+1})\right), \quad (35)$$

where

$$\begin{aligned} f(S_{t+1}) &= (S_{t+1} - S_{t+1|t})^T \Gamma_{t+1|t}^{-1} (S_{t+1} - S_{t+1|t}) \\ &\quad + (V_{t+1} - g_{t+1}(S_{t+1}) - \mu_{t+1}^d)^T (\Gamma_{\epsilon_{t+1}} + \Gamma_{t+1}^d)^{-1} \\ &\quad \times (V_{t+1} - g_{t+1}(S_{t+1}) - \mu_{\epsilon_{t+1}^d}^d) \end{aligned} \quad (36)$$

For linear Gaussian problems, the Kalman filter gives the conditional mean estimate for the state, which is the optimal estimate in the mean square sense. For nonlinear non-Gaussian cases the (extended) Kalman filters, however, yield estimates that do not exhibit any optimality with respect to the original state space estimation problem in the strict sense. Kalman filters give optimal estimates for linear systems with Gaussian errors. In general, optimal estimates can only be computed with the often computationally expensive particle filtering algorithms that are sequential versions of Markov chain Monte Carlo algorithms [Doucet et al., 2001].

In the case of IEKF the prediction is computed by propagating the evolution model to obtain an approximation for the conditional mean. The approximate predictor covariance is typically computed by a perturbation approach. In the filtering step, the estimate $S_{t+1|t+1}$ is computed as a maximum a posteriori estimate, which amounts to finding the minimum of the associated posterior potential, that is, the function f . The minimization problem can be solved, for example, iteratively using the Gauss-Newton algorithm with line search [Dennis and Schnabel, 1983]. The covariance $\Gamma_{t+1|t+1}$ is obtained by computing the Gaussian approximation for the posterior density at $S_{t+1|t+1}$. For a numerically efficient way to compute IEKF estimates, see for example Kaipio and Somersalo [2004].

3.3. Computing the statistics of the approximation error

The aim is to approximate $\mu_{t|t}^*$, $\mu_{t+1|t}^d$, $\Gamma_{t|t}^*$ and $\Gamma_{t+1|t}^d$ so that only crude qualitative assumptions for the permeability distribution are employed and all computationally intensive tasks can be done prior to the inversion. In this paper, we present two different approaches to compute the approximate statistics for ω_t^* and ϵ_t^d : one using a fixed approximation error model and one in which the approximation error model is efficiently updated during the extended Kalman filter recursion by employing an importance sampling approach.

In the first approach [Huttunen and Kaipio, 2007b] the conditional expectations and covariances are approximated with the conventional (unconditioned) expectations and covariances. This approximation is dictated by practical considerations: in nonlinear problems the computation of the conditional statistics calls for the solutions with the accurate model which is what we try to avoid in the first place. This choice will always correspond to an inflation of modelled uncertainty, which is the safe choice [Huttunen and Kaipio, 2007b].

The conventional expectations and covariances are determined by using an ensemble of samples as follows. First, we consider the determination of the expectation and covariance of ω_k^* . A sample k^j is drawn from the permeability distribution (details of this process will be discussed in Section 4.2). For the given realization k^j , the deterministic evolution model is used to calculate the water saturation distribution $S_t^j = S_t(k^j)$ at time t :

$$S_t^j = f_{t-1}(S_{t-1}^j, k^j). \quad (37)$$

The difference between the saturations for the homogeneous model and for the particular realization of the heterogeneous permeability field is calculated:

$$\omega_{t,j}^* = f_t(S_t^j, k^j) - f_t(S_t^j, k^*). \quad (38)$$

The $\omega_{t,j}^*$ are considered as samples from the distribution of the random variable ω_t^* . The process is repeated to obtain an ensemble of samples $\{\omega_{t,1}^*, \dots, \omega_{t,N^*}^*\}$. The expectation and covariance of ω_t^* are computed as sample averages:

$$\mu_t^* \approx \frac{1}{N^*} \sum_{j=1}^{N^*} \omega_{t,j}^*, \quad (39)$$

$$\Gamma_t^* \approx \frac{1}{N^* - 1} \sum_{j=1}^{N^*} (\omega_{t,j}^* - \mu_{\omega_t^*})(\omega_{t,j}^* - \mu_{\omega_t^*})^T. \quad (40)$$

The distribution of ω_t^* is approximated with the Gaussian distribution $\mathcal{N}(\mu_t^*, \Gamma_t^*)$. The Gaussian approximation is the key to efficient computational implementation. In reality, the approximation errors are seldom Gaussian. The Gaussian approximation has, however, turned out to be feasible in a number of earlier applications of the approximation error approach that have been cited above. Whether the approximation is feasible, remains to be verified with each application.

To obtain an approximate distribution for the approximation error related to the observation model, we generate an ensemble of samples $\{\epsilon_{t,1}^d, \dots, \epsilon_{t,N^d}^d\}$ as follows. We use the previously calculated saturation fields S_t^j . At each time t , Archie's law is applied to transform the saturation distribution S_t^j to an electrical conductivity distribution, which is then mapped onto both the fine mesh $\mathcal{M}^d$ and the coarse mesh $\mathcal{M}$. Then voltages are computed for these conductivity distributions using the discretized complete electrode model to get the values $g_t^d(S_t^j)$ and $g_t(S_t^j)$. A sample for ϵ_t^d is obtained as the difference between these voltage calculations at the measurement points, i.e., $\epsilon_{t,j}^d = g_t^d(S_t^j) - g_t(S_t^j)$. The expectation and covariance of ϵ_{t+1}^d are computed as

$$\mu_{t+1}^d \approx \frac{1}{N^d} \sum_{j=1}^{N^d} \epsilon_{t+1,j}^d, \quad (41)$$

$$\Gamma_{t+1}^d \approx \frac{1}{N^d - 1} \sum_{j=1}^{N^d} (\epsilon_{t+1,j}^d - \mu_{\epsilon_{t+1}^d})(\epsilon_{t+1,j}^d - \mu_{\epsilon_{t+1}^d})^T. \quad (42)$$

In this study we use also an alternative approach to approximate conditional covariances in which the conditional expectations and covariances are approximated by weighted averages. These weights are chosen based on the measurements. The main idea of this approach is loosely related to importance sampling step in particle filtering [Doucet et al., 2001].

Let f be a function that is either $f(x) = x$ for the conditional expectation or $f(x) = (x - \mu_{t|t}^*)(x - \mu_{t|t}^*)^T$ for the conditional covariance. The approximation error term ω_t^* depends on S_t and k . Thus, by Bayes rule,

$$\begin{aligned} \mathbb{E}[f(\omega_t^*)|D_t] &= \frac{\int \int f(\omega_t^*) p(S_{1:t}, k|D_t) dS_{1:t} dk}{\int \int p(S_{1:t}, k|D_t) dS_{1:t} dk} \\ &= \frac{\int \int f(\omega_t^*) \frac{p(D_t|S_{1:t}, k)}{p(D_t)} p(S_{1:t}, k) dS_{1:t} dk}{\int \int \frac{p(D_t|S_{1:t}, k)}{p(D_t)} p(S_{1:t}, k) dS_{1:t} dk} \\ &= \frac{\mathbb{E}[f(\omega_t^*) p(D_t|S_{1:t}, k)]}{\mathbb{E}[p(D_t|S_{1:t}, k)]} \end{aligned} \quad (43)$$

where $S_{1:t}$ is a notation for $(S_1, \dots, S_t)$. The expectations are approximated with the sample means,

$$\begin{aligned} \mathbb{E}[f(\omega_t^*)|D_t] &\approx \frac{\frac{1}{N^*} \sum_{j=1}^{N^*} f(\omega_{t,j}^*) w_j}{\frac{1}{N^*} \sum_{j=1}^{N^*} w_j} = \frac{\sum_{j=1}^{N^*} w_j f(\omega_{t,j}^*)}{\sum_{j=1}^{N^*} w_j}, \end{aligned} \quad (44)$$

where the weight is $w_j = p(D_t|S_{1:t}^j, k^j)$. If the states $S_{1:t}$ and the permeability field k are given, the measurements at different times are independent due to the independence assumption of the measurement noise ϵ_t . Thus

$$w_j = \prod_{i=1}^t p(V_i|S_{1:t}^j, k^j) \quad (45)$$

Furthermore, if the state S_j is known, information about the permeability field k and the other states $S_1, \dots, S_{j-1}, S_{j+1}, \dots, S_t$ does not provide any extra information about the measurement V_j . Hence

$$w_j = \prod_{i=1}^t p(V_i|S_1^j) \quad (46)$$

The conditional expectation $\mu_{t|t}^*$ and $\Gamma_{t|t}^*$ can be computed by using Equations (44) and (46) with the given choices of the function f .

The conditional expectation and covariance of ϵ_{t+1}^d can be computed similarly. Let g be a function which is either $g(x) = x$ for the conditional expectation $\mu_{t+1|t}^d$ or $g(x) = (x - \mu_{t+1|t}^d)(x - \mu_{t+1|t}^d)^T$ for the conditional covariance $\Gamma_{t+1|t}^d$. Then, by Bayes rule,

$$\begin{aligned} \mathbb{E}[g(\epsilon_{t+1}^d)|D_t] &= \frac{\int g(\epsilon_{t+1}^d) p(S_{t+1}|D_t) dS_{t+1}}{\int p(S_{t+1}|D_t) dS_{t+1}} \\ &= \frac{\int g(\epsilon_{t+1}^d) \frac{p(D_t|S_{1:t+1})}{p(D_t)} p(S_{1:t}, S_{t+1}) dS_{1:t+1}}{\int \frac{p(D_t|S_{1:t+1})}{p(D_t)} p(S_{1:t+1}) dS_{1:t+1}} \\ &\approx \frac{\sum_{j=1}^{N^d} \tilde{w}_j g(\epsilon_{t,j}^d)}{\sum_{j=1}^{N^d} \tilde{w}_j}, \end{aligned} \quad (47)$$

where the weights are $\tilde{w}_j = p(D_t | S_{1:t+1}^j)$. Due to a similar argument as above, $\tilde{w}_j = w_j$.

The conditional expectation $\mu_{t+1|t}^d$ and the conditional covariance $\mu_{t+1|t}^d$ can be computed by using Equation (47).

4. Synthetic Feasibility Study: Imaging Unsaturated Water Flow in Heterogeneous Soil

The solution of a dynamic imaging problem with approximation errors is demonstrated by conducting a synthetic, two-dimensional hydrological process monitoring study in which time-varying water saturation distributions are estimated using voltage measurements from a simulated ERT survey. Water is injected from a point source into an initially dry, heterogeneous porous medium. The ERT system consists of 16 electrodes, which are placed in two straight, vertical boreholes. The boreholes are five meters apart, and eight electrodes are installed in 1.2 meter intervals within each of the boreholes. The boundary of the computational domain is far away from the electrodes, and thus the error term due to domain truncation—discussed in detail in *Lehikoinen et al. [2007]*—is expected to be insignificant.

In Section 4.1 we generate the actual permeability field and the resulting evolution of the time-varying saturation, as well as the synthetic ERT measurements. In Section 4.2 we construct the approximation error related state and observation noise models corresponding to a statistical permeability (prior) model with a dynamical range of 8 orders of magnitude. Since the measurement geometry and the hydrological parameters are assumed to be known (except for the permeability), this stage involves only multiple simulations of the time-varying saturation in the accurate mesh with the inhomogeneous permeability field; and a simulation of the evolution in a sparse mesh with a single homogeneous permeability field which is used in the inversion. The actual permeability field is not known at this stage. In Section 4.3 we apply the proposed approach to the synthetic data and estimate the evolution of the saturation with different extended Kalman filter variants.

4.1. Generation of the synthetic data

The synthetic data for the study are generated as follows. As described above, the finite volume simulator TOUGH2

Table 1. Summary of parameters used in the generation of time-varying water saturation distributions to compute voltage observations

Parameters of Richards equation, Eqs. (1–2)	
k_v	$= 3 \times 10^{-12} \text{ m}^2$
k_h	$= 1 \times 10^{-12} \text{ m}^2$
ϕ	$= 0.3$
μ_w	$= 1.002 \times 10^{-3} \text{ Pa s}$
ρ_w	$= 1000 \text{ kg m}^{-3}$
Parameters of capillary pressure and relative permeability functions, Eqs. (3–5)	
m	$= 0.628$
α	$= 0.001 \text{ Pa}^{-1}$
S_{wr}	$= 0.083$
Parameters of Archie’s law, Eq. (12)	
b	$= 2.0$
n	$= 2.0$
σ_w	$= 0.01$
Parameters of spherical variogram model used to generate spatially correlated log permeability modifiers	
a	$= 0.4 \text{ m (range)}$
c	$= 1.0 \text{ (sill)}$
Anisotropy factor	$= 5$
Rotation angle	$= 25^\circ \text{ (from horizontal)}$

[Pruess et al., 1999] is used to solve the Richards equation in order to simulate the time-varying water saturation distributions. The uniform finite volume mesh consists of 18,271 elements and 36,270 connections. A heterogeneous field of spatially correlated permeability modifiers $\psi(x)$ is generated and mapped onto the mesh, whereby the locally anisotropic absolute permeability is calculated as

$$k_h(x) = k_h 10^{\psi(x)},$$

$$k_v(x) = k_v 10^{\psi(x)},$$

where k_h and k_v are the reference permeabilities in the horizontal and vertical directions, respectively. The permeability modifier $\psi(x)$ is a Markov random field which was generated using sequential Gaussian simulation [Deutsch and Journel, 1992]. The modifier field spans the interval $\psi(x) \in (-4, 4)$ which means that the permeability spans 8 orders of magnitude, see also Figure 3. All hydraulic parameters for this synthetic study are given in Table 1.

The synthetic voltage data are computed by a finite element solution of the complete electrode model (8)–(11), using a mesh with 43,031 nodes and 21,364 elements. The

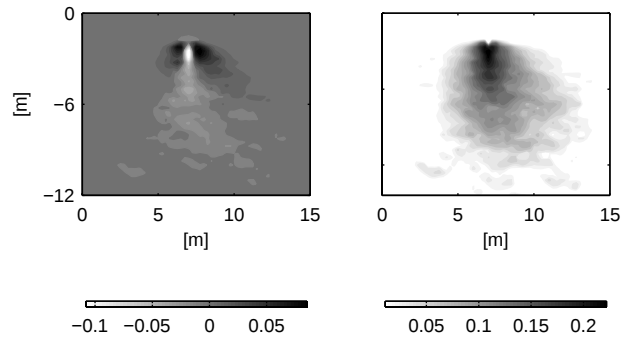


Figure 1. The approximation error ω_t^* 90 hours after beginning of water release. Left: mean of approximation error term; right: standard deviations.

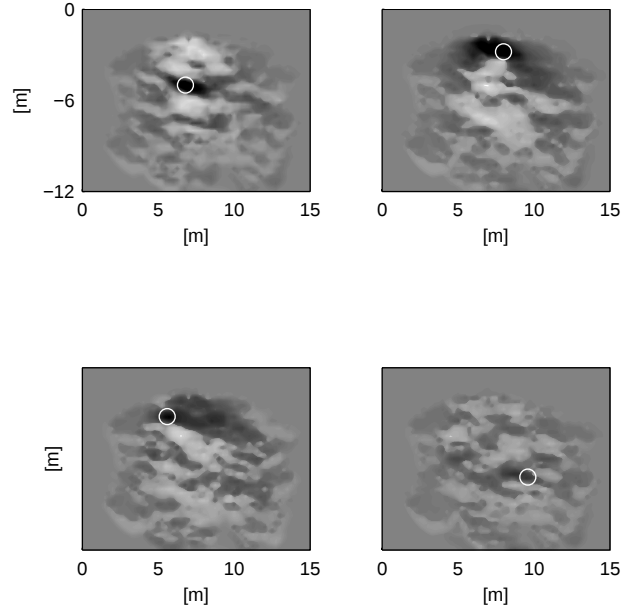


Figure 2. The signed deviations $\text{sign } \gamma(k, j) \sqrt{|\gamma(k, j)|}$ of four cross covariances at time $t = 90$ hours. The standard deviations (with $k = j$) are marked with white circles.

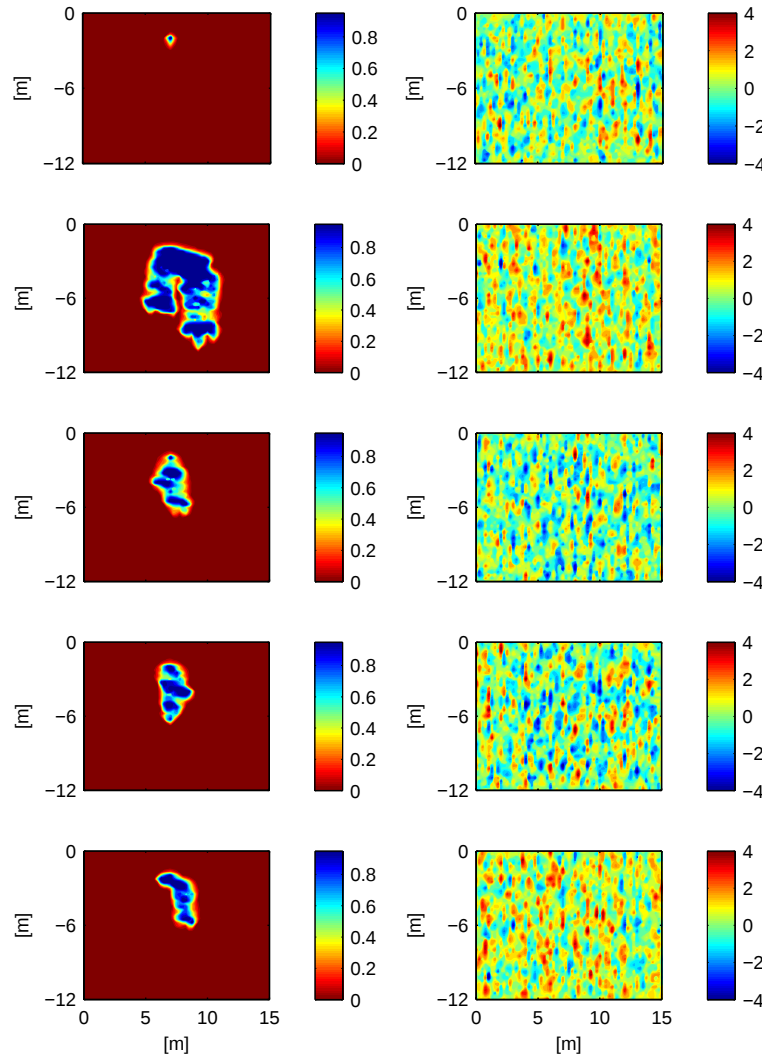


Figure 3. Simulated water distributions 90 hours after water release for 5 random permeability fields generated to construct the statistical model of the approximation error term. The saturation fields are shown on the left and the corresponding permeability modifier fields $\psi(x)$ are shown on the right.

potential u is approximated using second order basis functions.

Modern geophysical ERT systems consist of multiple electrodes for which the measurements and current injections are made parallel or multiplexed in order to reduce measurement time and to allow flexibility in configuring current injection patterns.

We simulate 16 different current patterns per frame, and the associated measurements are assumed to be obtained in a short time so that the monitored water saturation distribution does not change significantly during data acquisition. Here, a current pattern refers to a pair of electrodes between which the current is injected. The first eight current injections define a horizontal, zero off-set pattern between boreholes. The second set of eight injections follows a cross pattern, starting from the lowest electrode in the first borehole and the highest electrode in the second borehole, and subsequently using higher and lower electrodes in the respective boreholes. Each frame consists of 16 current injections, and for each current pattern 13 differential voltage measurements between two electrodes are taken, that is, no measurements that involve the injecting electrodes are used.

The voltage data are then corrupted with additive measurement noise consisting of two Gaussian components with zero mean. The standard deviation of the first error component is 2% of the measured value; the standard deviation

of the second component is 0.5% of the maximum observed voltage. This measurement error model corresponds to a system with both internal (electronics) errors and external electromagnetic field errors.

4.2. Generation of the Gaussian approximation error model

We follow the approach described in Section 2.3 to accommodate to the structural errors in the evolution model and discretization errors in the observation model. To develop the statistical model for ω_t^* , 1200 realizations of the permeability field are generated using sequential Gaussian simulation [Deutsch and Journel, 1992]. The variogram parameters are similar to those reported in Table 1, but intentionally slightly inaccurate. A rotation angle of 20° is chosen instead of 25° , and the reference permeability is assumed to be homogeneous and isotropic with a value of $k_h = k_v = 1 \times 10^{-12} \text{ m}^2$ instead of $k_h = 1 \times 10^{-12}$ and $k_v = 3 \times 10^{-12}$. Note that also here the permeabilities that are drawn from the prior distribution span 8 orders of magnitude. A flow simulation is performed with each permeability realization and the respective measurements are computed. The permeability field that is used in the inversion is a homogeneous one with $k_h = k_v \equiv 1 \times 10^{-12}$, that is, $\psi(x) \equiv 0$.

Five examples of the modifier fields and the corresponding saturations at 90 hours from the start of the water injection are shown in Figure 3. The saturation distribution calculated with the approximate, homogeneous model is subtracted from each of the realizations, and the means and covariances are computed as described in Section 2.3.

For the determination of the statistics of ϵ_t^d , which represents both the discretization errors in the observation model and the error due to using a fixed incorrect permeability model, the voltage data are simulated for each of the generated saturation fields (and corresponding conductivity fields) using two models: i) an accurate finite element model with 25,770 nodes and 12,771 elements, and ii) a coarse mesh with 9961 nodes and 4908 elements.

Figure 1 visualizes the approximation error term ω_t^* 90 hours after water release. The left hand image shows the mean of the state noise related approximation error and the right hand image the standard deviation (at 90 hours). The figure shows that the approximation errors are spatially highly heterogeneous. Moreover, since the mean is not zero, the estimates that would be obtained without the approximation error model would be highly biased.

The cross covariances $\gamma(k, j) = \text{cov}(\omega_t^*(k), \omega_t^*(j))$ are given by the rows of the covariance matrix $\Gamma_{\omega_t^*}$. The corresponding signed deviations $\text{sign} \gamma(k, j) \sqrt{|\gamma(k, j)|}$ are shown in Figure 2. These images depict the spatial correlation structure of the approximation errors. The traditionally used covariance model for the state noise process assumes that the state variables are mutually independent, and therefore all off-diagonal terms are zero. The four examples show that the approximation errors are spatially highly correlated. Hence, the traditionally used spatial white noise process model cannot appropriately model the approximation errors. For the interpretation of cross correlations of prior models, see *Kaipio et al. [1999]; Kaipio and Somersalo [2004]*.

4.3. Imaging of unsaturated water flow: results

To perform the dynamic reconstruction using Kalman filtering approaches, a computationally efficient, highly simplified evolution model is usually desirable or even mandatory when the computational resources are limited. In the inversion stage, that is, when the Kalman filters are employed, the prediction step for the unsaturated flow is computed using a coarse mesh (4636 elements and 9000 connections) with a homogeneous isotropic permeability field $k^* = k_h = k_v = 1 \times 10^{-12}$.

Running the (extended) Kalman filter requires iterative sequential computation of the model prediction and the inversion of the related covariance matrices. For this reason model reduction is almost invariably used in large dimensional filtering problems. On the other hand, when the approximation error statistics is computed, only the forward simulations are to be computed with the accurate model, in our case TOUGH2. Moreover, with a fixed measurement setup, the approximation error statistics only has to be computed once and can be used for all experiments (with the same setup).

The procedure used to solve the ERT inverse problem (described below) requires an initial guess for the state S_0 . Previous studies indicate that a homogeneous initial guess is usually sufficient. The homogeneous initial guess can be obtained by fitting a single homogeneous electrical conductivity σ_0 to a set of voltage measurements [*Järvenpää, 1996*].

The inversion of the ERT data for the estimation of time-varying water saturation distributions is performed using four different approaches: (1) a traditional, frame-by-frame method in combination with Tikhonov regularization and a smoothness prior, (2) the extended Kalman filter (EKF)

without inclusion of the approximation error method, (3) the EKF including the approximation error method, and (4) the iterated extended Kalman filter (IEKF) including the approximation error method.

The true and estimated water saturation distributions are shown in Figure 4. In the conventional inversion method, a Tikhonov regularization parameter needs to be specified. A relatively high regularization parameter results in a smooth image that generally underestimates the saturation near the center of the plume. Conversely, if the regularization parameter is reduced, the inverse problem becomes unstable. The regularization parameter was determined with the Morozov discrepancy principle.

Note that comparison of the new results with those obtained using the more conventional ERT inversion method is intended to provide some context for the current paper. It is possible that slightly better performance could be achieved with the conventional approach by using a different regularization criterion or with different error treatment. Furthermore, the inversion could be performed with an additional constraint that the mass of imaged water equals the amount injected. However, the main goal of this paper is limited to presenting a new approach for dynamic imaging with ERT data and approximation error treatment, highlighting its potential, rather than attempting to improve its superiority over conventional approaches for all cases.

The third column of Figure 4 shows the standard EKF without inclusion of an approximation error term, resulting in considerable inversion artifacts. The significant modeling errors (see Figure 1) are larger than the stochastic noise model employed in this case. The overall model is not able to capture the part of the plume that flows down and slightly to the right.

The fourth and fifth columns of Figure 4 show the improvements in the reconstructions that can be obtained if approximation errors are appropriately modeled. The images reasonably well reproduce the high absolute saturation values near the center of the plume, and they appropriately reflect the overall shape and structure of the plume.

To quantify the performance of the different reconstruction methods, the relative norm of the difference between the true and the estimated water saturation distributions is calculated and shown in Figure 5, demonstrating that the dynamic inversion method with the approximation error method provides better results than the traditionally used stationary reconstructions. Note that since the error measure is computed over the whole domain, the differences seem to be small. On the subdomain where the plume lives, the relative errors are much larger.

The estimates obtained using EKF and IEKF are almost at the same accuracy level, with only slightly improved results obtained with the IEKF. This is mainly due to the convergence of the measurement update step. The EKF with conditioned approximation error term gives the best estimates. We note that IEKF with the conditioned error term gives essentially the same level of accuracy as the EKF with conditioned error term. Generally, the question of whether the iterated extended Kalman filter will provide more accurate estimates than the plain sequentially linearized EKF, depends in a complicated way on i) the nonlinearities of the observation model and ii) the structure of the observation noise model. As a rule of thumb, however, we can state that the smaller the observation noise, the more meaningful it is to use the IEKF. In the case of this particular example, the total observation noise model (comprising of both the measurement error and the approximation error) was large enough to render the difference between EKF and IEKF insignificant.

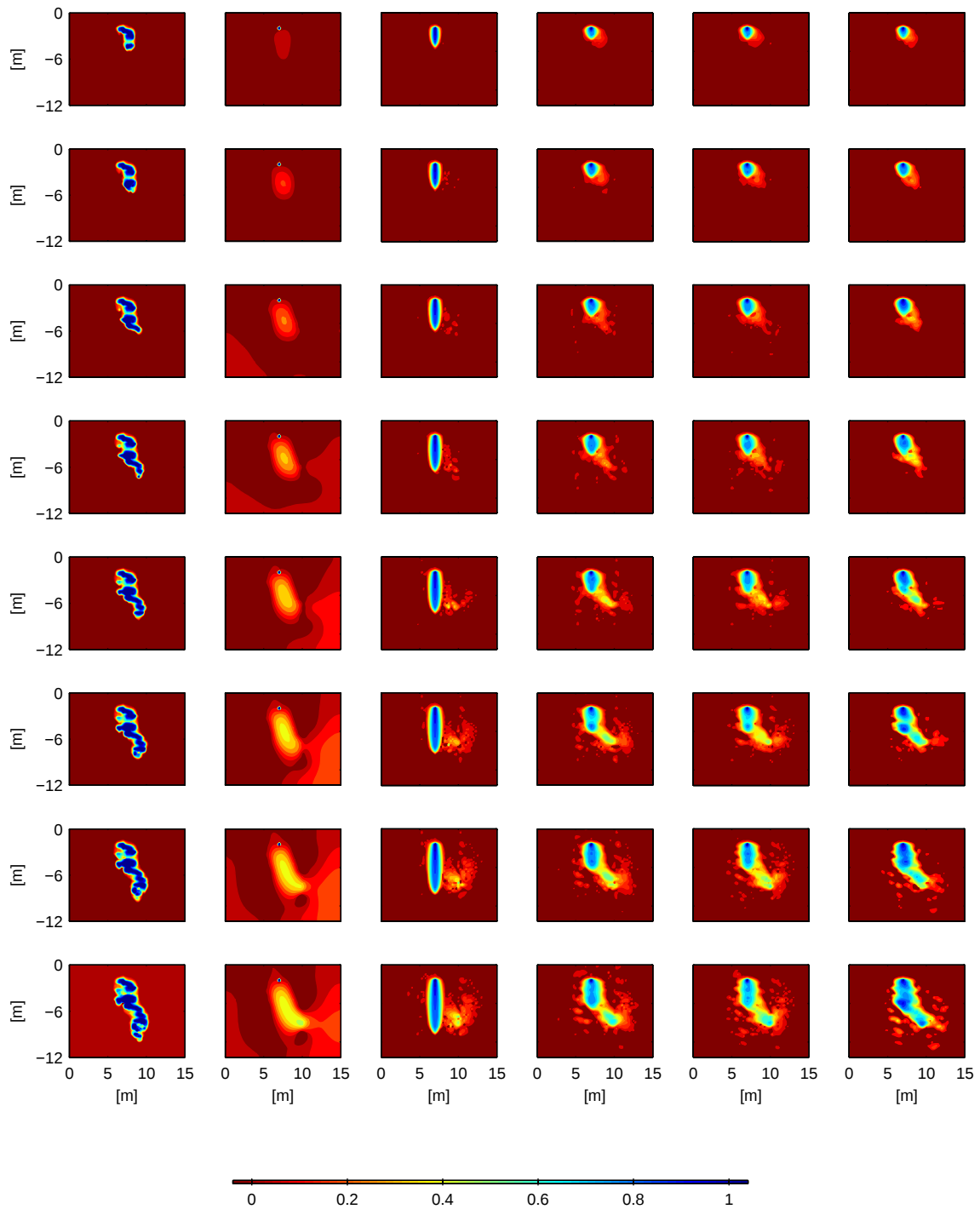


Figure 4. First column: true, simulated water saturation distribution in heterogeneous porous medium; second column: stationary reconstructions using Tikhonov regularization with a smoothness prior; third column: dynamic reconstructions using EKF, without approximation error term; fourth column: dynamic reconstructions using EKF and approximation error term; fifth column: dynamic reconstructions using IEKF and approximation error term; sixth column: dynamic reconstructions using EKF and conditioned approximation error term; rows are 12 hours apart.

5. Conclusions

We have discussed the dynamic approach for the inversion of time-lapse ERT data for absolute imaging of water saturation distributions in highly heterogeneous, partially saturated porous media.

The inverse problem was formulated as a Bayesian state estimation problem and solved using the extended Kalman filter and the iterated extended Kalman filter algorithms. The evolution model (which is based on a solution to Richards equation for unsaturated flow) provides a time-varying prior model of the water saturation distribution, and the observation model (which is based on Archie's law and the complete electrode model) relates the water saturation distribution to voltage observations.

Both the evolution and observation models contain approximation errors as a result of structural errors, uncertain parameters, and discretization errors. Traditional methods either ignore these errors or include them in an ad hoc fashion despite the fact that they are significantly larger than measurement noise and the state noise in the evolution model.

We adopted the Bayesian approximation error theory of *Kaipio and Somersalo* [2004], as it provides a framework in which the approximation errors are taken into account by building a statistical model. The statistics of the modeling errors are estimated by sampling. The statistical model representing approximation errors are incorporated in the computation of the posterior probability density. This approach leads to significantly improved state estimates.

The feasibility study proposes that the dynamic approach allows the estimation of time-varying water saturation distributions with reasonable accuracy using geophysical time-lapse ERT even with a very simplified flow model. The setting up of the approximation error model is a CPU intensive task. This task has to be done, however only once for a set up. In addition, the accurate models are never needed to be used in the inversion stage.

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References

- Anderson, B. D. O., and J. Moore (1979), *Optimal Filtering*, Prentice-Hall, Eaglewood Cliffs, NJ.
- Archie, G. E. (1942), The electrical resistivity logs as an aid determining some reservoir characteristics, *Trans. AIME*, 146, 54–61.
- Arridge, S., J. Kaipio, V. Kolehmainen, M. Schweiger, E. Somersalo, T. Tarvainen, and M. Vauhkonen (2006), Approximation errors and model reduction with an application in optical diffusion tomography, *Inverse Problems*, 22, 175–195.
- Binley, A., G. Cassiani, R. Middleton, and P. Winship (2002), Vadose zone flow model parametrisation using cross-borehole radar and resistivity imaging, *Journal of Hydrology*, 267, 147–159.
- Cheng, K.-S., D. Isaacson, J. Newell, and D. G. Gisser (1989), Electrode models for electric current computed tomography, *IEEE Trans. Biomed.*, 36, 918–924.
- Daily, W. D., and A. L. Ramirez (2000), Electrical imaging of engineered hydraulic barriers, *Geophysics*, 65(1), 83–94.
- Daily, W. D., A. L. Ramirez, D. J. LaBrecque, and J. Nitao (1992), Electrical resistivity tomography of vadose water movement, *Water Resour. Res.*, 28, 1429–1442.
- Dennis, J., and R. Schnabel (1983), *Numerical Methods for Unconstrained Optimization and Nonlinear Equations*, Prentice-Hall, Englewood Cliffs, NJ.
- Deutsch, C. V., and A. G. Journel (Eds.) (1992), *GSLIB—Geostatistical Software Library and User's Guide*, Oxford University Press, New York, NY.
- Dobson, D. C., and F. Santosa (1996), Recovery of blocky images from noisy and blurred data, *SIAM J Appl Math*, 56(4), 1181–1198.
- Doucet, A., N. de Freitas, and N. Gordon (2001), *Sequential Monte Carlo Methods in Practice*, Statistics for Engineering and Information Science, Springer-Verlag, NY.
- Eppstein, M. J., and D. E. Dougherty (1998), Efficient three-dimensional data inversion: Soil characterization and moisture monitoring from cross-well ground-penetrating radar at a Vermont test site, *Water Resour. Res.*, 34, 1889–1900.
- Evensen, G. (1994), Sequential data assimilation with a nonlinear quasigeostrophic model using monte carlo methods to forecast error statistics, *J. Geophys. Res.*, 99(C5), 10143–10162.
- Ferre, T., A. Hinnell, and J. Blainey (2006), Examining the potential for inferring hydraulic properties using surface-based electrical resistivity during infiltration, *The Leading Edge*, 25(6), 720–723.
- Finsterle, S. (2004), Multiphase inverse modeling: Review and iTOUGH2 applications, *Vadose Zone J.*, (3), 747–762.
- French, H., C. Hardbottle, A. Binley, P. Winship, and L. Jakobsen (2002), Monitoring snowmelt induced unsaturated flow and transport using electrical resistivity tomography, *Journal of Hydrology*, (267), 273–284.
- Hughson, D., and T.-C. J. Yeh (2000), An inverse model for three-dimensional flow in variably saturated porous media, *Water Resour. Res.*, 36(4).
- Huttunen, J., and J. Kaipio (2007a), Approximation errors in nonstationary inverse problems, *Inverse Problem and Imaging*, 1(1), 77–93.
- Huttunen, J., and J. Kaipio (2007b), Approximation error analysis in nonlinear state estimation with an application to state-space identification, *Inverse Problems*, submitted.
- Järvenpää, S. (1996), Finite element model for inverse conductivity problem, Ph.D. thesis, University of Helsinki, Finland.
- Kaipio, J., and E. Somersalo (1999), Nonstationary inverse problems and state estimation, *Inverse and Ill-Posed Problems*, 7, 273–282.
- Kaipio, J., and E. Somersalo (2004), *Statistical and computational inverse problems*, Applied Mathematical Sciences 160, Springer-Verlag.
- Kaipio, J., and E. Somersalo (2007), Statistical inverse problems: Discretization, model reduction, and inverse crimes, *J. Comput. Appl. Math.*, 198, 493–504.
- Kaipio, J. P., M. Vauhkonen, and E. Somersalo (1999), Inverse problems with structural prior information, *Inverse Problems*, 15, 713–729.
- Kaipio, J. P., V. Kolehmainen, E. Somersalo, and M. Vauhkonen (2000), Statistical inversion and Monte Carlo sampling methods in electrical impedance tomography, *Infrared Phys.*, 16, 1487–1522.
- Kalman, R. E. (1960), A new approach to linear filtering and prediction problems, *Trans. ASME J. Basic Eng.*, (82D), 35201345.
- Kemna, A., J. Vanderborght, B. Kulesa, and H. Vereecken (2002), Imaging and characterisation of subsurface solute transport using electrical resistivity tomography (ERT) and equivalent transport models, *Journal of Hydrology*, 267(3), 174–198.
- Lehikoinen, A., S. Finsterle, A. Voutilainen, and J. P. Kaipio (2007), Approximation errors and truncation of computational domains with application to geophysical tomography, *Inverse Problems and Imaging*, 1(2), 371–389.
- Lehikoinen, A., S. Finsterle, A. Voutilainen, M. B. Kowalsky, and J. P. Kaipio (2009), Water saturation estimation by dynamical filtering of geophysical data using an unsaturated flow evolution model, *Inverse Problems in Science and Engineering*, in press.
- Linde, H., S. Finsterle, and S. Hubbard (2006a), Inversion of hydrological tracer test data using tomographic constraints, *Water Resources Research*, 42, W04410, doi:10.1029/2004WR003806.
- Linde, N., A. Binley, A. Tryggvason, L. Pedersen, and A. Revil (2006b), Improved hydrogeophysical characterization using joint inversion of cross-hole electrical resistance and ground penetrating radar traveltime data, *Water Resour. Res.*, 42(12), W12404, doi:10.1029/2006WR005131.

- Nissinen, A., L. M. Heikkinen, and J. P. Kaipio (2008), Approximation errors in electrical impedance tomography - experimental study, *Measur. Sci. Technol.*, doi:10.1088/0957-0233/19/1/015501.
- Park, S. K. (1998), Fluid migration in the vadoze zone from 3-d inversion of resistivity monitoring data, *Geophysics*, 63, 41–51.
- Pruess, K., C. Oldenburg, and G. Moridis (1999), Tough2 user's guide, version 2.0, *Report LBNL-43134*, Lawrence Berkeley National Laboratory, Berkeley, California.
- Ramirez, A., W. Daily, D. LaBrecque, E. Owen, and D. Chesnut (1993), Monitoring an underground steam injection process using electrical resistance tomography, *Water Resour. Res.*, 29, 73–87.
- Ramirez, A., W. Daily, A. Binley, D. LaBrecque, and D. Roelant (1996), Detection of leaks in underground storage tanks using electrical resistance methods, *J. Environ. Engng Geophys.*, 1(3), 189–203.
- Richards, L. (1931), Capillary conduction of liquids through porous medium, *Physic*, 1, 318–333.
- Seppänen, A., M. Vauhkonen, P. J. Vauhkonen, E. Somersalo, and J. P. Kaipio (2001), State estimation with fluid dynamical models in process tomography - an application to impedance tomography, *Inverse Problems*, 17, 455–471.
- Slater, L., A. Binley, W. Daily, and R. Johnson (2000), Cross-hole electrical imaging of a controlled saline tracer injection, *J. Appl. Geophys.*, 44, 85–102.
- van Genuchten, M. T. (1980), A closed-form equation for predicting the hydraulic conductivity of unsaturated soils, *Soil. Sci. Soc. Am. J.*, 44, 892–898.
- Vauhkonen, P. J. (2004), Image reconstruction in three dimensional electrical impedance tomography, Ph.D. thesis, University of Kuopio, Finland.
- Vauhkonen, P. J., M. Vauhkonen, T. Savolainen, and J. Kaipio (1999), Three dimensional electrical impedance tomography based on the complete electrode model, *IEEE Trans. BME*, 46, 1150–1160.
- Voutilainen, A., and J. Kaipio (2009), Model reduction and pollution source identification from remote sensing data, *Inverse Probl Imaging*, in press.
- Voutilainen, A., T. Pyhlahti, K. Y. Kallio, J. Pulliainen, H. Haario, and J. Kaipio (2007), A filtering approach for estimating lake water quality from remote sensing data, *International Journal of Applied Earth Observation and Geoinformation*, 9, 50–64.
- Vrugt, J. A., B. A. Robinson, and V. V. Vesselinov (2005), Improved inverse modeling for flow and transport in subsurface media: Combined parameter and state estimation, *Geophysical Research Letters*, 32, doi:10.1029/2005GL023940.
- Yeh, T.-C., and J. Simunek (2002), Stochastic fusion of information for characterizing and monitoring the vadose zone, *Vadose Zone Journal*, 1, 207–221.
- Yeh, T.-C. J., S. Liu, R. J. Glass, K. Baker, J. R. Brainard, D. Alumbaugh, and D. LaBrecque (2002), A geostatistically based inverse model for electrical resistivity surveys and its applications to vadose zone hydrology, *Water Resour. Res.*, 38(12), doi:10.1029/2001WR001204.
- Zhang, J., and T.-C. J. Yeh (1997), An iterative geostatistical inverse method for steady flow in the vadose zone, *Water Resour. Res.*, 33(1), doi:6371.
- Zhou, Q. Y., J. Shimada, and A. Sato (2001), Three dimensional spatial and temporal monitoring of soil water content using electrical resistivity tomography, *Water Resour. Res.*, 37, 273–285.

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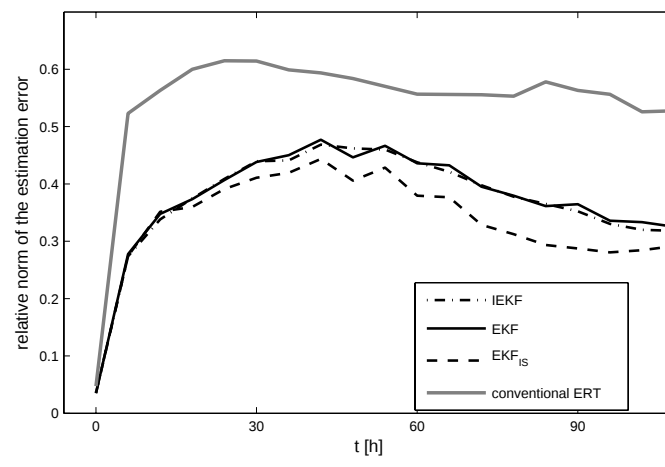


Figure 5. The relative norm of estimation error as a function of time.