Inverse modeling of unsaturated flow parameters using dynamic geological structure conditioned by GPR tomography

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Received 12 June 2007; revised 4 February 2008; accepted 11 March 2008; published 1 August 2008.

[1] A method is presented to estimate flow parameters and geological structure in the vadose zone by combining time-lapse Ground Penetrating Radar (GPR) traveltime tomography and inverse flow modeling. The traveltime tomography is used to determine the spatial electromagnetic velocity distribution in the vadose zone. These time-lapse velocity images are converted to time-lapse volumetric soil water content images using petrophysical relationships. Subsequently, the water content images are used as constraints in the flow inversion. The influence of the tomographic artifacts on the flow inversion is minimized by assigning weights that are proportional to the ray coverage. Our flow inversion algorithm estimates the flow parameters and calibrates the geological structure. The geological structure is defined using a set of control points, the positions of which can be modified during the inversion. After the inversion, the final geological and flow model are used to compute GPR traveltimes to check the consistency between these computed traveltimes and the observed traveltimes. The method is first tested on two synthetic models (a steady state and a transient flow models). Subsequently, the method is applied to characterize a real vadose zone at Oslo Airport Gardermoen, Norway, during the snowmelt in 2005. The flow inversion method is applied to locate and quantify the main geological layers at the site. In particular the inversion method identifies and estimates the location and properties of thin dipping layers with relatively low-permeability. The flow model is cross validated using an independent infiltration event.

1. Introduction

[2] Estimation of flow parameters is of fundamental importance for the modeling and understanding of hydrological processes in the subsurface. Traditionally, flow parameters have been determined in the laboratory using small scale samples and/or by in situ field tests. However, using estimates of the flow parameters based on these methods to characterize larger areas normally carries significant uncertainty because of scale discrepancies and sparse spatial sampling. This is due to the ubiquitous heterogeneity of natural soil. Furthermore, laboratory and in situ field tests are invasive, time consuming and expensive. An alternative method to estimate flow parameters is provided by inverse flow modeling conditioned on flow measurements. The purpose of this paper is to present a method to estimate the flow parameters by conditioning the flow model on spatially continuous volumetric soil water content obtained at various times during a natural infiltration event. The water content estimates are obtained by applying petrophysical relationships [Topp et al., 1980] to time-lapse Ground Penetrating Radar (GPR) velocity tomograms.

[3] GPR and seismic tomograms have been used to estimate the location and shape of lithologic zones [Hyndman et al., 1994; Hyndman and Gorelick, 1996; Linde et al., 2006] as well as the volumetric soil water content using petrophysical relationships [Hubbard et al., 1997; Binley et al., 2001; Alumbaugh et al., 2002; Farmani et al., 2008]. In recent years, GPR data have also been used to estimate flow parameters such as permeability and porosity [e.g., Lambot et al., 2004; Kowalsky et al., 2004, 2005; Linde et al., 2006]. Most of these studies used the observed GPR traveltimes for conditioning. Only Linde et al. [2006] used GPR tomograms, but their work was limited to synthetic data.

[4] There is a general consensus about the qualitative power of GPR tomography to image the electromagnetic (EM) velocity distribution. However, because of the presence of artifacts in the images, the quantitative application of tomograms should be performed with caution. Kowalsky et al. [2005] show an example of image distortion after tomography inversion, and Day-Lewis et al. [2005] demonstrate the importance of resolution and parameterization in GPR tomography. Since we use the GPR images quantitatively in the flow inversion, it is important to mitigate the influence of artifacts in the images. We propose a method that minimizes the influence of these artifacts by assigning weights that are proportional to ray coverage. The method...
suggested is similar, but not identical, to maximum likelihood inverse modeling. In our method the weights in the objective function are computed using an a priori covariance matrix as well as the ray coverage.

[5] In addition to estimating the flow parameters, the flow inversion method presented here also calibrates the geological structure. In general, determination of the geological structure in a heterogeneous medium is performed by soil sampling and/or indirect measurements such as tomograms and surface reflection profiles. However, it is not trivial to locate the positions of various geological units quantitatively. To overcome this problem, we define the geological geometry by using a set of control points. We calibrate the positions of these control points as part of the inversion algorithm. The position of the points can be changed independently or, alternatively, the points can be clustered into different groups. The proposed flow inversion method, therefore, differs from the traditional procedure where the geological structure is predefined and fixed [e.g., Kitterød and Finsterle, 2004]. This is an important improvement because geological structure strongly influences the flow. If geological structure is incorrectly implemented, the optimization of flow parameters may be biased.

[6] As a final step of our method, the EM wave traveltimes through the flow model are computed by applying the inverse petrophysical relationships and compared with the observed traveltimes. This way, consistency between the computed and observed traveltimes can be used to accept or reject the inversion results. Furthermore, this coupling between measurements and inverse modeling results can be further developed in joint inversion of indirect measurements and flow modeling, which is an interesting topic for further studies.

[7] The concept of moveable control points differs from the concept of pilot points in geostatistics [RamaRao et al., 1995]. Control points are used to define and calibrate the geometry during the inversion. Pilot points are used to simulate heterogeneity without any assumption of geological structure. Instead, pilot points are selected in unmeasured locations of the model using geostatistics and sensitivity analysis which, in turn, can be used for conditioning the inversion.

[8] To validate the proposed inversion method we generated two realistic case studies based on synthetic data. The first test consists of a steady state flow model; the second test is a transient infiltration event. The synthetic steady state model is generated by assigning EM velocities to each geological unit. In this model, the soil water content distribution is assumed to be homogenous within each layer. The synthetic velocity tomogram for this example is obtained using both straight ray and curved ray traveltome

graphy. The second synthetic model, which is run using an observed transient infiltration event, is generated by assigning flow parameters to each geological unit. Soil water content is computed as a continuous function in space and sampled at three different times corresponding to the time of conditioning (or “observation”). Synthetic tomograms are then computed using curved ray traveltome

graphy and converted to soil water content. After this, the flow parameters are estimated and the geological structure is calibrated using the proposed flow inversion method.

We then apply the method to a real-world problem: the estimation of flow parameters and calibration of geological structure of an ice-contact delta in Norway. The GPR field data were acquired during the snowmelt in 2005. The resulting flow model is cross validated by using infiltration data due to the snowmelt in 2006. These infiltration data are not used in the flow inversion and are, therefore, independent data. The simulated groundwater recharge reproduces the observed retention of water flux, but the initial response is simulated with a delay compared to the observations.

2. Methodology

2.1. Ground Penetrating Radar Traveltime Tomography

[9] EM waves generated by GPR antennas used in this study are in the frequency band where ray theory is valid [e.g., Kline and Kay, 1965; Vasco et al., 1997]. According to this theory, energy propagates along raypaths. In isotropic heterogeneous media the raypaths are given by a set of coupled ordinary differential equations:

\[
\frac{dX}{ds} = \nu P, \quad \frac{dP}{ds} = \frac{\partial}{\partial X} \left( \frac{1}{v} \right),
\]

where \(X = (X_1(s), X_2(s), X_3(s))\) is the raypath; \(P = (P_1(s), P_2(s), P_3(s))\) is the slowness vector (tangent vector to the raypath); \(v = v(X)\) is the velocity at \(X\); and the independent parameter \(s\) is the arc length along the ray. The initial conditions for the ray equations are \(X(0) = X_0\), \(P(0) = P_0\). Here, \(X_0\) is the position of the source antenna, and \(P_0\) is the slowness vector at the source, i.e., the vector pointing in the direction in which the ray leaves the source antenna. In this paper the velocity values are given on square grids with a grid size of 10 cm by 10 cm. The acquisition geometry of the data is a cross-well geometry. This means that the sources are located in one well, and the receivers in another well. For each ray (source-receiver combination) \(i\), the traveltime of the first arrival is picked from the waveforms [see Farmani et al., 2008]. These traveltimes are used to estimate an average velocity through the medium between the two wells. Using this average velocity model, the starting velocity model, the traveltime residuals \((\delta T_i = T_{i,c} - T_{i,o})\) can be computed. Here \(T_{i,c} = \int \frac{ds}{v}\) is the traveltime of the ray traveling through the model, \(v_i\) is the velocity model computed using tomography, and \(T_{i,o}\) is the observed traveltime. In traveltime tomography, the traveltime residuals are related to the velocity variation \(\delta v_i\) [Nolet, 1987] (the difference between the computed velocity and the true velocity) by:

\[
\delta T_i = \sum_k \frac{l_k}{v_k} \delta v_k, \quad \text{(2)}
\]

Here, \(l_k\) is the length of ray \(i\) through velocity cell \(k\) and the starting velocity in cell \(k\) for each iteration is denoted by \(v_k\). In our study, equation (2) is extended to account for small errors in the source and receiver locations [Keers et al., 2000] and stabilized by adding two terms to minimize a
combination of velocity variation (damping) and velocity gradients (smoothing):

$$
\begin{pmatrix}
\delta T \\
0 \\
0
\end{pmatrix} = \begin{pmatrix}
L & L_R & L_S \\
\lambda_1 I & 0_R & 0_S \\
\lambda_2 D & 0_R & 0_S \\
\end{pmatrix} \begin{pmatrix}
\delta V \\
\delta V_R \\
\delta V_S \\
\end{pmatrix}.
$$

(3)

Here $L$ is the coefficient matrix consisting of the factors $l_{ik}/v_k$ in equation (2); $L_R$ and $L_S$ are matrices containing zeros and ones depending on whether the source/receiver is active; $\delta V_R$ and $\delta V_S$ represent the source and receiver statics; $\lambda_1$ is the damping factor; $\lambda_2$ is the smoothing factor; $I$ is the identity matrix; $D$ is the smoothing operator; and $0_R$ and $0_S$ are zero matrices. In this study the damping and smoothing factors are kept constant for all inversions. $L$ is a sparse matrix and, therefore, it can be solved efficiently using the LSQR algorithm [Paige and Saunders, 1982]. We use this algorithm to solve equation (3) iteratively. Velocities obtained for one iteration are used as the starting velocities for the next iteration.

[10] The final tomogram gives a spatial velocity distribution of the vadose zone between the source and receiver wells. We apply the conventional assumption that the EM velocity of the soil $v$, is described by:

$$
v \approx \frac{c_v}{\sqrt{\varepsilon}},
$$

(4)

where $c_v$ is the velocity of an EM wave through the air and $\varepsilon$ is the relative dielectric permittivity of the soil [Davis and Annan, 1989]. For a range of sediments (from clay to sandy loam), Topp et al. [1980] found a general experimental relationship between volumetric soil water content and apparent permittivity. They also introduced separate relationships for different types of soils. Since the vadose zone at our research field site in Norway consists mainly of sand, Topp’s model for sandy loam is included in this study:

$$
\theta = a + b\varepsilon_a + c\varepsilon_a^2 + d\varepsilon_a^3,
$$

(5)

where $a = -5.75 \times 10^{-2}$, $b = 3.09 \times 10^{-2}$, $c = -7.44 \times 10^{-4}$, $d = 9.634 \times 10^{-6}$. According to Topp et al. [1980] the absolute standard error in the values of $\theta$ in equation (5) is about $\sigma_{\theta_{Topp}} = 0.0089$. For low-loss materials we have $\varepsilon_a \approx \varepsilon$ so that $\theta$ can be determined from the velocity $v$ using equations (4) and (5).

[11] The applicability of Topp’s model for sandy loam in our field site was cross validated using neutron probe measurements and water balance comparison [see Farmani et al., 2008]. Furthermore, we noted that the differences in volumetric soil water content estimated by either Topp’s general model or Topp’s model for sandy loam did not exceed 0.2%. Although Topp et al. did not use sand samples to derive their general model, some other studies [e.g., Ponizovsky et al., 1999] applied Topp’s model to laboratory measurements of soil water content and dielectric permittivity of sand and found a satisfactory fit.

2.2. Forward Flow Modeling

[12] Water flow in a heterogeneous variably saturated porous medium is modeled by Richards’ equation [Richards, 1931; Comsol Multiphysics, 2004]:

$$
[C + S_o S] \frac{\partial p}{\partial t} + \nabla \left[ - \frac{k_s}{\eta} \nabla (p + \rho g z) \right] = Q_s,
$$

(6)

where $p$ is the dependent variable; $C$ is the specific capacity ($C = \frac{s}{C_0}$) expressed in equation (9); $S_o$ is the effective saturation; $S$ is the storage coefficient related to the compression and expansion of the pore space and the water; $k_s$ is the intrinsic or absolute permeability; $\eta$ is the fluid viscosity; $k_r$ is the relative permeability; $\rho$ is the density of water; $g$ is the gravitational acceleration; $z$ is the vertical coordinate (positive upwards); and $Q_s$ represents a source or a sink.

[13] Richards’ equation is highly nonlinear because $p$ and $k_r$ vary as a function of volumetric water content $\theta$. For these parameters constitutive relations are needed. In this study we use the relations of Mualem [1976] and Van Genuchten [1980]:

$$
\theta = \theta_r + S_s (\theta_s - \theta_r),
$$

(7)

$$
S_s = \left(1 + \frac{ap}{\rho g z} \right)^{-m},
$$

(8)

$$
C = \frac{am}{1 - m} (\theta_s - \theta_r) S_s^{1/m} \left(1 - S_s^{1/m} \right)^m,
$$

(9)

$$
k_r = S_s^{1/m} \left[1 - \left(1 - S_s^{1/m} \right)^m \right]^2,
$$

(10)

Here $\theta_r$ is the residual water content; and $\theta_s$ is the maximum water content. $\alpha$, $m$, $n$, and $L$ are parameters which characterize the porous medium. In this paper we set $Q_s$ and $S_o$ to zero, $L = 0.5$, and $m = 1 - 1/n$. We solve Richards’ equation using the finite element code FEMLAB3.1 [Comsol Multiphysics, 2004].

2.3. Inverse Flow Modeling

[14] The volumetric soil water content, $\theta$, estimated by several GPR traveltime tomography models and Topp’s model, gives the soil water content distribution at various times. These soil water content distributions are the observed soil water content for the inverse flow modeling. Given a combination of flow parameters and a geological structure, the flow model predicts the soil water content distribution at the same times as the observed soil water content. By minimizing the difference between the observed and computed soil water content, we can invert for the flow parameters and calibrate the geological structure. The initial geometry of the flow model is typically built using various data, such as knowledge of local geology, measurements on soil samples, seismic and GPR data. Because forward flow modeling is time consuming, the flow model consists of a
relatively small number of distinct homogeneous geological units, in this paper referred to as sub domains. Since the sizes of these sub domains are much larger than the size of the velocity cells used in the traveltime tomography, the inversion performs an upscaling of the measurements. After solving Richards’ equation for the flow model, the saturation obtained for the finite elements are mapped to the square velocity cells to compute the difference between the observed and computed soil water content. The sub domains themselves are defined by a number of discrete control points (vertices). In the optimization, the locations of these control points are allowed to vary. It is also possible to put constraints on these points. If, for example, for geological reasons an interface between two sub domains is assumed to be more or less horizontal, the corresponding control points can be constrained accordingly. Because control points are included in the objective function (equation (11)), discontinuity problems may arise. To avoid such discontinuities and to make the derivatives of water content with respect to the coordinates of the control points as smooth as possible, it is necessary to use a fine mesh in the flow modeling. In this study, we use approximately 5200 finite elements to solve Richards’ equation.

The objective function to be minimized is the sum of the squared weighted-residuals for all data sets:

\[ F = \sum_{j=1}^{n_p} \sum_{k=1}^{N} \sigma_{jk}^{-2} (\theta_{jk} - \theta(p_1, p_2, \ldots, p_M, g_1, \ldots, g_Q))^2 \]  \hspace{1cm} (11)

where \( p_1, \ldots, p_M \) are the flow parameters that are optimized; \( g_1, \ldots, g_Q \) are the local coordinates of the control points that are modified; \( \theta_{jk} \) and \( \theta_j \) are respectively the observed and the computed volumetric soil water content at a given cell \( k \) and survey time \( j \); \( N \) is the number of velocity cells; \( n_p \) is the number of surveys; and \( \sigma_{jk}^{-2} \) are the weights, which are defined as:

\[ \sigma_{jk}^{-2} = W_{jk} \sigma_{Topp}^{-2} \]  \hspace{1cm} (12)

where,

\[ W_{jk} = \max \left( \frac{\sum_{i=1}^{r} l_{jk}}{\max_k \left( \sum_{i=1}^{r} l_{ijk} \right)} , \chi \right) \]  \hspace{1cm} (13)

and \( \sigma_{Topp}^{-2} \) is the error variance of Topp’s model. \( W_{jk} \) is the weight derived from the ray coverage and \( \sum_{i=1}^{r} l_{jk} \) is the total length of the rays passing through the \( k \)-th cell in the \( j \)-th survey, \( r \) is the total number of raypaths, and \( \chi \) is a small number which is used as a lower bound in case there are some cells with no or very little ray coverage in the medium. The lower bound \( \chi \), assures that no weights get zero value. The reason for including a lower bound for the weights is that all cells inherit some information, partly from the initial guess and partly because we include a smoothing factor as part of the tomographic inversion. For this study we let \( \chi = 0.05 \). No cell in the synthetic examples receives this weight. In the field example, however, less than 1.5% of the cells located in the capillary zone, received the boundary value. To derive the weights we assume that regions with relatively larger ray coverage are less influenced by artifacts. In the synthetic examples, we show that this is a reasonable assumption. In addition, Curtis [2004] showed mathematically that if a tomography survey is designed to maximize the total ray coverage, then error in the final velocity estimates is minimized. Therefore there is a correlation between ray coverage and artifact. We also assume that the observed volumetric soil water contents are uncorrelated.

[15] The objective function is minimized using the Levenberg-Marquardt (LM) algorithm [Bixby, 1992]. For the synthetic transient model, we test the accuracy of the LM algorithm by comparing it with the Shuffled Complex Evolution (SCE) global search algorithm [Duan et al., 1992]. The objective function in equation (11) is minimized iteratively. In our experience convergence is obtained after 10 to 20 iterations. Because of the scale difference between the tomograms and the flow model the objective function does not converge to zero. This is an effect of the upscaling which is discussed later. For the LM algorithm, each iteration consists of all function evaluations through the search direction for that iteration and updates of the Jacobian before the search direction is changed. For the SCE algorithm, on the other hand, each iteration consists of all function evaluations to evolve complexes before shuffling them and updating the array of samples. It is worthwhile to mention that if the locations of the control points are changed, then the meshing is updated accordingly. Because a fine meshing is applied, the impact of the remeshing on the solution is negligible. The remeshing option makes the inverse flow modeling flexible and robust.

[17] Once convergence of the objective function has been obtained, the estimates of the flow parameters and the calibrated geological structure are used to compute the EM wave traveltimes through the velocity image obtained from the flow model. These computed traveltimes are compared with the observed traveltimes. A quantitative measurement of the accuracy of the velocity image is obtained using the following misfit function:

\[ T_m = \frac{1}{r} \left( \sum_{i=1}^{r} (T_{i,c} - T_{i,o})^2 \right)^{\frac{1}{2}} \]  \hspace{1cm} (14)

If the value of the misfit function is not acceptable, the initial guess of the parameters search space and/or the number of sub domains in the geological model should be reconsidered. This is a manual step in the algorithm which is used, if necessary, to test other possible scenarios. The objective function may be considered as the final criterion for acceptance or rejection of the inversion results. By using the objective function as the final criterion, the traveltimes criterion of equation (14) can be avoided. Alternatively, the traveltimes could be included directly in the objective function. However, because of the scale difference between tomograms and flow model, the objective function does not converge to zero. The inversion result may still be acceptable, but in order to validate the result it is necessary to use the traveltimes misfit function as the final criterion. The alternative approach, by including the traveltimes directly in the objective function, is caused to miss the opportunity to compute the weights in the objective
function. A flowchart of the complete inverse flow modeling outlined above is given in Figure 1.

After the optimization, the sensitivities are estimated to assess the relative importance of all the parameters that are varied in the optimization. The sensitivity coefficients are defined using the Jacobian matrix [Carrera and Neuman, 1986]:

$$ J_{jk} = \frac{\partial q_{jk}}{\partial p_l} \quad \text{or} \quad \frac{\partial q_{jk}}{\partial g_l}, $$

where $l = 1, 2, \ldots, M + Q$. Here $M$ and $Q$ are the number of flow parameters and control points, respectively. The sensitivity coefficients are used to evaluate the impact of flow parameters and control points on the final volumetric soil water content estimates. Because the parameters have different units, the sensitivity coefficients are made dimensionless. This is done by scaling the coefficients by $\sigma^*$ and the standard deviation of each parameter, $\sigma_p$ or $\sigma_g$. The standard deviation of a parameter is calculated from an a priori search space by assuming a Gaussian distribution:

$$ J_{\lambda l} = J_{\lambda l} \frac{\sigma_p}{\sigma_{\lambda l}} \quad \text{or} \quad J_{\lambda l} \frac{\sigma_g}{\sigma_{\lambda l}}. $$

The sum of the sensitivity coefficients for each parameter assesses the total impact of that parameter on the model:

$$ S_{\lambda} = \sum_{j=1}^{n} \sum_{k=1}^{N} |J_{\lambda j}|. $$

The sensitivity analysis is performed for the optimal values and is only locally meaningful. A more robust estimation of sensitivities can be obtained by doing a global sensitivity analysis over the whole search space. However, a global sensitivity analysis is not feasible for the number of parameters we use in this study because it is too time consuming. The local sensitivity analysis is still of interest because it indicates how the volumetric soil water content is influenced by small changes in the optimal parameter values. In the next section we illustrate the proposed inversion method using a synthetic steady state as well as a transient flow model.

3. Synthetic Test Models

The geometry and the scale of the synthetic models are designed to capture the main features of the real field site. The geometry of the synthetic models contains two
main geological structures: the delta topset and the delta foreset. Each of these two structures consists of two or three sub domains. These sub domains are horizontal layers in the case of the topset and slightly dipping (approximately 15°) layers in the case of the foreset. The wells used in the cross-well tomography are located in the center of the flow model. The flow model is extended in both directions to eliminate the influence of boundary conditions on the monitoring area (see Figure 2a).

3.1. Steady State Model

The methodology is first tested on a steady state flow model. We assume that the volumetric soil water content distribution within each layer of the model is homogeneous (see Figure 2a). The interfaces between the layers are not discontinuous but somewhat smoothed. Smooth interfaces give more accurate ray tracing results. The smoothing is physically justified because the capillary forces of fine grained material cause a smooth change in the water content, even across a geological discontinuity. Using equations (4) and (5), the EM velocity distribution can be obtained from the soil water content. This gives the synthetic velocity models used in this example. Flow parameters are not used to generate the model. However, the model is rather close to the field tomograms which are discussed later. The idea is to check if the presented methodology is able to estimate physically meaningful flow parameters for the soil layers. This is similar to what we encounter in a real-world problem where measurements or estimates of soil water content usually are the starting point for inverse flow modeling. In the next section, we present a synthetic example where we check the robustness of the algorithm to reproduce the known flow parameters.

After application of equations (4) and (5), the two horizontal layers in the topset of the model have an EM-velocity of 130 m/μs and 140 m/μs, respectively. The foreset contains two low-velocity layers with an EM velocity of 108 m/μs. The other dipping foreset layers have an EM velocity of 120 m/μs. The lower boundary of the model is the groundwater table, which is at 4.4 m depth. There are two boreholes in the model that are 2.4 m apart (Figure 2a). From the surface, cross-well GPR data are collected to a depth of 4.2 m with 0.2 m spacing for both source and receiver antennas; thus, the total of 484
traveltimes are obtained. However, only traveltimes from source-receiver pairs with offset angles equal to or smaller than 45° are used in the tomographic inversion. This is done to keep the synthetic examples as close to the field example as possible. Higher angle paths of the field data were too noisy and were not used in the tomographic inversion. Consequently, 352 traveltimes were used in the inversion. Since we assume a steady state condition with infiltration of 0.5 mm/day (equation (6)), only one GPR data set is acquired. The starting velocity model has a constant velocity. All subsequent inverted velocity models are heterogeneous. The traveltimes through these models are computed using two methods: straight ray tomography, which is approximate, but used regularly in GPR tomography, and curved ray tomography, which uses the exact raypaths. The results are shown in Figure 2b (straight ray tomogram) and Figure 2c (curved ray tomogram). This is Step 3 in the flow diagram of Figure 1.

[22] The straight ray tomogram does not result in a clearly defined interface between the two topset layers. Also the low-velocity dipping layer in the foreset, which crosses the two wells, is not well resolved. The low-velocity dipping layer at the bottom of the tomogram is absent. The curved ray tomogram, on the other hand, recovers both the interface in the topset as well as the shape of the dipping layers in the foreset.

[23] During the inverse flow modeling some of the flow parameters of the various sub domains (porosity, residual water content, and viscosity) are fixed; the others (the intrinsic permeability, and the van Genuchten parameters $n$ and $\alpha$) are optimized during the inversion (see Table 1). The fixed parameters, the initial guess and the a priori search space were derived by interpreting the available data and previous studies done at the field site [Pedersen, 1994; Kitterød et al., 1997; Kitterød and Finsterle, 2004]. The basic geological structure (i.e., the number of sub domains and their approximate shapes) is assumed to be known. However, the exact location and shape (thicknesses, dip angle etc.) of the sub domains are unknown and estimated using the optimization. The initial locations of the control points in the starting flow model, which define the geological structure, are located ±20 cm from their correct locations. This way the ability of the optimization algorithm to find the correct geometry is tested. Two pairs of the control points, the two points labeled $g_5$ and two points labeled $g_6$ (see Figure 2a), define the horizontal interfaces. These points are constrained in such a way that the corresponding interfaces stay horizontal during the inversion. Search space for the control points is ±40 cm from their initial location in both vertical and horizontal directions (Table 1). By this, each control point can freely change its location in 18% of the total vertical length and 6% of the total horizontal length of the model. The flow inversion is done three times. The first inversion is conditioned on the straight ray tomogram without using the weights in the objective function, the second inversion is conditioned on the straight ray tomogram while using the weights, and the third inversion is conditioned on the curved ray tomogram again by using the weights. The weights in the objective function for the straight and curved ray tomograms are shown in Figures 2d and 2e, respectively. The flow inversion results are presented in Table 1. The corresponding velocity images between the wells are shown in Figures 2f, 2g, and 2h.

[24] The flow inversion conditioned on the straight ray tomogram without using the weights (Figure 2f) is able to calibrate the overall geological structure quite well. However, it fails to recover the true velocities in the topset layers. This is especially evident for the lower topset layer. On the other hand, when the weights are taken into account in the objective function, the velocities of all layers are recovered well but the geological structure is not precisely calibrated (Figure 2g). The position of the interface between the two topset layers is lower than its true position. Also, the thickness of the low-velocity layer in the foreset is underestimated.

[25] To show the impact of the weights on the inversion results, we focus on the two topset layers where the tomographic artifact is strongly correlated to the weights. In the foreset, the correlation between the tomographic artifact and ray coverage is less strong in the case of straight ray tomography. The straight ray tomogram (Figure 2b) clearly contains artifacts at the center of the upper layer of the topset and underestimates the velocity because of poor ray coverage (Figure 2d). However, the optimized flow parameters correctly recover the velocity of this layer (Figure 2g). The reason is that the weights of the cells near the wells are larger than the weights of the central cells (equation (11)). As a result, the optimized flow parameters reconstruct the velocities at the side cells of the layer better than at the central cells. Since the velocities of the side cells are very close to the true velocity of the layer in the model, the final velocity estimate from the optimized flow parameters is correct. The same phenomenon is observed for the lower layer of the topset. The velocity estimate from the optimized flow parameters for this layer (Figure 2g) is closer to the velocity estimates at the central cells of the tomogram which have larger weights and better estimate the true velocity. The algorithm does not correctly estimate the position of the interface between the two topset layers. This is because there is no clearly defined interface between these layers in the straight ray tomogram (Figure 2b).

[26] The flow inversion conditioned on the curved ray tomogram gives better results (Figure 2h). Especially the geological structure is better calibrated. Figure 3a shows the reduction of the objective function during the inverse flow modeling conditioned on the curved ray tomogram. After 15 iterations the objective function was minimized to only 4% of its initial value. Figure 3b shows the estimated velocities obtained using cross-well GPR tomography (Step 3 of Figure 1), the initial (Step 5 of Figure 1) and the optimized flow (Step 11 of Figure 1) models versus the true velocities for all individual cells. The final flow model estimates the velocities of the cells almost as well as the cross-well tomography, even though considerable upscaling has been used in the former. GPR volumetric soil water content estimates are obtained at the spatial resolution of 10 cm by 10 cm. The flow model upcales the high resolution GPR volumetric soil water content estimates into a few sub domains. The only, minor, artifact is that the velocity of the low-velocity dipping layers is not completely resolved. This is because there are relatively few cells in these layers and the weights of these cells are relatively low (Figure 2e). Thus the flow model overestimates the velocity of these
Table 1. Fixed, Initial, True and Optimized Flow Parameters for the Steady State Example, the Transient Example and the Natural Snowmelt Event at Moreppen (Near Oslo’s Gardermoen Airport)*

<table>
<thead>
<tr>
<th>Dom.</th>
<th>$\theta_s$</th>
<th>$\theta_r$</th>
<th>$\eta$</th>
<th>$\alpha$</th>
<th>$n$</th>
<th>$k_s (\log_{10})$</th>
<th>$\alpha$</th>
<th>$n$</th>
<th>$k_s (\log_{10})$</th>
<th>$\alpha$</th>
<th>$n$</th>
<th>$k_s (\log_{10})$</th>
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<td></td>
<td>Synthetic Steady State Flow Model</td>
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<td>Synthetic Transient Flow Model</td>
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<td>Moreppen Research Field Flow Model</td>
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<td>Fixed</td>
<td>Initial Guess</td>
<td>Optimized: Curved Ray Tomography</td>
<td>Optimized: straight ray Tomography</td>
<td>Optimized: straight ray tomography, no weights</td>
<td>Optimized with LM Algorithm</td>
<td>Optimized with SCE algorithm</td>
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<tr>
<td>1</td>
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<td>1.75E-03</td>
<td>33.35</td>
<td>2.04</td>
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<td>30.90 (15.07)</td>
<td>1.98 (0.06)</td>
<td>-10.80 (0.29)</td>
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<td>1.70E-03</td>
<td>20.15</td>
<td>2.14</td>
<td>-10.3</td>
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<td>2.35 (0.23)</td>
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<tr>
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<td>1.60E-03</td>
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<td>1.93 (0.02)</td>
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<td>22.75 (12.88)</td>
<td>1.73 (0.06)</td>
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<td>19.25</td>
<td>2.52</td>
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<td>1.60E-03</td>
<td>32.90</td>
<td>1.47</td>
<td>-11.54</td>
<td>22.75 (12.88)</td>
<td>1.73 (0.06)</td>
<td>-11.82 (0.39)</td>
<td>19.25</td>
<td>2.52</td>
<td>-12.70</td>
</tr>
</tbody>
</table>

*The steady state example is a velocity model. Its optimized flow parameters were estimated by inverse flow modeling conditioned on curved ray tomography as well as straight ray tomography with or without using the weights in the objective function (sub domains labeled in Figure 2). The inverse flow modeling of the transient example and Moreppen were conditioned on time-lapse curved ray tomography (sub domains labeled in Figure 5a). Standard deviations in parenthesis were calculated with assumption of normality and linearity. $\theta_s$ is porosity, $\theta_r$ is residual water content, $\eta [kgm^{-1}s^{-1}]$ is water viscosity, $\alpha [m^{-1}]$ and $n$ are van-Genuchten parameters and $k_s [m^2]$ is intrinsic permeability. We assume $Q_s = 0$, $l = 0.5$ and $m = 1^{-l}/n$. 
are the most important parameters. Clearly the analysis indicates that the sensitivity to these control points indicates a reasonable robust estimation of the geological structure. For example, the position error of control points $g_5$, $g_6$, and $g_3$ decreased, respectively, to 15%, 5%, and 20% of their initial error value (20 cm) after the inversion. Of course in a real case there are not perfectly horizontal or straight interfaces, but in the proposed method, the interfaces can easily be changed to any desirable shapes by introducing more control points. This increased flexibility comes at a cost however: the CPU-time increases with the number of control points. So the total number of control point has to be limited to keep the inversions feasible. Of the flow parameters the intrinsic permeability $k_0$, and the van Genuchten parameter $n$ (which is a measure for the heterogeneity of each geological unit) are slightly more sensitive than the van Genuchten parameter $\alpha$ (which is related to the air entry pressure).

The misfit of the traveltimes (equation (14), Step 12 of Figure 1) for the best final estimates is 0.16 ns, which is 0.68% of the average traveltimes. This is comparable to the misfit of the traveltimes for the curved ray tomogram (Step 3 of Figure 1), which is 0.13% of the average traveltimes. The latter is expected to be a lower as many more parameters were used in that inversion.

3.2. Transient Model

The geological structure for the transient flow test model (see Figure 5a) is very similar to that of the steady state model. We have only added one low-permeability dipping layer in the foreset to obtain a synthetic example that is as close as possible to a real image of the delta structure. There are, therefore, three different dipping layers in the foreset. The fixed values and initial guesses for the flow parameters and the true values for the parameters that are inverted for in each sub domain are given in Table 1. For the latter is expected to be a lower as many more parameters were used in that inversion.

Before doing the flow inversion, the model is run to steady state with a daily infiltration of 0.5 mm in order to estimate the initial pressure state. This 0.5 mm infiltration rate is assumed to be the average infiltration rate during the long winter before the snowmelt started. However, based on previous work done at the field site, the steady state infiltration has no significant impact on the transient inversion result if observations are started some days after the infiltration starts [Kitterød and Finsterle, 2004].

The synthetic GPR data for this example are derived in the same way as the steady state model, but now on three different dates (indicated by the three red dots in Figure 6) from the cross-well pairs w1–w2 and w2–w3. These GPR data are obtained from forward flow modeling using the flow parameters given in Table 1. The computed volumetric soil water content between wells w1 and w3 on these 3 d are converted to EM velocity using Topp’s model for sandy loam and equation (4). The resulting velocity models on the different dates (indicated by the three red dots in Figure 6) are also the same as the field data example. The infiltration was due to the melting of snow at the field site in Norway in March and April of 2005.
(1 April) and 5d (22 April). Curved ray traveltime tomog-
raphy is then used to obtain the velocity tomograms. The
resulting velocity tomograms are shown in Figures 5e, 5f,
and 5g. All five sub domains are clearly visible in the tomo-
grams. Furthermore, flow focusing and dry zones of water,
respectively, at the top and bottom of the low-permeability
dipping layer between wells w2 and w3 in 22 April 2005 are
reasonably well recovered. The tomograms are converted to
volumetric soil water content using equations (4) and (5) and
are used as conditioning data for inverse flow modeling.

\[ \text{(32)} \]

Even though the curved ray traveltime tomograms
recover the true velocity models quite well, it is still difficult
to identify the correct positions of the control points from
these images. We assume that the basic geological structure
(i.e., the number of sub domains and their shapes) is known.
However, as in the previous example, the exact locations of
the sub domains are unknown and estimated during the flow
optimization. For the inversion, some of the interfaces are
constrained to be horizontal (\( g_1 \) and \( g_2 \) in Figure 5a). The
dipping layers are constrained by imposing a constant
thickness and dip. Compared to the optimization of each
individual control point of the dipping layers separately, this
reduces the number of control points from 12 to 4. This way
we lose some flexibility, but the flow inversion becomes
faster. The initial positions of the control points, which
define the geological structure, are located ±20 cm away
from their correct locations.

\[ \text{(33)} \]

In the inverse flow modeling, the absolute permea-
bility (\( k_1 \)) and the van Genuchten parameters (\( n \) and \( \alpha \)) as
well as the location of the control points are modified.
Minimization of the objective function is performed by
using both the LM as well as the SCE algorithm. For the
SCE algorithm an initial population of 117 points (3 com-
plexes of 39 points) was used. The remainders of the
algorithm’s variables were identical to those used by Duan
et al. [1992]. However, the SCE algorithm was stopped after
13 iterations because of its slow performance on a normal
PC (Pentium 4 with CPU 3 GHz and 3 GB of RAM). Since
the SCE algorithm uses the simplex method for the
optimization, it needs a large amount of function evalua-
tions to find the global minima. Each function evaluation of
the flow model took around 15 min and, therefore, it was
not feasible to continue the algorithm. The optimized flow
parameters are given in Table 1. After 13 iterations of the
flow inversion, the objective function is minimized to
approximately 7% of its initial value using both the LM and
SCE algorithm (see Figure 7a). In the first iterations, the
LM algorithm is much more efficient than the SCE
algorithm. However, after 10 iterations the SCE algorithm
minimizes the objective function slightly better than the LM
algorithm. The results presented in Figure 7a and Table 1
show that within the indicated confidence interval, the LM
algorithm is able to find the true parameters for most of the
parameters. The same is true for the SCE algorithm with the
same number of iterations as for the LM algorithm.

\[ \text{(34)} \]

The velocities estimated by cross-well tomography,
the initial and the optimized (using LM) flow models (Steps
3, 5 and 11 of Figure 1 respectively) versus the true
velocities for all individual cells are shown in Figure 7b.
The velocities estimated using the optimized flow model are
quite close to the true velocities. However, like the steady
state model, the final residuals of the flow model are not
Gaussian or randomly distributed, but show systematic
deviations between the model and data. The corresponding velocity images between the wells are shown in Figures 5h, 5i, and 5j.

In general, the flow parameters are reasonably well estimated and the geological structure is well calibrated with the proposed method. The best and worst estimates correspond to the second and first sub domains, respectively. The inversion algorithm uses tomograms to condition the flow inversion. Since the influence of the tomographic artifacts on the inverse flow modeling cannot be totally removed, the final estimates do not exactly match the true parameters.

Standard deviations of the estimates in Table 1 were calculated by assuming normality and linearity. In some cases, the true parameters are not located in the 95% confidence interval. This is expected since the assumption of normality and linearity is not valid (Figure 7b). The uncertainty is, therefore, probably underestimated. It should be emphasized that the results of this synthetic inversion indicate the theoretical uncertainty which is present in all inversion methods using high resolution measurements for estimation of upscaled flow parameters.

A sensitivity analysis shows that for the transient flow example, the position of the control points are the most
sensitive parameters during the inversion (Figure 8). This again demonstrates the importance of including the geometry in the inversion algorithm. The misfits of the travel-times for the final estimates vary between 0.53% and 0.63% of the average traveltimes of the corresponding cross-well data sets. This is comparable to the misfit of the traveltimes for the tomograms, which vary between 0.31% and 0.65%.

In the next section we apply the inversion algorithm to real field data.

4. Application of the Inverse Flow Modeling Algorithm to the Time-Lapse Field Data

4.1. Description of the Field Site and Data

[37] We apply the inverse flow modeling algorithm on real field data obtained at Moreppen, near Oslo’s Gardermoen airport in Norway (Figure 9). This subsection contains a brief description of the field site. The inversion results are discussed in the next subsection.

[38] Moreppen has been the subject of numerous studies related to sedimentological, hydrological, geophysical and geochemical processes in the saturated and unsaturated zone [see for example Aagaard et al., 1996; Langsholt et al., 1996; Tuttle and Aagaard, 1996; French and Binley, 2004; Farmani et al., 2008]. Moreppen is a part of the Gardermoen delta, an ice-contact delta formed after the last ice age about 9500 years ago, with an area of approximately 80 km². The delta is vertically divided into three main sedimentary structures: bottomset, foreset and topset. The thickness of the structures within the delta varies considerably and is a function of distance from the main glacial portals and depth to the bedrock. The vadose zone at Moreppen is about 4 to 5 m thick. The vadose zone contains the topset unit (roughly the upper two meters) as well as the upper part of the foreset unit.

[39] The foreset at Moreppen consists of about 95% fine sand. The remainder of the structure contains coarse sand and gravel as well as some fine lenses of sandy silt. It was deposited in a shallow marine environment and progrades in southwesterly direction (dip directions vary between 180 and 240°) with dips between 15 and 30°. The topset was deposited in a fluvial environment. It consists mainly of pebbly sand. The bedding in the topset is subhorizontal [Tuttle et al., 1996; Tuttle and Aagaard, 1996].

[40] Moreppen has a continental precipitation regime with an annual mean of 860 mm. Average temperatures range from −4.9°C in January to up to 16.6°C in July. The GPR time lapse data sets were collected in March and April 2005 (see Figure 6). During this time the snow that had fallen during the winter of 2004/2005 started to melt. The equivalent water infiltration rate, based on the measurements at Moreppen and a meteorological station nearby, is shown in Figure 6. The groundwater level at Moreppen during this time was at a depth of approximately 4.4 m.

[41] Moreppen contains a number of PVC cased wells (wells k14, k16 and k18; see Figure 9). The distances...
between k14-k16 and k16-k18 are 2.4 m and 2.5 m, respectively. Multioffset cross-well GPR data were collected from wells k14–k16 and wells k16–k18 on March 22 (just before the snow started to melt), 1 April (during the snowmelt) and 22 April (after the snowmelt). The groundwater well shown in Figure 9 was used to measure the groundwater level on these dates.

All six GPR data sets were collected using a step frequency radar provided by the Norwegian Geotechnical Institute [Kong and By, 1995]. Start and stop frequencies for data acquisition were 50 MHz and 900 MHz, respectively, with 199 evenly stepped frequencies. The cross-well GPR data were acquired from the surface to a depth of 4.2 m with 0.2 m spacing between the source antennas and between the receiver antennas. Data recorded from the surface to a depth of 0.8 m were not used in the inversion because of the possible existence of ice lenses as well as tree roots and other organic material. The relative dielectric permittivity of the ice ($\varepsilon_i$) is very different from water ($\varepsilon_w$ at 2°C, [Collie et al., 1948]). Therefore the amount of ice in the soil cannot be estimated by Topp’s model. In addition, organic materials usually contain considerable amount of residual water which is not directly involved in water flow. Also traveltimes from source-receiver pairs with offset angles higher than 45° were not used in the tomographic inversion because of the tomographic inversion. Thus from the 484 traces collected in each survey, only 294 traces were used in the tomographic inversion (Step 3 of Figure 1). As a first step traveltime tomography was applied to all the 6 data sets. The soil water content distribution was found using equations (4) and (5) (Step 4 of Figure 1) is shown in Figures 10a, 10b, and 10c. These volumetric soil water content estimates were consistent with various quality checks, such as the estimates from a calibrated neutron probe in a nearby well, water balance computation, continuity of the tomograms across well k16 and knowledge of the local geology [see Farmani et al., 2008 for more details]. One of the main things to note about these estimates is that the difference in water content between Figures 10a and 10b is much smaller than that between Figures 10b and 10c. This is to be expected from the infiltration data (Figure 6). Only a small amount of the snow melted between the time of the first (Figure 10a) and the second (Figure 10b) data acquisition. Most of the snow melted between the second (Figure 10b) and the third (Figure 10c) data acquisition.

In addition to the cross-well GPR data, air temperature, soil temperature and precipitation data in 2005 were available. Furthermore, a zero offset surface GPR reflection profile was acquired in May 2006 (see Figure 11a). Finally, core samples of the wells were also available.

4.2. Inverse Flow Modeling Using GPR Data From Moreppen

The initial guess of the geological structure is derived from the surface GPR reflection profile (Figure 11a), the difference in volumetric soil water content between the third and first surveys (Figure 11b), the tomograms themselves, the core samples and knowledge of the local geology/sedimentology. For more details on the tomographic inversion and discussion of the initial geological model, see Farmani et al. [2008]. The initial geological structure is similar to that of Figure 5a. Wells k14, k16 and k18 are located at relative horizontal coordinates of 0 m, 2.4 m, and 4.9 m in this Figure. Following the principle of parsimony in hydrology [McLeod, 1993], the number of parameters to
be optimized and the number of geological sub domains, were kept at a minimum. If more flow parameters and/or sub domains are used, a better fit can be expected. However, the purpose of the inverse flow modeling is not to reproduce details in the observations. An important goal is the ability to transfer the modeling results to areas with no observations. Increasing the number of parameters usually decreases the predictive power of the model. Furthermore, the computational cost increases dramatically if more parameters are introduced.

The interface between the topset and foreset is not clearly visible in the tomograms. This interface is more clearly visible in the core samples and surface GPR reflection data and also expected on the basis of sedimentological knowledge from the area. The same is true for the interface between the two topset layers. The exact locations of the interfaces are not known and are, therefore, variable parameters in the optimization problem. Some minor structures are omitted from the topset beds. For example, the dry zone next to well k14 is left out. This zone probably consists of coarse material [Farmani et al., 2008]. The foreset, on the other hand, is more homogeneous and, therefore, it is easier to define an initial geological structure for this unit. Some thin dipping layers are evident in this unit in Figures 10, 10b, 10c, and 11b. On the basis of these figures and other available data (such as the presence of such layers in local outcrops), we define three different sub domains in the foreset.

The infiltration history at Moreppen during snowmelt in 2005 is shown in Figure 6. The infiltration history depicts a spatial average of the infiltration into the monitoring area. However, the spatial distribution of infiltration is not uniform. For example, the shadow of trees near well k18 caused a local delay in snowmelt near this well. Moreover, small scale topography also caused a spatial variation in the infiltration, especially at the beginning of the snowmelt [French and Binley, 2004]. These irregularities are not taken into account in the inversion, and a uniform infiltration rate is used instead. Porosities and residual water contents of the individual sub domains are taken from previous laboratory and field measurements [Pedersen, 1994; Kitterød et al., 1997]. The water viscosity in each sub domain is estimated using the average soil temperature during the period of infiltration.

Inverse flow modeling is performed in the same way as the synthetic transient flow model with the same fixed flow parameters (Table 1) and initial locations of the control points. Initial guesses of the flow parameters and
A priori information of the parameters search space to be optimized are obtained by interpreting available data and previous studies performed at the field site [Pedersen, 1994; Kitterød et al., 1997; Kitterød and Finsterle, 2004]. As before, the inversion is conditioned on the soil water content estimates derived from the time-lapse cross-well GPR tomography. The value of the objective function (as defined in equation (11)) decreases by 50% after 19 iterations (Figure 12). The inversion results are presented in Table 1, and the corresponding volumetric soil water content estimates are shown in Figures 10d, 10e, and 10f. The main change for the location of the control points happened for $g_3$, which defines the location of sub domain 5 (Figure 5a). This control point shifted +16 cm in the horizontal direction. This was expected because the initial position of this layer did not quite match the interface with changing water content between the first and the third survey (see Figure 11b). The flow models can be converted back to velocity using Topp’s model, and the traveltimes can be computed (Step 11 of Figure 1). The misfits of the traveltimes for the final estimates vary between 1.8% (k14–k16, 22 April 2005) and 5.2% (k16–k18, 22 March 2005) of the average traveltimes. The misfits of the traveltimes for the tomograms vary between 0.42% and 0.57%. The best match between volumetric soil water content estimates from the tomograms and the flow model is at the end of the snowmelt on 22 April 2005 (Figures 10c and 10f).

An interesting flow phenomenon occurs underneath the low-permeability layers in the foreset: dry areas are persistent during the whole monitoring period. This is very clear between wells k16 and k18, but it is also evident between wells k14 and k16. The area with low volumetric water content beneath sub domain 4 overshadows sub domain 5. This clearly indicates that the EM-velocity tomograms are more sensitive to the water content distribution than to the soil structure heterogeneity. Thus inverse flow modeling conditioned on EM-velocity tomograms is not only a robust method to estimate the flow parameters in the vadose zone; it can also lead to new geological information of the subsurface.

The volumetric soil water content derived from the tomograms and flow simulations does not match well for the data sets acquired on 22 March 2005 and 1 April 2005 (Figure 10). This mismatch is especially clear for the low-permeability layer in the foreset between wells k16 and k18.
are a function of changes in inflow (a) Surface GPR reflection profile between the D Kowalsky et al. [2004] used homo- =0 . D W08401 = D Lambot et al. D matrix (equation (12)). Synthetic =/C0 Linde et al. + D D is constant during the infiltration event, and (red line in Figure 13). Outflux of the D Hyndman et al. We assume the inflow to the saturated zone was negligible: D R0/2006 to 31 May 2006. This covers the snowmelt event of 2005). Dashed lines show the initial geometry of the flow model.

There are several reasons for this, which are discussed in more detail in the next section. The main reason is likely to be the much smaller number of parameters in the flow inversion (as compared to the velocity inversion) and errors in the data. Other possible reasons are the non uniform spatial infiltration, as mentioned above, the 3D geometry of the forestet rather than the 2D and the use of isotropic, rather than anisotropic, parameters in the inversion.

4.3. Cross Validation of the Inversion Results

In order to illustrate the predictive power of the method presented above, we include a simple cross validation example by using an infiltration event at the same site, which is not used in the inverse flow modeling. The independent infiltration data were monitored from 1 January 2006 to 31 May 2006. This covers the snowmelt event of 2006 (the blue line in Figure 13). The observed flow into the saturated zone was derived from continuous observations of the groundwater level from an automatic monitoring station at Moreppen. Changes in the groundwater table \( \Delta h \) are a function of changes in inflow \( \Delta G \), and changes in outflow \( \Delta R \): \( \Delta h = \Delta G - \Delta R \). During the winter period, inflow to the saturated zone was negligible: \( \Delta G / \Delta t = 0 \). Hence a drop in the groundwater table during this period is due to steady state outflow: \( \Delta h / \Delta t = -\Delta R / \Delta t \). We assume that \( \Delta R / \Delta t \) is constant during the infiltration event, and inflow into the saturated zone was estimated by \( \Delta G / \Delta t = \Delta h / \Delta t + \Delta R / \Delta t \) (red line in Figure 13). Outflux of the model was computed by forward modeling using the estimated flow parameters from the 2005 snowmelt event and compared to the flow of the water into the saturated zone (black line in Figure 13). We obtain a reasonable match between the observed groundwater inflow and simulated water flux out of the vadose zone. The timing and amplitude of the peak as well as the shape of the curve after the peak are well recovered. However, the shape of the curve before the peak is not well recovered. This result shows that the estimated flow model does not only reproduce spatial-temporal changes in soil water content, but the model can also be used to simulate groundwater recharge.

5. Discussion

In this paper we present a flow inversion method (Figure 1) that uses time-lapse GPR velocity tomograms and petrophysical relationships, together with a priori geological knowledge, to determine the flow and calibrate the structural properties in the vadose zone. The conditioning of the flow inversion to water content estimates from travel-time tomography contains several sources of uncertainties (e.g., error in data, petrophysical relationships, tomograms, flow model). In this study, the influences of two main uncertainties, the uncertainty of the applied petrophysical relationships and the uncertainty in the tomograms, on the inversion results are minimized by including them in the inverse flow modeling procedure (equation (11)) by calculating the \( \sigma^2 \) matrix (equation (12)). Synthetic examples show that there is a strong correlation between ray coverage and errors in the GPR tomograms for the type of models studied here. By doing ray tracing rather than using straight rays, we demonstrate that the results of the flow inversion are improved. Because of this, we apply the ray tracing methodology to the Moreppen field data. We think it can be important to use ray tracing in GPR tomography in general.

Previous studies estimated flow parameters using the GPR data directly (rather than tomograms or geological structure). For example Lambot et al. [2004] used homogenous sand samples to derive flow parameters, and avoided the problem of defining the optimal geological structure. Kowalsky et al. [2005] used the concept of pilot points and variograms to define the spatial variability of the flow parameters of interest. In their method, statistical parameters (i.e., variograms) were assumed to be given in a deterministic sense and to be independent from other parameters. Their inversion was conditioned on the GPR traveltimes directly, rather than the tomograms. In this approach, artifacts associated with the tomograms are not an issue.

However, there are two important advantages in using tomograms. First, the initial geological structure can be derived from the tomograms [Hyndman et al., 1994; Tronicke et al., 2004; Linde et al., 2006]. By defining the initial geological structure we can derive flow parameters for different sub domains which usually are more realistic. Second, spatially continuous images are derived using...
physical principles, which improve the quality of the estimates compared to statistical interpolation techniques which always inherit the uncertainties of the statistical assumptions.

[54] If the geological structure is only derived from the tomograms, then there is always a risk of misinterpretation. For example, in Figure 5g the high-velocity area below the low-permeability layer between wells w2 and w3 (sub domain 4) can be misinterpreted to be a part of that layer or a separate layer. Also, the low-permeability layer between wells w1 and w2 (sub domain 5) is apparently truncated above the capillary zone. This phenomenon is due to the dry conditions in the shadow zone caused by the funneling of water from the low-permeability layer above (sub domain 4). For the field data shown in Figure 10, we are able to explain the water content discontinuity in sub domain 5 from the flow simulations without introducing any corresponding geological discontinuity. This is because EM waves are much more sensitive to the water content than to the soil composition. However, heterogeneity in the soil water content distribution is not always correlated to the heterogeneity in the soil composition because of the possi-
ble existence of flow focusing and shadow zones of water flow caused by the geological structure. Zoning algorithms [Hyndman et al., 1994; Linde et al., 2006] relate velocity (or water content) heterogeneity to geological structure. If flow focusing and shadow zones are not taken into account then there is a risk of misinterpretation if these algorithms are applied to the vadose zone. To overcome this problem, the use of prior information of the geological structure is critical.

[55] Two alternative methods to self-identify the number of sub domains, including their shapes are the level set method [Berre et al., 2007; Duan et al., 2008; Lu and Robinson, 2006] and the global-local optimization method presented by Tsai et al. [Tsai et al., 2003, 2005; Tsai and Yeh, 2004]. The level set method is a promising method for geological characterization. However, if flow parameters should be estimated in addition to the geological structure, other methods need to be used first to estimate the flow parameters. After that, the level set method can be used to find the optimal geological structure. For example Berre et al. [2007] used an adaptive multiscale estimation method to estimate the permeability and coarse-scale geological structure. Then, they used the level set method to modify the geological structure. Another example is provided by Lu and Robinson [2006], who simplified the optimization problem by assuming that the saturated hydraulic conductivity was known and demonstrated that the level set method was able to estimate the geological structure consisting of two sub domains. In our study, we suggest a method that is simpler and more intuitive than the general level set method, but uses simultaneously inverting for the flow parameters and calibrating the geological structure. The global-local optimization method presented by Tsai et al. is a useful method when the inverse flow modeling is conditioned on sparse measurements and observations. In these kinds of problems, the geological structure is usually unknown and an algorithm is needed to automatically estimate the number of sub domains and their shapes as well as the flow parameters of interest. However, estimating the number of sub domains is not usually needed when tomograms are used and basic knowledge of the geological structure (the existence of the topset and foreset layers in this case) exist. This is particularly true in the saturated zone. The tomograms are continuous images of reality and, therefore, give us a good indication about the geological structure which can be used as initial geological structure in the flow model. What we usually need is calibration of the shape of the sub domains during the inverse flow modeling, which is what we do, rather than, changing the number of sub domains.

[56] Therefore we do not change the conceptual model when we optimize the geological structure. In other words, we do not evaluate different geological concepts in this paper. The question we want to answer in this study is: within the geological concept of a delta structure, is it possible to use GPR-tomography to optimize geological structure and flow parameters in one coupled inverse algorithm? Within the same conceptual model, it is still relevant to ask: How significant is the discrepancy between the final model result and the starting point, namely the GPR-tomograms? Therefore we include computation of “artificial” GPR-traveltimes by ray tracing given the optimized flow model and compare them to the real observations. This is relevant because the flow model might be an oversimplification of the real geology.

[57] The misfit reduction of the flow inversion functional is about 95% for the synthetic examples and about 50% for the field data case. This difference is to be expected as various assumptions were made for the field data case. The main assumptions probably are: the flow is 2D rather than 3D; the permeability is isotropic, not anisotropic; the infiltration is uniform and not spatially dependent; and, most importantly, the geological model consists of a few number of discrete layers. Higher misfit for the final flow model of the field data is mainly caused by neglecting smaller scale structures which exist in the study area. Introduction of more sub domains in the field model would decrease the misfit. However, more sub domains give more parameters, which reduce the capacity of the model to predict flow phenomena in settings with similar geological structures.

[58] It is important to reemphasize that a misfit reduction of 100% for the synthetic examples presented in this study is not possible because of theoretical reasons. By doing flow modeling, we upscale the synthetic observations (GPR volumetric soil water content estimates) that hold the same tomographic artifacts as the real data. This point is demonstrated in the steady state example: EM-velocity in two neighboring cells within a homogeneous velocity layer should be identical (Figure 2a). However they are not always identical due to the artifacts (Figures 2b and 2c). The correlation between artifacts and ray coverage is also revealed in the synthetic steady state example (Figures 2b versus 2d, and 2c versus 2e). Thus there are sound physical reasons to use ray coverage to minimize the influence of artifacts on the inversion results. Even though ray coverage is low in some areas, we do not allow the weights to be zero. The reason is that all cells contain some valuable information because of the effect of smoothing factor on the tomographic inversion results. Therefore all observations contribute in the objective function. In our example, observations have a resolution of 10 cm by 10 cm. However, the high resolution observations contain uncertainties because of the artifacts. The flow model, on the other hand, consists of four homogeneous sub domains. Volumetric soil water content distribution in the flow model depends on the hydrological parameters of these sub domains. Up-scaling of observations by doing flow modeling can never reproduce volumetric soil water content distribution at the resolution of observations. That is the reason why the misfit reduction for the synthetic steady state case ends up at 96% instead of 100%.

[59] One of the major problems in performing inverse flow modeling is equifinality or non uniqueness. For example, Binley and Beven [2003] estimated flow parameters using a natural recharge to a sandstone aquifer using 1D flow modeling. They reported a significant degree of equifinality when the flow simulations were compared to the geophysical data. To minimize this problem it is important to constrain the inversion to the expected parameter range, for example, by using available a priori information. In addition, equifinality may be an indication of a conceptual mismatch between the simulation model and reality. If the problem is in reality 2D or 3D, then
equifinality is unavoidable when 1D modeling is used. By increasing the dimensionality of the model (making it 2D or 3D), the equifinality problem is often suppressed. For example, having dipping layers with different physical properties will introduce flow focusing and dry zones of water in the model. These zones are detectable with cross-well GPR traveltime tomography. As a result, generated tomograms will contain much more inherent information than the 1D models.

One of the main quality checks for all kinds of simulations is to test their capability of reproducing phenomena of interest without calibration. This is the core point of cross validation. In the context of this paper, this means answering the question: can the flow model conditioned on GPR data successfully predict other observations? To indicate an answer we included a simple test where we compared the simulated outflux of the model to observed flux after the snowmelt event in 2006. The simulated outflux reproduced the main character of the observations, which confirms that the flow model can reasonably predict other observations.

6. Conclusions

In this paper, we presented a method to estimate vadose zone flow parameters and calibrate the geological structure by combining cross-well GPR traveltime tomography (obtained in 2005), petrophysical relationships, prior geological knowledge and inverse flow modeling. We used traveltime tomography to determine the spatial EM-velocity distribution in the vadose zone. These velocities were converted to volumetric soil water content using Topp’s model, and were used as constraints in the inverse flow modeling.

Sensitivity analyses demonstrated the importance of including geometry calibration in the flow inversion. A fixed geometry introduces significant uncertainties in the estimated flow parameters. Therefore calibrating the initial geological structure was made part of the flow inversion. We evaluated the uncertainty of the algorithm using synthetic models and subsequently applied the algorithm to a natural infiltration event.

In the synthetic examples given in this study, there was a correlation between ray coverage and the quality of the tomogram. We used ray coverage to compute weights of the observations, which were used to increase the robustness of the inverse flow modeling significantly. This requires a physically correct ray tracing procedure. If the geological structure includes dipping low-permeability layers, conditioning the model on volumetric soil water content derived from straight ray tomography fails to estimate the flow parameters and calibrate the geological structure. Of that reason we recommend the use of curved ray tracing.

The inverse flow modeling of the snowmelt data from Gardermoen airport indicated clearly that real geological structure can be camouflaged by flow focusing and dry zones due to the unsaturated water flow. Flow modeling combined with GPR-tomography improves the interpretation of soil structure and quantifies the impact of flow phenomena. By the proposed method, thin low-permeability layers in the forested area were identified which explained the existence of preferential flow and dry zones. Finally, the inverted flow model indicates encouraging results with respect to prediction of groundwater recharge and preferential flow due to flow focusing effects in the vadose zone. We suggest further cross-validation to elucidate the combined use of flow modeling and geophysical observations.

Acknowledgments. The authors thank Per Aagaard at the Department of Geosciences, University of Oslo, for financial and scientific support. The authors also thank Fan Nian Kong from the Norwegian Geotechnical Institute for advice and the use of NGI’s step-frequency radar, the COMSOL support team, and staff at the Bioforsk Soil and Environment.

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