Inversion and sensitivity analysis of Ground Penetrating Radar data with waveguide dispersion using deterministic and Markov Chain Monte Carlo methods

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Abstract

Ground Penetrating Radar (GPR) has found widespread application for the non-invasive characterization of the subsurface. Nevertheless, the interpretation of GPR measurements remains difficult in some cases, particularly when the subsurface contains thin horizontal layers with contrasting dielectric properties that might act as waveguides for electromagnetic wave propagation. GPR data affected by waveguide dispersion are typically interpreted using the so-called dispersion curve, which describes the phase velocity as a function of frequency. These dispersion curves are commonly analyzed with deterministic optimization algorithms and which return dielectric properties of the subsurface as well as the location and depth of the respective soil layers. Unfortunately, current state-of-the-art inversion methods do not provide estimates of the associated uncertainty of the inferred subsurface properties. Here, we apply a Bayesian inversion methodology using the recently developed DiffeRential Evolution Adaptive Metropolis DREAM(ZS) algorithm. This Markov Chain Monte Carlo simulation method is admirably suited to estimate (nonlinear) parameter uncertainty and treat measurement error explicitly. Analysis of synthetic GPR data showed that the frequency range used in the inversion has an important influence on the estimated values of the parameters. This is related to the parameter sensitivity that varies with frequency. Our results also demonstrate that measurement errors of the dispersion curve are frequency dependent, and that the estimated model parameters become severely biased if this error is not properly treated. We demonstrate how frequency dependent measurement errors can be estimated jointly with the model parameters using the DREAM(ZS) algorithm. The posterior distribution of the model parameters derived this way compared well with inversion results for a reduced frequency bandwidth which is another method to reduce the bias introduced through measurement error. Altogether, the inversion procedure presented herein provides an objective methodology for analysis of dispersive GPR data, and appropriately treats measurement error and
parameter uncertainty. The full frequency bandwidth is deliberately used to reduce the need for subjective decisions regarding which frequencies to use in the inversion.

**Keywords:**
GPR, Inversion, Monte Carlo Markov Chain, Dispersive data, Measurement error, Uncertainty

**Introduction**

Ground penetrating radar (GPR) is a geophysical technique that emits electromagnetic waves into the soil using a transmitter antenna, and measures the intensity of the electrical field at receiver antenna(s) as a function of time. Typically, the transmitting and receiving antennas are placed on the ground (i.e. on-ground GPR). The waves that are transmitted into the soil will be partly reflected and partly transmitted when contrasts in dielectric permittivity associated with subsurface structures occur. The propagation velocity of the GPR waves depends on the dielectric permittivity, which in turn can be related to soil moisture content and soil porosity amongst other factors.

GPR is widely used in many research fields, including civil and environmental engineering, archeology, pavement and infrastructure characterization, mining, and extraterrestrial exploration. In recent years, GPR has especially found widespread use in the field of hydrogeophysics because of its ability to non-invasively monitor and map soil water content and to characterize the near-surface structures controlling hydrological processes (e.g. van Overmeeren et al. 1997; Huisman et al. 2001; Galagedara et al. 2003, Huisman et al. 2003a, Moysey 2004, Bradford 2008, Westermann et al. 2010; Haarder et al. 2011; Rhim 2011; Steelman and Endres 2011). Both subsurface characterization and soil water content determination using GPR rely on an accurate determination of the propagation velocity of GPR waves. For on-ground GPR, this propagation velocity and therewith the dielectric permittivity can be determined when GPR measurements are made with multiple offsets between the antennas, for example using a common midpoint (CMP) measurement where the antenna separation is increased while keeping the same midpoint. In such a CMP measurement, reflected GPR waves can be identified by their hyperbolic shape that can be used to estimate the depth of the reflecting layer and the average propagation velocity of the subsurface above the reflecting layer (Greaves et al. 1996; van Overmeeren et al. 1997; Dannowski and Yaramanci, 1999; Endres et al., 2000; Bohidar and Hermance, 2002; Garambois et al., 2002, Grote et al., 2003; Lunt et al., 2005; Turesson A. 2006; Gerhards et al., 2008). Another wave that has been used for soil water content determination is the ground wave, which is the direct transmission from sender
to receiver antenna through the top of the soil. The ground wave can be recognized in a CMP measurement by the linear increase in arrival time with antenna separation, and the ground wave propagation velocity can be easily determined from the slope of this increase. The ground wave velocity has been widely used to measure the spatio-temporal development of soil water content variability (e.g. Galagedara et al. 2003; Huisman et al. 2003b; Weihermüller et al., 2007).

Although the use of the ground wave is a promising method for soil water content measurements, difficulties arise when the subsurface exhibits strong vertical variability due to the presence of distinct soil layers or gradients in soil moisture content that introduce thin horizontal layers with a strong contrast in dielectric permittivity. If the depth of the layers are comparable to or smaller than the wavelength of the GPR signal, these layers can act as a waveguide in which the electromagnetic waves are trapped. This leads to positive interference related to total reflection of the trapped wave at the boundaries of the layer. Field situations where such waveguides have been reported include a thin ice sheet floating on water (Arcone 1984; van der Kruk et al., 2007), a water infiltration front in a dry soil (Arcone et al. 2003), a thin organic-rich sandy silt layer overlying a gravel unit (van der Kruk et al. 2006), a mountain slope with a 1 m soil cover (Strobbia and Cassiani, 2007), and thawing of a frozen soil layer (van der Kruk et al., 2009; Steelman et al., 2010). In the presence of such waveguides, CMP measurements are difficult to interpret because the arrival time and the first cycle amplitude of the ground wave cannot be identified due to interfering waves.

In order to enable interpretation of GPR data with waveguide dispersion, van der Kruk et al. (2006) presented a deterministic inversion algorithm to estimate the thickness and permittivity of the dispersive waveguide and the permittivity of the soil below the waveguide. This work drew inspiration from inversion algorithms that are used to interpret dispersive Rayleigh and Love waves commonly observed in multi-offset seismic data. The deterministic inversion method of van der Kruk et al. (2006) was later extended for higher order modes by van der Kruk (2006) and van der Kruk et al. (2007). More recent extensions now enable inversion for the case that multiple layers act as waveguides (van der Kruk et al. 2010).

Inversion of GPR data affected by waveguide dispersion requires a forward model that accurately describes the dispersive characteristics of GPR data for a given subsurface structure described by a set of model parameters. Optimization methods are then used to seek a set of model parameters that minimizes the discrepancy between simulated and measured GPR data. Because such an inversion is nonlinear and ill-posed, a unique ‘best’ model might not exist or might be hard to find. In general, numerical modeling and inversion methods for GPR data have been greatly improved in the last decade, which obviously enhances the quality of inversion
results as well as the range of GPR data that can be inverted. Yet, traditional GPR inversion algorithms are deterministic, and estimate only a single ‘best’ set of model parameters without consideration of parameter uncertainty (e.g. Pettinelli et al. 2007; Steelman and Endres 2010; Wollschläger et al. 2010). Therefore, it is not yet well established how errors in GPR measurements and models propagate through the processing and inversion of dispersive GPR data. For non dispersive data, confidence intervals of the wave velocity and hence implicitly of the electrical permittivity have been reported which vary widely depending on the field settings and methods used (e.g. Jacob and Hermance 2004). Typical sources of error in GPR measurements introduced during GPR data acquisition are inaccuracies in offset, timing, antenna orientation, and other antenna effects (Slob 2010). An additional error source that is more complicated to address is model structural uncertainty, which is introduced by the use of simplifying assumptions in the modeling of GPR data.

Clearly, it is desirable to simultaneously estimate the ‘best’ model parameters and their associated uncertainty. Bayesian inversion algorithms based on Markov Chain Monte Carlo (MCMC) methods are particularly well suited for this task. MCMC methods use random walks through the parameter space to sample the joint posterior probability distribution of the model parameters that describes parameter uncertainty. MCMC methods are not new in the field of geophysical inversion (Mosegaard and Tarantola, 1995; Sambridge and Mosegaard, 2002), but the ever increasing computational power has resulted in their increased use in recent years, especially in the field of hydrogeophysics (e.g. Strobbia and Cassiani 2007; Irving and Singha, 2010; Hinnell et al. 2010; Huisman et al. 2010).

In this study, we invert synthetic and experimental GPR data with waveguide dispersion and determine the posterior model parameter distribution using a state-of-the-art MCMC algorithm. This posterior probability density function is used to investigate parameter uncertainty and sensitivity. In particular, we show that the posterior parameter estimates are sensitive to the frequency bandwidth of the data used in the inversion and that the measurement error is frequency dependent. To provide stable parameter estimates, we introduce a novel MCMC framework that simultaneously infers the model parameters and the frequency dependent measurement error.

The remaining part of this paper is organized as follows. We first describe the deterministic and MCMC inversion methods. Then, a synthetic case study is used to illustrate the effects of frequency bandwidth selection and measurement error on the final parameter estimates. Next, a real-world GPR data set is analyzed and used to demonstrate how model parameters and
measurement errors can be jointly retrieved from the measured dispersion curve. Finally, the last section of this paper summarizes our main results and provides some conclusions.

Methodology

The general flow of our deterministic and Bayesian inversion strategies is summarized in Figure 1. First, the CMP data, \( E(x, t) \), depending on the offset, \( x \), of the antennas and time \( t \), are processed to obtain a so-called dispersion curve (Park et al. 1998; van der Kruk 2006). The first processing step is to transform \( E(x, t) \) into the frequency domain, \( \hat{E}(x, f) \), with a Fourier transformation. Then, the phase-velocity spectrum is calculated by:

\[
D(v, f) = \left| \sum_x \frac{\hat{E}(x, f)}{\hat{E}(x, f)} \exp \left( i \frac{2\pi f}{v} x \right) \right|
\]

where \( v \) is the phase velocity, \( f \) is frequency and \( i \) is the square root of -1. In the final processing step, the dispersion curve, \( v_{\text{meas}}(f) \), is obtained by selecting the phase velocity with maximum amplitude for each frequency. This dispersion curve constitutes the measured data in the following deterministic and Bayesian inversion strategies.

The forward model to simulate a dispersion curve is based on modal theory (Budden 1961; van der Kruk, 2006). It assumes that the waveguide consists of a single high permittivity layer overlying a halfspace with lower permittivity (Figure 2). The model parameters of the single layer model are the dielectric permittivity and height of the waveguide (\( \varepsilon_1 \) and \( h \)) and the permittivity of the halfspace (\( \varepsilon_2 \)). The highest phase velocity of a single-layer guided wave is given by \( c_0 / \sqrt{\varepsilon_2} \), where \( c_0 \) denotes the speed of light (van der Kruk 2006; van der Kruk et al. 2006). It is obtained for low frequencies because the dispersion curve decreases monotonically with frequency. A first rough estimate of \( \varepsilon_2 \) can thus be calculated from the highest measured phase velocity. This also suggests that an adequate representation of low frequencies is required to obtain accurate estimates of \( \varepsilon_2 \). For high frequencies, the phase velocity approaches an asymptote given by \( c_0 / \sqrt{\varepsilon_1} \), which similarly suggests that an adequate representation of high frequencies is required for accurate estimates of \( \varepsilon_1 \). However, the direct estimation of \( \varepsilon_1 \) and \( \varepsilon_2 \) from the dispersion curve can be difficult because of the low signal to noise ratio for low and high frequencies.
Inversion algorithms

Two inversion algorithms are used in this study: the deterministic inversion algorithm presented in van der Kruk et al. (2006) and the DiffeRential Evolution Adaptive Metropolis (DREAM(ZS)) algorithm presented in Vrugt et al. (2009).

Deterministic inversion

The deterministic inversion approach of van der Kruk (2006) aims to find the model parameters \( \mathbf{m} = \varepsilon_1, \varepsilon_2, h \) that minimize the difference between modeled and measured dispersion curves. In contrast to van der Kruk et al. (2006), we minimize the mean squared difference between modeled and measured dispersion curves (\( L_2 \) norm). In the first step of the deterministic inversion approach, the feasible parameter space is sampled using a regular grid. In the second step, each of these parameter combinations is used as a starting value for a local search using the Simplex method (Lagarias et al. 1998). The model parameters with the smallest misfit are assumed to represent the best possible subsurface model describing the dispersive GPR data. Application of this inversion algorithm to synthetic and measured dispersive GPR data showed robust and reliable results (van der Kruk 2006; van der Kruk et al. 2006; van der Kruk et al. 2007; van der Kruk et al. 2010).

Markov Chain Monte Carlo Simulation: The DREAM(ZS) algorithm

MCMC algorithms have found widespread application and are used to estimate the most likely values of model parameters along with their posterior probability distribution. This posterior probability distribution contains all the necessary information to estimate parameter uncertainty and sensitivity. Unfortunately, standard MCMC algorithms are generally inefficient, and even very simple problems typically require many thousands of model evaluations to converge to the posterior probability distribution. This work capitalizes on recent developments in MCMC simulation and uses the DiffeRential Evolution Adaptive Metropolis (DREAM(ZS)) algorithm (Vrugt et al. 2009). The algorithm runs multiple Markov chains (random walk trajectories) in parallel, and maintains detailed balance and ergodicity. Whereas standard MCMC algorithms require extensive tuning, DREAM(ZS) automatically scales the orientation and scale of the proposal distribution during sampling. This proposal distribution is used to generate new points in each Markov chain. The only information to be specified by the user is the parameter ranges, and the likelihood function to compare model predictions with respective observations. A detailed description of the algorithm can be found in Vrugt et al. (2009), and is beyond the scope of the current paper.

Many likelihood functions have been developed in the literature, and these functions differ in their underlying treatment of the error residuals. We adopt a relatively simple likelihood
function, \( L(m \mid v_{\text{meas}}) \) that assumes that the residuals between modeled and measured dispersion curve are normally distributed and mutually independent:

\[
L(m \mid v_{\text{meas}}) = \prod_{k=1}^{K} \frac{1}{\sqrt{2\pi \sigma_{\text{me}}^2(f_k)}} \exp\left(-\frac{1}{2} \left( \frac{v_{\text{mod}}(f_k, m) - v_{\text{meas}}(f_k)}{\sigma_{\text{me}}(f_k)} \right)^2 \right)
\]

where \( v_{\text{mod}}(f_k, m) \) is the modeled dispersion curve given the model parameters \( m \) and the \( k \)th frequency, \( K \) denotes the number of frequencies, and \( \sigma_{\text{me}}(f_k) \) signifies the standard deviation of the measurement error. The likelihood function of Eq. [2] constitutes only one part of the posterior distribution, \( p(m \mid v_{\text{meas}}) = p(m) \cdot L(m \mid v_{\text{meas}}) \). The other term, commonly referred to as prior distribution, \( p(m) \) conveys all the information about the parameters prior to any data being collected and processed. In the absence of detailed prior information about the properties of the subsurface, we typically ignore \( p(m) \) by assuming a uniform prior parameter distribution. In other words, \( \alpha \)-priori each different parameter combination is equally likely. In this case, the likelihood function, \( L(m \mid v_{\text{meas}}) \), is similar to the posterior distribution, and hence the model parameters are solely conditioned on the GPR data.

It is particularly important to select a reasonable value for the measurement error standard deviation, \( \sigma_{\text{me}}(f_k) \) in Eq. [2]. If this value is too large, the posterior distribution will be too dispersive, and the uncertainty of the parameters will be exaggerated. On the contrary, a conservative choice for the measurement error might significantly underestimate the actual parameter uncertainty. Unfortunately, in many applications it is not immediately obvious which value of \( \sigma_{\text{me}}(f_k) \) to take. Most common is to assume that \( \sigma_{\text{me}}(f_k) \) is equal to the Root Mean Square Error (RMSE) of the best possible model fit to the data. This error deviation is estimated during the inversion with the DREAM\textsubscript{(ZS)} algorithm, and thus its value does not need to be specified \( \alpha \)-priori. This approach assumes that all deviations between model predictions and observations are attributed to a single homoscedastic (frequency independent) measurement error (e.g. Vrugt and Bouten 2002). In the case of dispersive GPR data, \( \sigma_{\text{me}} \) comprises a wide range of possible error sources introduced during GPR data acquisition and subsequent processing. It is not evident that \( \sigma_{\text{me}} \) is homoscedastic, and, therefore, we allow that \( \sigma_{\text{me}} \) can be frequency dependent, \( \sigma_{\text{me}}(f) \), also referred to as heteroscedastic error.

We run the DREAM\textsubscript{(ZS)} algorithm with prior ranges of the parameters specified in Table 1. These bounds are in agreement with the deterministic inversion approach and consistent with the information contained in the synthetic and real-world dispersion curve. In each MCMC trial, convergence of DREAM\textsubscript{(ZS)} to the limiting posterior distribution was monitored using the \( R \)-statistic of Gelman and Rubin (1992). After convergence, the last 5,000 parameter sets of the
joint Markov Chains created with DREAM(zs) were used to represent the posterior parameter distribution.

**Synthetic Data**

CMP data corresponding to a single layer model (Figure 2) were simulated using a numerical solution of an exact forward model for a horizontally layered medium (van der Kruk et al. 2006). The resulting dispersive CMP data for a waveguide with a height of 0.25 m and a relative permittivity of $\varepsilon_1 = 20$ overlying a halfspace with $\varepsilon_2 = 10$ are shown in Figure 3a. The shingling events indicate different phase and group velocities, which is characteristic for waveguide dispersion. Additionally we created a noisy radargram by adding normally distributed random noise to the simulated CMP data (Figure 3b). This random noise had a zero mean and the variance was set to 1% of the maximum amplitude of the simulated CMP data. The visual impression of higher noise level for larger offsets comes from the use of trace normalization in the visualization of the CMP data and the lower signal strength for large offsets. The phase-velocity spectra of the noise-free data and the noisy data together with the ‘measured’ and modeled dispersion curves are presented in Figure 3c and d.

Each of the three model parameters has a distinct influence on the dispersion curve, which is illustrated in Figure 4. The permittivity of the waveguide, $\varepsilon_1$, determines the high frequency asymptote whereas $\varepsilon_2$ determines the highest phase velocity observed for low frequencies. The height of the waveguide mostly determines the slope of the dispersion curve.

**Inversion results for synthetic GPR data**

To investigate how the use of different frequency ranges influence the model parameter estimation, we selected three frequency ranges (43 - 219 MHz, 71 - 219 MHz, and 43 - 145 MHz) from the measured dispersion curve obtained from the synthetic noise-free CMP data (Figure 3c). The marginal posterior probability distributions of $\varepsilon_1$, $\varepsilon_2$, and $h$ obtained using DREAM(zs), and the results of the deterministic inversion (green points) are shown in Figure 5. The mean of the marginal posterior probability distributions (red triangle) and the true model parameters used to generate the synthetic GPR data (red line) are included as well. Compared to the marginal posterior probability distributions for the complete frequency range (top row of Figure 5), a decreasing frequency range resulted in an increasing uncertainty in model parameter estimates as expressed by the width of the marginal posterior probability distribution. Removing the low frequencies (middle row of Figure 5) resulted in a significant increase in the parameter uncertainty for $\varepsilon_2$. In comparison, the parameter uncertainty for $\varepsilon_1$ and $h$ increased only slightly, although a small shift of the mean was observed. The effect of excluding the high frequencies is illustrated in the lower row of Figure 5. The uncertainty in the model parameters $\varepsilon_1$ and $h$ is now
larger, whereas the uncertainty in $\varepsilon_2$ has only slightly increased. These results clearly show that $\varepsilon_1$ and $h$ are more sensitive to high frequencies than $\varepsilon_2$. In addition, the close agreement of the mean of the marginal posterior probability distributions and the results for the deterministic inversion inspire confidence that both algorithms have located the global minimum.

Next, we investigated the effect of measurement error in GPR data on model parameter estimates. First, we consider noise in the radargram and its influence on the measurement error of the dispersion curve. A first indication can be obtained from a comparison of the average frequency spectra shown in Figure 6a. The ratio of the average frequency spectrum of the noise-free data (blue line) and the noise itself (green line) determines the signal to noise ratio (SNR). A large SNR indicates that noise has little influence on the measured signal, whereas a small SNR indicates that noise is more dominant. The differences in the SNR shown in Figure 6a imply a heteroscedastic (frequency dependent) measurement error. Another indication that noise mostly influences low and high frequencies was already provided in Figure 3d, where the measured dispersion curve deviates more from the modeled dispersion curve for high and low frequencies. This was not the case for the measured dispersion curves obtained from the noise-free CMP data (Figure 3c).

As a first step in our inversion, we nevertheless assume that the measurement error is homoscedastic (independent of frequency) and equal to the RMSE of the best fit to the measured dispersion curve obtained from noisy CMP data (Figure 3d) for the frequency range from 34 to 219 MHz. This resulted in a measurement error of $\sigma_{1\text{me}} = 0.0013 \text{ m/s}$. Figure 3d shows that most of this error is associated with the highest frequencies. Therefore, it is common to consider a reduced frequency range to exclude the error-prone frequency ranges (van der Kruk et al. 2006). Here, we also consider a reduced frequency range from 45 MHz to 201 MHz, which resulted in significantly lower estimate of the measurement error ($\sigma_{2\text{me}} = 0.0003 \text{ m/s}$). The signal-to-noise ratio illustrated in Figure 6a indicated that the measurement error is most likely heteroscedastic, which we considered in a third scenario ($\sigma_{3\text{me}}(f)$). To assign values to $\sigma_{3\text{me}}(f)$, we created 50 different realizations of noisy CMP data. The corresponding modeled dispersion curves after processing of the CMP data are shown in Figure 6b. The standard deviation of these 50 different dispersion curves served as an estimate of $\sigma_{3\text{me}}(f)$ and is plotted in Figure 6c together with the two homoscedastic measurement errors.

The inversion results for the three different choices of the measurement errors of the dispersion curve are shown in Figure 7. For the wide frequency range (34 - 219 MHz) and the homoscedastic measurement error $\sigma_{1\text{me}}$, the posterior probability distributions do not contain the true values for $\varepsilon_1$ and $h$ (top row of Figure 7). Clearly, too much confidence is placed on the
uncertain ends of the dispersion curves during inversion, which results in biased parameter estimates. When the most uncertain part of the dispersion curve is not considered and the corresponding homoscedastic measurement error $\sigma_{me}^2$ is used, the means of the marginal posterior probability distributions are much closer to the true values used to generate the synthetic data (middle row of Figure 7b). Moreover, the uncertainty of the estimated model parameters is smaller compared to the use of the full frequency bandwidth, illustrating that smaller measurement error reduces parameter uncertainty. The deterministic inversion results show similar behavior as the mean of the posterior probability distribution as long as a homoscedastic measurement error is considered.

To obtain accurate and precise model parameter estimates using $\sigma_{me}^2$, it was necessary to discard the uncertain parts of the dispersion curve. Alternatively, the frequency-dependent measurement error $\sigma_{me}(f)$ and the full frequency range can be used. Although the uncertain parts of the dispersion curve are now considered in the inversion, they receive less weight because of their relatively high $\sigma_{me}(f)$ values. The inversion results with this heteroscedastic measurement error are shown in the third row of Figure 7. We indeed obtain marginal posterior probability distributions that encapsulate the true values demonstrating that a better description of the measurement error results in more realistic parameter estimates. The results from the deterministic inversion are not considered in this case because the deterministic inversion was not extended to include heteroscedastic measurement error.

**Experimental Data**

The measured GPR data were obtained on a terrace of braided river sediments in New Zealand (van der Kruk et al. 2006). The CMP data were recorded with a pulseEKKO 100A system and 100 MHz antennas. The sampling window was 600 ns with a discretization of 0.5 ns and the spatial sampling resolution was 0.2 m. The trace-normalized CMP data are shown in Figure 8a. For the inversion, the air wave and the reflected waves were muted. The phase-velocity spectrum corresponding to the region enclosed by the black lines in Figure 8a is shown in Figure 8b. The measured dispersion curve obtained from this spectrum is indicated with the yellow line.

**Inversion results for experimental GPR data**

To investigate the sensitivity of the estimated model parameters to the use of different frequency bandwidths in the inversion of the dispersion curve, we select three different frequency ranges: a) 44 - 141 MHz, b) 54 - 141 MHz, and c) 44 - 131 MHz. These frequency ranges are highlighted in Figure 8b with arrows. The marginal posterior distributions for these different frequency ranges and the deterministic inversion results are displayed in Figure 9. As with the
synthetic data, we see that the marginal posterior distributions of $\varepsilon_1$ and $h$ remain similar when the low frequencies are removed (top and second row of Figure 9). In contrast, the model parameter uncertainty for $\varepsilon_2$ is nearly doubled and the mean of the marginal posterior distribution changed slightly. Again, this confirms that $\varepsilon_2$ is mostly sensitive to lower frequencies. The inversion results that exclude the high frequencies in the measured dispersion curve are shown in the third row of Figure 9. The marginal posterior distribution of $\varepsilon_2$ was similar to the results for the full frequency bandwidth. However, significant differences were observed in the mean of the marginal posterior distribution of $\varepsilon_1$ and $h$, which changed from $\varepsilon_1^{mean} = 20.4$ to $\varepsilon_1^{mean} = 21.6$ and from $h^{mean} = 0.182$ m to $h^{mean} = 0.166$ m, respectively. Again, this confirms the sensitivity of $\varepsilon_1$ and $h$ to high frequencies.

Figure 9 shows that filtering of high frequencies results in marginal posterior parameter distributions that are disjoint. The analysis of the synthetic data indicated that this might be related to an inappropriate definition of the measurement error. Indeed, it was already shown that the measurement error associated with the dispersion curve is frequency dependent, but this was not considered in our analysis of the measured GPR data thus far. Unfortunately, it is not straightforward to obtain a reliable estimate of this frequency dependent measurement error. Recently, several studies using MCMC simulation have included the measurement error as an additional parameter to be estimated (e.g. Vrugt et al. 2009). To test the usefulness of this approach for our dispersive GPR data, we first assume a single, frequency independent measurement error and estimate $\sigma_{me}$ along with the model parameters using the DREAM$_{zs}$ algorithm. The median value of this homoscedastic error corresponds very well with the RMSE of the best model fit for the entire frequency bandwidth (black arrow, Figure 10), and the posterior uncertainty of $\sigma_{me}$ (blue area, Figure 10) nicely encapsulates this RMSE value. Consequently, the marginal posterior parameter distributions (top row, Figure 11) are very similar to those derived previously using the full frequency bandwidth (Figure 9, top row).

It is rather encouraging to conclude that the measured GPR dispersion curve enables the inference of the measurement error. Yet, our approach has considered $\sigma_{me}$ to be homoscedastic; an assumption that is unrealistic given the strong dependence of the measurement errors on the frequency. We therefore proceed with another DREAM$_{zs}$ trial in which the measurement error of Eq. [2] is assumed to be frequency dependent, $\sigma_{me}(f)$. This requires specification of three additional parameters that need to be estimated by calibration against the measured dispersion curve. The four parameters beside the model parameter specify the measurement error at four different frequencies which are equally distributed along the frequency axis (Figure 10). Cubic Hermite interpolation between these four points is subsequently used to estimate the (heteroscedastic) measurement error at the remaining frequencies. About 70,000 model runs were
needed with DREAM\textsuperscript{(ZS)} to converge to the posterior model parameter and measurement error distribution. This is significantly more than the 20,000 model runs originally required for the model parameters. Indeed, the measurement error parameters increased the computational burden of the inversion problem.

In Figure 10, the median and corresponding 95% uncertainty ranges of the posterior $\sigma^{me}(f)$ function is plotted. For completeness, we also include the results of the homoscedastic error, $\sigma^{me}$. The shape of the measurement error curve illustrates that the measured dispersion curve is most reliable in the frequency range between 70 and 110 MHz. Above 120 MHz, the measurement error of the GPR data is significantly larger implying that the data is considered less important. Consequently the marginal posterior parameter distributions (bottom row, Figure 11) are very similar to those derived with a reduced frequency bandwidth (bottom row, Figure 9). The measurement error curve depicted in Fig. 10 is in close agreement with its counterpart plotted previously in Fig. 6 for synthetic GPR data. This attests the ability of our inversion procedure to return the properties of the measurement error.

We argue that the posterior parameter distributions presented in Figure 11 (bottom row) best summarize the actual subsurface properties considered herein based on the results of our synthetic study. It is demonstrated that the model parameters can only be correctly retrieved when the full frequency bandwidth together with a heteroscedastic measurement error is used or a meaningful a-priori reduction to the frequency bandwidth is applied. The latter approach is rather subjective and in practice it remains difficult to pinpoint an appropriate frequency bandwidth to invert the dispersion curve. Moreover, the synthetic and the experimental case studies illustrate the strong sensitivity of the model parameters to high and low frequencies and with a reduction of the frequency bandwidth we risk to lose valuable information. However, the MCMC inversion approach introduced herein removes the need for subjective selection of the frequency bandwidth and is especially designed to retrieve the (heteroscedastic) measurement error and subsurface properties, and their underlying posterior distribution.

**Summary and Conclusions**

We applied a deterministic and a Bayesian inversion method to synthetic and experimental on-ground GPR data with waveguide dispersion assuming a single layer model of the subsurface. Bayesian inversion used DREAM\textsuperscript{(ZS)}, a recently developed MCMC method that provides fast convergence. Unlike deterministic inversion methods, MCMC sampling with DREAM\textsuperscript{(ZS)} additionally approximates the joint posterior probability distribution of the model parameters,
which enables the investigation of parameter uncertainty and sensitivity. Overall, the estimated ‘best’ parameters derived from synthetic and measured dispersion curves depended strongly on the frequency bandwidth used in the inversion. More precisely, the relative permittivity of the subsurface below the waveguide was sensitive to the low frequencies of the dispersion curve, whereas the relative permittivity and the height of the waveguide were sensitive to high frequencies. Detailed analysis of the synthetic data showed that the measurement error associated with the dispersion curve was frequency dependent. In particular, the extreme ends of the dispersion curve were more uncertain. When such frequency-dependent measurement errors were not properly handled during the inversion, the resulting model parameters were biased. One possible way to resolve this issue is to remove the low and high frequency parts of the dispersion curve during the inversion. Although this procedure led to plausible results for both the deterministic inversion and MCMC simulation with DREAM\textsubscript{(ZS)}, the choice of an appropriate frequency bandwidth is quite arbitrary. A better solution is presented herein and consists of estimating the measurement error properties simultaneously with the model parameters. This resulted in plausible estimates of all three model parameters that compared well with inversion results for a reduced frequency bandwidth. Moreover, the heteroscedastic measurement error function derived in our study compared well with a homoscedastic error model and prior information. Altogether, the Bayesian inversion framework presented herein is entirely objective, explicitly handles measurement error and parameter uncertainty, and circumvents the need to make subjective decisions on the frequency bandwidth to be used in the inversion.

**Acknowledgements**

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References


Table 1
True parameter values and their prior ranges used for the synthetic and experimental data.

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Figure 1
Schematic outline of the algorithm. The measured CMP data is transformed into a dispersion curve which is a combination of the true dispersion curve and measurement error which comprises a wide range of possible errors. The forward model gives the theoretical dispersion curve. A deterministic and Bayesian inversion method are applied of which MCMC simulation with DREAM(ZS) can treat measurement error explicitly.

Figure 2
Single-layer model of a surface waveguide. Due to total reflection beyond the critical angle $\theta_c$, multiple reflections occur that are trapped within the waveguide layer. The model parameters that influence the dispersion characteristics of the electromagnetic waves are the height $h$, the relative permittivity of the waveguide $\varepsilon_1$ and the relative permittivity of the subsurface $\varepsilon_2$.

Figure 3
Numerically created CMP data (a) without and (b) with noise, and (c, d) the corresponding phase-velocity spectra. The theoretical dispersion curve is plotted in green, whereas the picked dispersion curves are plotted in yellow. The theoretical upper and lower bound of the dispersion curve are indicated with dashed-dotted white lines. The different frequency ranges used in the inversion are indicated with the white arrows.

Figure 4
Theoretical dispersion curves with differences in parameter values. In each plot one parameter is varied to investigate its influence on the dispersion curve. The fixed parameter values are $\varepsilon_1 = 20$, $\varepsilon_2 = 10$, and height $h = 0.25m$.

Figure 5
Histograms of the marginal posterior distributions of the model parameters using the dispersion curve shown in Figure 3c with frequency ranges; a) 43<f<219MHz, b) 71<f<219 MHz, and c) 43<f<145MHz
These histograms are created using the last 5,000 samples generated with DREAM\textsubscript{ZS}. The green circles represent the results of the deterministic waveguide inversion, the red triangles denote the mean of the marginal posterior distributions, and the red lines indicate the true parameter values used to generate the synthetic data.

(a) Average frequency spectra of the noise-free data (Figure 3a), the noisy synthetic data (Figure 3b), and the noise. (b) Black lines show different realizations of noisy CMP data. The red lines indicate the standard deviation from the mean of all dispersion curves (68\% of all the dispersion curves lay between the red lines). (c) Three different measurement error variances: $\sigma_{j}^{me}$ (blue line) is the homoscedastic measurement error, which is determined from the RMSE of the best fit to the data, $\sigma_{j}^{me}$ (green line) is obtained by limiting the frequency range of the dispersion curve to $45<f<201$ MHz, $\sigma_{j}^{me}(f)$ (red line) is determined from the standard deviation of the 50 different dispersion curve shown in Figure 6b.

Histograms of the marginal posterior parameter distributions corresponding to the dispersion curve shown in Figure 3d using the three different measurement error variances shown in Figure 6c: a) $\sigma_{j}^{me}$ and $34<f<219$ MHz, b) $\sigma_{j}^{me}$ and $45<f<201$, and c) $\sigma_{j}^{me}(f)$, and $34<f<219$ MHz. The red triangles signify the mean of the DREAM\textsubscript{ZS} derived marginal posterior distributions, the green dots represent the results of the deterministic waveguide inversion, and the red lines indicate the true model parameters.

a) Trace-normalized measured CMP data, b) corresponding phase-velocity spectrum using the data enclosed by the black lines. The yellow line indicates the selected dispersion curve and the different frequency ranges used in the inversions are indicated with magenta arrows.

Histograms of the marginal posterior parameter distributions using the dispersion curve of Figure 8b and three different frequency ranges: a) 44-141 MHz, b) 54-141 MHz (low frequency filtered), and c) 44-131 MHz (high frequency filtered). The measurement error is assumed to be frequency independent, normally distributed with standard deviation similar to the RMSE of the best possible fit to the GPR data. The red
triangles denote the mean of the marginal posterior distributions and the green dots illustrate the results of the deterministic waveguide inversion.

Figure 10
The estimated homoscedastic and heteroscedastic measurement errors in blue and red, respectively with their 95 percentile confidence interval. The red dots represent the median of the estimated points and were used to calculate the median of the heteroscedastic measurement error. The black and green arrows indicate the RMSE of the best fit of the results shown in Figure 9a and 9c, respectively.

Figure 11
Parameter posterior distributions when measurement error variance $\sigma_{me}$ and parameter are estimated simultaneously. In the first row $\sigma_{me}$ is homoscedastic and in the second row heteroscedastic. The red triangles denote the mean of the marginal posterior distributions.
Figure 1
Schematic outline of the algorithm. The measured CMP data is transformed into a dispersion curve which is a combination of the true dispersion curve and measurement error which comprises a wide range of possible errors. The forward model gives the theoretical dispersion curve. A deterministic and Bayesian inversion method are applied of which MCMC simulation with DREAM(ZS) can treat measurement error explicitly.
Figure 2

Single-layer model of a surface waveguide. Due to total reflection beyond the critical angle $\theta_c$, multiple reflections occur that are trapped within the waveguide layer. The model parameters that influence the dispersion characteristics of the electromagnetic waves are the height $h$, the relative permittivity of the waveguide $\varepsilon_1$ and the relative permittivity of the subsurface $\varepsilon_2$. 
Figure 3

Numerically created CMP data (a) without and (b) with noise, and (c, d) the corresponding phase-velocity spectra. The theoretical dispersion curve is plotted in green, whereas the picked dispersion curves are plotted in yellow. The theoretical upper and lower bound of the dispersion curve are indicated with dashed-dotted white lines. The different frequency ranges used in the inversion are indicated with the white arrows.
Figure 4

Theoretical dispersion curves with differences in parameter values. In each plot one parameter is varied to investigate its influence on the dispersion curve. The fixed parameter values are $\varepsilon_1 = 20$, $\varepsilon_2 = 10$, and height $h = 0.25\text{m}$. 
Figure 5

Histograms of the marginal posterior distributions of the model parameters using the dispersion curve shown in Figure 3c with frequency ranges; a) 43 < f ≤ 219 MHz, b) 71 < f ≤ 219 MHz, and c) 43 < f ≤ 145 MHz (see also arrows in Figure 3c). These histograms are created using the last 5,000 samples generated with DREAM$_{ZS}$. The green circles represent the results of the deterministic waveguide inversion, the red triangles denote the mean of the marginal posterior distributions, and the red lines indicate the true parameter values used to generate the synthetic data.
Figure 6

(a) Average frequency spectra of the noise-free data (Figure 3a), the noisy synthetic data (Figure 3b), and the noise. (b) Black lines show different realizations of noisy CMP data. The red lines indicate the standard deviation from the mean of all dispersion curves (68% of all the dispersion curves lay between the red lines). (c) Three different measurement error variances: \( \sigma_{1}^{me} \) (blue line) is the homoscedastic measurement error, which is determined from the RMSE of the best fit to the data, \( \sigma_{2}^{me} \) (green line) is obtained by limiting the frequency range of the dispersion curve to \( 45 < f < 201 \) MHz, \( \sigma_{3}^{me}(f) \) (red line) is determined from the standard deviation of the 50 different dispersion curve shown in Figure 6b.
Figure 7

Histograms of the marginal posterior parameter distributions corresponding to the dispersion curve shown in Figure 3d using the three different measurement error variances shown in Figure 6c: a) $\sigma_{1}^{me}$ and $34 < f < 219$ MHz, b) $\sigma_{2}^{me}$ and $45 < f < 201$, and c) $\sigma_{3}^{me}(f)$, and $34 < f < 219$ MHz. The red triangles signify the mean of the DREAM(28) derived marginal posterior distributions, the green dots represent the results of the deterministic waveguide inversion, and the red lines indicate the true model parameters.
Figure 8

a) Trace-normalized measured CMP data, b) corresponding phase-velocity spectrum using the data enclosed by the black lines. The yellow line indicates the selected dispersion curve and the different frequency ranges used in the inversions are indicated with magenta arrows.
Figure 9

Histograms of the marginal posterior parameter distributions using the dispersion curve of Figure 8b and three different frequency ranges: a) 44-141 MHz, b) 54-141 MHz (low frequency filtered), and c) 44-131 MHz (high frequency filtered). The measurement error is assumed to be frequency independent, normally distributed with standard deviation similar to the RMSE of the best possible fit to the GPR data. The red triangles denote the mean of the marginal posterior distributions and the green dots illustrate the results of the deterministic waveguide inversion.
Figure 10
The estimated homoscedastic and heteroscedastic measurement errors in blue and red, respectively with their 95 percentile confidence interval. The red dots represent the median of the estimated points and were used to calculate the median of the heteroscedastic measurement error. The black and green arrows indicate the RMSE of the best fit of the results shown in Figure 9a and 9c, respectively.
Figure 11
Parameter posterior distributions when measurement error variance $\sigma^{me}$ and parameter are estimated simultaneously. In the first row $\sigma^{me}$ is homoscedastic and in the second row heteroscedastic. The red triangles denote the mean of the marginal posterior distributions.