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► To cite this version:

Corinna Kopke, James Irving, Delphine Roubinet. Stochastic inversion for soil hydraulic parameters in the presence of model error: An example involving ground-penetrating radar monitoring of infiltration. *Journal of Hydrology*, 2019, 569, pp.829-843. 10.1016/j.jhydrol.2018.12.016 . hal-02073122

HAL Id: hal-02073122

<https://hal.science/hal-02073122>

Submitted on 22 Feb 2024

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Stochastic inversion for soil hydraulic parameters in the presence of model error: an example involving ground-penetrating radar monitoring of infiltration

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Revised manuscript for *Journal of Hydrology*

November 11, 2018

1 **Abstract**

2 Proxy forward solvers are commonly used in Bayesian solutions to inverse problems in hydrology and geophysics in order to make sampling of the posterior distribution, for example using
3 Markov-chain-Monte-Carlo (MCMC) methods, computationally tractable. However, use of
4 these solvers introduces model error into the problem, which can lead to strongly biased and
5 overconfident parameter estimates if left uncorrected. Focusing on the specific example of esti-
6 mating unsaturated hydraulic parameters in a layered soil from time-lapse ground-penetrating
7 radar data acquired during a synthetic infiltration experiment, we show how principal com-
8 ponent analysis, conducted on a suite of stochastic model-error realizations, can for some
9 problems be used to build a sparse orthogonal basis for the model error arising from known
10 forward solver approximations and/or simplifications. Projection of the residual onto this
11 basis during MCMC permits identification and removal of the model error before calculation
12 of the likelihood. Our results indicate that, when combined with an informal likelihood metric
13 based on the expected behaviour of the ℓ_2 -norm of the residual, this methodology can yield
14 posterior parameter estimates exhibiting a marked reduction in bias and overconfidence when
15 compared to those obtained with no model-error correction, at reasonable computational cost.
16

17 1 Introduction

18 Stochastic parameter estimation and inversion have become increasingly popular in hydrology
19 and geophysics over the past decade. In particular, it is now computationally feasible and
20 common to solve many inverse problems in these domains in a Bayesian manner, whereby prior
21 knowledge about the subsurface parameters of interest is combined with measured data to
22 yield a posterior probability distribution. The latter is typically sampled using Markov-chain-
23 Monte-Carlo (MCMC) methods (*Linde et al.*, 2017). Notable advantages of the Bayesian-
24 MCMC approach are that (i) it is highly flexible and can incorporate any information that
25 can be expressed as a probability density into the inverse problem; (ii) it provides a natural
26 framework for data integration; and (iii) it has the potential to provide more accurate pa-
27 rameter uncertainty estimates than traditional methods based on linearization. This does,
28 however, come at the cost of being highly computationally expensive. Indeed, many thou-
29 sands if not millions of MCMC iterations, each requiring a numerical solution of the forward
30 problem, are typically required to obtain a sufficient number of posterior samples for use in
31 subsequent probabilistic forecasting and risk analysis (e.g., *Ruggeri et al.*, 2015).

32 A critical component of framing an inverse problem in a Bayesian context is proper char-
33 acterization of the expected statistical nature of the residual. This is, in order to formulate
34 the likelihood, we must have detailed knowledge about the statistical distribution of the dif-
35 ference between the measured data and those calculated through the numerical solution of the
36 forward problem on the “true” set of subsurface model parameters. In arguably most cases,
37 the residual is attributed solely to data-measurement errors and described as multi-Gaussian,
38 usually with independent and identically distributed elements (e.g., *Bodin and Sambridge*,
39 2009; *Gallagher et al.*, 2009; *Irving and Singha*, 2010; *Linde and Vrugt*, 2012; *Scholer et al.*,
40 2013; *Vrugt et al.*, 2008). This is despite the fact that, in order to improve the computational
41 tractability of the Bayesian-MCMC approach, approximate versions of the forward solver,
42 for example using coarsened discretizations and/or simplifications of the underlying physics,
43 are typically employed (e.g., *Christen and Fox*, 2005; *Cui et al.*, 2011; *Efendiev et al.*, 2008;
44 *Hinnell et al.*, 2010; *Ray et al.*, 2015; *Scholer et al.*, 2013). The use of such computationally
45 efficient “proxy solvers” leads to model error, which if left uncorrected has the potential to

46 overwhelm the effects of data measurement uncertainties and lead to strongly biased and
47 overconfident posterior distributions (*Brynjarsdóttir and O’Hagan, 2014*).

48 In recent years, a number of studies in the hydrological and geophysical literature have
49 attempted to address the issue of model error in Bayesian inversions, with the aim of making
50 more effective use of proxy solvers when dealing with computationally expensive forward oper-
51 ators. In general, the approaches that have been presented can be divided into two categories.
52 In the first category, researchers have focused on the overall or “global” statistical characteri-
53 zation of the model error, with the goal of using this information to develop more appropriate
54 parametric likelihood functions that better reflect the true nature of the residual. This has
55 generally been accomplished through the analysis of stochastic model-error realizations, which
56 are generated by running the full and approximate forward solvers for randomly drawn sets
57 of model parameters. Typically, multi-Gaussian statistics for the model error are assumed,
58 meaning that means and covariances estimated from the realizations can be incorporated into
59 a Gaussian likelihood (e.g., *Arridge et al., 2006; Hansen et al., 2014; Kaipio and Somersalo,*
60 *2007; Lehikoinen et al., 2010; Stephen, 2007*), but other parametric likelihood functions have
61 also been considered (e.g., *Del Giudice et al., 2013; Schoups and Vrugt, 2010; Smith et al.,*
62 *2010; Smith et al., 2015*). Accounting for model error in this manner has been shown to
63 lead to broadened posterior distributions and a reduction in parameter bias. One key issue,
64 however, concerns the validity of the assumption that the errors can be adequately described
65 by a given parametric distribution. In many inverse problems in geophysics and hydrology,
66 for example, model errors will exhibit complex statistics and correlations that arise from
67 the typically high dimension of the data and/or model-parameter spaces in these problems,
68 combined with the non-linearity of the forward operators involved. Indeed, there has been
69 much increased interest in “likelihood-free” inference methods such as approximate Bayesian
70 computation (ABC) (e.g., *Vrugt and Sadegh, 2013*) and generalized likelihood uncertainty
71 estimation (GLUE) (e.g., *Beven and Binley, 1992*), to a large extent because of this issue.

72 In the second category of developed approaches for addressing model error, researchers
73 have focused on building a parameter-dependent or “local” error model in order to describe
74 the discrepancy between the full and approximate forward solvers. As with the approaches

75 mentioned above, this is constructed based on computed realizations of the model error for
76 different parameter sets. However, in this case the results are used to effectively correct
77 the output of the approximate solver rather than to develop a more appropriate Bayesian
78 likelihood function. Construction of the error model can be done in a number of different
79 ways. This includes simple nearest-neighbour or linear interpolation between model-error
80 realizations (e.g., *Cui et al.*, 2011; *O’Sullivan and Christie*, 2006), representing the discrepancy
81 as a Gaussian process conditioned to the points in the parameter space where the model error
82 is known (e.g., *Kennedy and O’Hagan*, 2001; *Xu and Valocchi*, 2015), or using statistical
83 regression approaches (e.g., *Doherty and Christensen*, 2011; *Josset et al.*, 2015). In all of this
84 work, the implicit assumption is that the full and approximate model-response surfaces are
85 regular enough such that the model error for a set of parameter values where it is unknown can
86 be effectively predicted through some kind of interpolation between the existing realizations.
87 While this may be the case for some inverse problems, difficulties can arise in the presence of
88 strongly non-linear forward solvers and/or large numbers of model parameters. That is, it may
89 not be possible to sufficiently sample the model-parameter space with model-error realizations
90 such that interpolation between these realizations will provide a reliable model-error estimate
91 at some new location.

92 Recently, *Köpke et al.* (2018) presented a new approach to account for the model error
93 arising from the use of proxy forward solvers in Bayesian-MCMC inversions, whereby infor-
94 mation about the error is gathered during the inversion procedure through occasional runs of
95 the approximate and full solvers together, the results of which are stored in a dictionary. In
96 contrast to the existing methods mentioned above, the approach of *Köpke et al.* (2018) focuses
97 on the projection-based identification of the model-error component of the residual through
98 the construction of a local, parameter-dependent, orthogonal model-error basis, rather than
99 on attempting to fit the overall model-error statistics to a prescribed statistical distribution
100 or develop an interpolation-based error model. The model error estimated by projecting onto
101 the basis is then subtracted from the residual before computing the likelihood of a proposed
102 set of model parameters in MCMC. Application of the approach of *Köpke et al.* (2018) to
103 a high-dimensional spatially distributed tomographic example was found to yield parame-

104 ter estimates exhibiting a notable reduction in bias compared to those obtained when the
 105 model error was ignored. The presented method does, however, still require occasional runs
 106 of the full forward solver along the Markov chain as MCMC iterations progress, which can be
 107 computationally costly depending on the problem at hand.

108 In this paper, we build on the work of *Köpke et al.* (2018) and show that, for some inverse
 109 problems, it may be possible to derive a suitable global basis for the model error over the entire
 110 parameter space through the application of principal component analysis to a large number
 111 of stochastic model-error realizations. These realizations can be conveniently computed in
 112 parallel prior to MCMC, and they must be properly organized in the data space before analysis
 113 to maximize similarity in their spatial characteristics. We begin in Section 2 with an overview
 114 of Bayesian-MCMC inversion, followed by a detailed description of our developed approach.
 115 This is followed in Section 3 with application to synthetic data corresponding to a vadose-
 116 zone inverse problem that has been the subject of much investigation in previous work, which
 117 is the estimation of unsaturated soil hydraulic parameters from time-lapse zero-offset-profile
 118 (ZOP) ground-penetrating radar (GPR) data acquired during infiltration. We compare the
 119 results obtained with our methodology to those obtained when no model-error correction is
 120 applied, and conclude in Section 4 with an overall assessment of the method with regard to
 121 its advantages and limitations.

122 2 Methodological background

123 2.1 Bayesian-MCMC inversion

124 Consider to begin the forward problem linking a set of M subsurface model parameters of
 125 interest $\mathbf{m}_{true} \in \mathbb{R}^M$ to a set of N measured or observed data $\mathbf{d}_{obs} \in \mathbb{R}^N$:

$$126 \quad \mathbf{d}_{obs} = F(\mathbf{m}_{true}) + \mathbf{e}_d, \quad (1)$$

127 where forward operator $F : \mathbb{R}^M \rightarrow \mathbb{R}^N$ contains the physics and geometry of the measurements
 128 and \mathbf{e}_d is vector of data measurement errors. The goal of the corresponding inverse problem
 129 is to estimate \mathbf{m}_{true} given \mathbf{d}_{obs} , which requires knowledge of F and in most cases some prior

130 information about the model parameters. From a probabilistic point of view, this can be
 131 formulated using Bayes' theorem, whereby an initial prior state of information for the model
 132 parameters $\rho(\mathbf{m})$ is updated to a more refined posterior state of knowledge $\sigma(\mathbf{m})$ based on
 133 the available data (e.g., *Tarantola, 2005*). That is,

$$134 \quad \sigma(\mathbf{m}) = k L(\mathbf{m}) \rho(\mathbf{m}), \quad (2)$$

135 where normalization constant k ensures that the posterior probability distribution integrates
 136 to unity, and likelihood $L(\mathbf{m})$ expresses the conditional probability of model parameter set \mathbf{m}
 137 given the observed data \mathbf{d}_{obs} . Assuming that (i) the underlying physics are completely known
 138 and considered in the inverse problem; and (ii) the data measurement errors are independent
 139 and identically normally distributed having mean zero and standard deviation s_d , $L(\mathbf{m})$ takes
 140 on the simple multi-Gaussian form

$$141 \quad L(\mathbf{m}) = \frac{1}{(2\pi s_d^2)^{N/2}} \exp \left[-\frac{\|\mathbf{r}(\mathbf{m})\|^2}{2s_d^2} \right], \quad (3)$$

142 where $\|\cdot\|$ denotes the ℓ^2 -norm and $\mathbf{r}(\mathbf{m})$ is the residual or difference between the observed
 143 data and those predicted for some model parameter set \mathbf{m} using F . The latter quantity is
 144 given by

$$145 \quad \mathbf{r}(\mathbf{m}) = \mathbf{d}_{pred} - \mathbf{d}_{obs}$$

$$146 \quad = \underbrace{F(\mathbf{m}) - [F(\mathbf{m}_{true})]}_{\substack{\text{parameter-error} \\ \text{component}}} + \mathbf{e}_d, \quad (4)$$

147

148 where \mathbf{d}_{pred} denotes the predicted data. We see in equation (3) that $L(\mathbf{m})$ will be maximized
 149 when the ℓ^2 -norm of $\mathbf{r}(\mathbf{m})$ is minimized, which corresponds to the case where $\mathbf{m} = \mathbf{m}_{true}$ and
 150 the parameter-error component as defined in equation (4) is zero. The spread of the likelihood
 151 distribution about the maximum value is controlled by the data measurement error standard
 152 deviation s_d along with the number of data N , with larger errors and lesser amounts of data
 153 yielding broader likelihoods.

154 Equations (2) through (4) together provide a means of calculating the posterior probability

155 of a set of model parameters \mathbf{m} . This is commonly used within MCMC sampling algorithms
 156 to quantify posterior uncertainty, thereby solving the inverse problem, since it is not generally
 157 possible to perform the multi-dimensional integrations needed to obtain the statistical mo-
 158 ments of $\sigma(\mathbf{m})$. In this regard, a basic Metropolis-Hastings algorithm (*Metropolis et al.*, 1953;
 159 *Hastings*, 1970) that is guaranteed (after burn-in) to generate a Markov chain of samples
 160 $\{\mathbf{m}_1, \dots, \mathbf{m}_k\}$ from the Bayesian posterior distribution proceeds as follows:

- 161 1. Draw the first model in the Markov chain \mathbf{m}_1 from the Bayesian prior distribution $\rho(\mathbf{m})$.
 162 Set $i = 1$.
- 163 2. Draw a perturbed model-parameter set \mathbf{m}' from the proposal distribution $Q(\mathbf{m}'|\mathbf{m}_i)$,
 164 whose width around \mathbf{m}_i is chosen so as to provide a balance between efficiently moving
 165 through the parameter space and generating proposals that have a reasonable probability
 166 of being accepted.
- 167 3. Calculate the probability of accepting \mathbf{m}' as the next model in the Markov chain using

$$P_{acc} = \min \left[1, \frac{\sigma(\mathbf{m}') Q(\mathbf{m}_i|\mathbf{m}')}{\sigma(\mathbf{m}_i) Q(\mathbf{m}'|\mathbf{m}_i)} \right]. \quad (5)$$

- 168 4. Draw a random number $x \in U(0, 1)$. If $x \leq P_{acc}$, then set $\mathbf{m}_{i+1} = \mathbf{m}'$. Otherwise set
 169 $\mathbf{m}_{i+1} = \mathbf{m}_i$.
- 170 5. Set $i = i + 1$ and go to Step 2.

171 Note that, in the case where the proposal distribution is symmetric (i.e., $Q(\mathbf{m}'|\mathbf{m}_i) = Q(\mathbf{m}_i|\mathbf{m}')$),
 172 the above algorithm reduces to the original MCMC sampler of *Metropolis et al.* (1953) where
 173 the acceptance probability is given by $P_{acc} = \min[1, \sigma(\mathbf{m}')/\sigma(\mathbf{m}_i)]$. We consider the latter
 174 sampler for the example inversions presented in Section 3.

175 2.2 Accounting for model error

176 Likelihood equation (3) is perfectly theoretically valid for the case where the only contribution
 177 to the difference between the observed and predicted data, when considering the correct set
 178 of model parameters \mathbf{m}_{true} , is a set of Gaussian data-measurement errors having standard

179 deviation s_d . However, as mentioned previously, approximate forward solvers are typically
 180 used in hydrological and geophysical problems to improve the computational efficiency of the
 181 Bayesian-MCMC procedure, meaning that the residual more realistically takes the form

$$\begin{aligned}
 182 \quad \mathbf{r}(\mathbf{m}) &= \hat{F}(\mathbf{m}) - [F(\mathbf{m}_{true}) + \mathbf{e}_d] \\
 183 \quad &= \underbrace{\hat{F}(\mathbf{m}) - F(\mathbf{m})}_{\text{model-error component}} + \underbrace{F(\mathbf{m}) - [F(\mathbf{m}_{true}) + \mathbf{e}_d]}_{\text{parameter-error component}}, \quad (6) \\
 184
 \end{aligned}$$

185 where \hat{F} is the approximate forward operator. The presence of an additional model-error term
 186 in equation (6) as compared with equation (4), which is commonly of large magnitude, strongly
 187 correlated, and/or highly non-Gaussian (*Kaipio and Somersalo, 2007; Schoups and Vrugt,*
 188 *2010; Smith et al., 2010*), makes use of likelihood expression (3) inappropriate. In particular,
 189 it means that (i) the residual will not necessarily be minimized when $\mathbf{m} = \mathbf{m}_{true}$, implying
 190 posterior parameter bias; and (ii) feasible model parameter sets may have an extremely low
 191 likelihood when considering realistic levels of data error. Although simple inflation of s_d can
 192 be used to broaden the Gaussian likelihood and reduce the latter issue, it cannot address the
 193 former and be viewed as an effective solution for reliable posterior uncertainty quantification.

194 In order to address the model-error issue, we build on the work of *Köpke et al. (2018)* in this
 195 paper and focus on learning about the nature of the model error through stochastic simulation
 196 such that it may be identified and removed from the residual during MCMC. The overall idea is
 197 that, for some problems, a representative set of stochastic model-error realizations, computed
 198 prior to MCMC for random model parameter sets using the full and approximate forward
 199 solvers, can be used to construct an orthonormal basis for the model error. Projection of the
 200 residual onto this basis in each MCMC iteration is used to isolate the model-error component,
 201 which is subtracted from $\mathbf{r}(\mathbf{m})$ before calculating the likelihood. Note that, whereas *Köpke*
 202 *et al. (2018)*, used a dictionary-based K-nearest-neighbour (KNN) approach to construct a
 203 different local model-error basis for each proposed set of model parameters in MCMC, with
 204 runs of the full forward solver being required periodically along the entire Markov chain,
 205 we focus here on the development of a global basis (i.e., over the entire model parameter
 206 space) before posterior sampling begins. Although not appropriate for all problems, this

207 methodology has the advantage that all expensive forward solver computations can be run in
 208 a simple parallel manner outside of the MCMC iterations. The corresponding set of model-
 209 error realizations can also be directly reused in any subsequent inversions. Our approach
 210 proceeds as follows:

- 211 1. Generate k random sets of model parameters $\{\mathbf{m}_1, \dots, \mathbf{m}_k\}$ from the Bayesian prior
 212 distribution $\rho(\mathbf{m})$.
- 213 2. Compute the corresponding set of stochastic model-error realizations $\{\mathbf{E}_1, \dots, \mathbf{E}_k\}$, where
 214 $\mathbf{E}_i = \hat{F}(\mathbf{m}_i) - F(\mathbf{m}_i)$.
- 215 3. If necessary, organize the information in each realization to improve coherency for sub-
 216 sequent analysis (see Section 3.3).
- 217 4. Perform principal component analysis (PCA) on the model-error realizations $\{\mathbf{E}_1, \dots, \mathbf{E}_k\}$
 218 in order to obtain a sparse orthonormal basis $\mathbf{B} = [\mathbf{b}_1, \dots, \mathbf{b}_b]$ for the model error. The
 219 number of basis vectors b should be chosen to be the minimum required to capture a
 220 high percentage of the variance of the realizations, typically around 98%. In this way,
 221 the basis will be able to capture the model-error behaviour, but will have minimal abil-
 222 ity to represent contributions to the residual that do not resemble model error such as
 223 data measurement uncertainties.
- 224 5. For each set of model parameters \mathbf{m}' tested within MCMC, calculate the best approx-
 225 imation of the residual $\mathbf{r}(\mathbf{m}') = \hat{F}(\mathbf{m}') - \mathbf{d}_{obs}$ using the model-error basis, obtained in
 226 a least-squares sense using $\mathbf{B}\mathbf{B}^T\mathbf{r}(\mathbf{m}')$, and remove this result from the residual. This
 227 yields the remainder

$$\mathbf{R}(\mathbf{m}') = \mathbf{r}(\mathbf{m}') - \mathbf{B}\mathbf{B}^T\mathbf{r}(\mathbf{m}') \quad (7)$$

- 228 6. Use $\mathbf{R}(\mathbf{m}')$ to determine $L(\mathbf{m}')$ within MCMC (see Section 2.3).

229 It is important to note that the success of the modified MCMC approach described above,
 230 in terms of providing refined and unbiased posterior parameter estimates using an approximate
 231 forward operator, hinges on our ability to effectively separate the model-error component

232 of equation (6) from (i) data-measurement errors, and (ii) parameter-related errors. The
 233 implicit assumption in our work is that these two other sources of error lie orthogonal to the
 234 elements of \mathbf{B} , such that projection of the residual onto the basis will preserve only the model-
 235 error component. With regard to (i), we have found that this is a reasonable expectation
 236 as the limited number of model-error basis vectors, which tend to possess a high degree of
 237 spatial correlation, are generally not capable of representing random data-measurement errors
 238 through a linear combination (*Köpke et al., 2018*). With respect to (ii), although there is no
 239 guarantee that the basis cannot represent at least part of the parameter-error term through
 240 a linear combination, our experience has been that the model and parameter-related errors
 241 typically possess significantly different statistical characteristics meaning that the latter tend
 242 to be quite effectively attenuated through projection onto \mathbf{B} . If this is not the case and a
 243 particular incorrect model-parameter set tested within MCMC happens to yield a parameter-
 244 error component that resembles what was observed in the model-error realizations, this error
 245 will be removed and the parameter set will have a reasonably high chance of being accepted
 246 (*Köpke et al., 2018*). This latter point is discussed in further detail in Section 3.5.

247 **2.3 Likelihood evaluation**

248 Ideally, the remainder $\mathbf{R}(\mathbf{m})$ in equation (7) should represent the residual in (6) with the
 249 model-error component perfectly removed, meaning that it should be identical to equation (4)
 250 and thus suitable for inclusion into Gaussian expression (3) to evaluate the likelihood. In
 251 reality, however, small but correlated and non-Gaussian errors in the approximation of the
 252 model-error component of the residual, related to our inability to perfectly separate model
 253 error from data measurement and parameter uncertainty using the sparse basis \mathbf{B} , mean
 254 that $\mathbf{R}(\mathbf{m}_{true})$ will deviate somewhat from multi-Gaussian and use of equation (3) can be
 255 problematic. Indeed, the strong ranking of models provided by a Gaussian likelihood function
 256 is well understood to pose difficulties for Bayesian inference when the underlying statistical
 257 assumptions regarding the residual are violated, in the sense that sets of model parameters
 258 that are perfectly acceptable may be mapped to extremely low likelihoods (e.g., *Beven and*
 259 *Binley, 1992; O’Sullivan and Christie, 2006*). To address this issue, we evaluate the likelihood

260 in this work using a statistically informal but more practical metric based on the expected
 261 univariate distribution of the ℓ_2 -norm of the remainder in equation (7), as opposed to the
 262 expected multivariate distribution of the vector $\mathbf{R}(\mathbf{m})$. Specifically, assuming for lack of
 263 better information that the elements of $\mathbf{R}(\mathbf{m})$ are uncorrelated and normally distributed
 264 having mean zero and standard deviation s_R , it can be shown that the ℓ_2 -norm $\|\mathbf{R}(\mathbf{m})\|$ will
 265 follow a scaled chi distribution (*Forbes et al.*, 2010), leading to the following equation:

$$L(\mathbf{m}) = \frac{2^{1-\frac{N}{2}}}{\Gamma(\frac{N}{2}, 0)} s_R^{-N} \|\mathbf{R}(\mathbf{m})\|^{N-1} \exp\left[-\frac{\|\mathbf{R}(\mathbf{m})\|^2}{2s_R^2}\right], \quad (8)$$

266 where $\Gamma(\cdot, \cdot)$ is the incomplete gamma function.

267 For the typical case where s_R is unknown and can only be bounded between lower and
 268 upper values s_{R_1} and s_{R_2} , respectively, equation (8) can be integrated over s_R yielding

$$L(\mathbf{m}) \propto \Gamma\left(\frac{N-1}{2}, \frac{\|\mathbf{R}(\mathbf{m})\|^2}{2s_R^2}\right)\Bigg|_{s_{R_1}}^{s_{R_2}}. \quad (9)$$

269 Figure 1 shows $L(\mathbf{m})$ calculated using equation (9) as a function of $\|\mathbf{R}(\mathbf{m})\|$ for $N = 1000$
 270 with $s_{R_1} = 0.1$ and $s_{R_2} = 0.2$. We see that there is a range for the ℓ_2 -norm of $\mathbf{R}(\mathbf{m})$ over
 271 which the likelihood is approximately constant, outside of which it falls off rapidly to near-
 272 zero values. In other words, sets of model parameters for which $\|\mathbf{R}(\mathbf{m})\|$ is consistent with
 273 the ℓ_2 -norm of a vector of normally distributed values with $s_R \in [0.1, 0.2]$ are considered to
 274 be approximately equally likely, whereas those that do not fit this criterion are given almost
 275 zero likelihood. Equation (9) is much less sensitive to small changes in $\mathbf{R}(\mathbf{m})$ compared with
 276 equation (3), and represents a significantly more relaxed and inherently conservative constraint
 277 than that provided by a formal Gaussian likelihood function. Indeed, the use of such informal
 278 likelihood measures within stochastic inverse methods has gained widespread acceptance in
 279 hydrology and other domains in recent years (e.g., *Beven and Freer*, 2001; *Beven and Binley*,
 280 2014; *Blasone et al.*, 2008; *Nott et al.*, 2012; *Sadegh and Vrugt*, 2013a,b; *Wilkinson*, 2013),
 281 as researchers have realized the shortcomings of placing too much importance on the detailed
 282 statistical properties of the residual for many real-world problems. Equation (9) can in fact be
 283 considered as a slight variation of the generalized likelihood uncertainty estimation (GLUE)

284 approach, originally proposed by *Beven and Binley (1992)*, where the distinction between
285 “behavioural” and “non-behavioural” models is quantified by using the ℓ_2 -norm of the data
286 misfit. Models whose remainder norm falls within the bounds indicated in Figure 1 will have
287 a high chance of being accepted in MCMC, whereas those falling significantly outside these
288 bounds will tend to be rejected.

289 [Figure 1 about here.]

290 **3 Example: GPR monitoring of infiltration**

291 We now apply the model-error methodology presented in Section 2 to a synthetic example
292 involving GPR monitoring of an infiltration experiment. Zero-offset-profile (ZOP) GPR data,
293 acquired between two boreholes over the course of the experiment, provide estimates of hor-
294 izontally averaged soil water content as a function of depth and time (e.g., *Annan, 2006*).
295 Together with a numerical model for the infiltration process, the latter results are then used
296 to estimate unsaturated soil hydraulic properties in a layered subsurface. This particular prob-
297 lem has been the focus of much previous research in the field of hydrogeophysics (e.g., *Binley*
298 *and Beven, 2003; Cassiani and Binley, 2005; Looms et al., 2008; Rucker and Ferré, 2004;*
299 *Rucker, 2011*), and was most recently investigated within the context of Bayesian-MCMC
300 inversion by *Scholer et al. (2011, 2012, 2013)*. Here, we consider the model errors arising from
301 a simplifying assumption common to all past work, which is that water movement occurs in
302 a purely vertical direction through the subsurface.

303 **3.1 Governing equations and model simplifications**

304 The general movement of water through unsaturated soils is described by Richards’ equation
305 (*Richards, 1931*), given by

$$306 \quad \frac{\partial \theta(h)}{\partial t} = \nabla \cdot [K(h) \nabla h] + \frac{\partial K(h)}{\partial z}, \quad (10)$$

307 where θ is the volumetric water content, K is the unsaturated hydraulic conductivity, h is
308 pressure head, t is time, and z is elevation. The relationships $\theta(h)$ and $K(h)$ for different

309 soils are commonly described using the van Genuchten - Mualem (VGM) model (*Mualem,*
 310 1976; *van Genuchten,* 1980). With this model, the soil water retention, expressed in terms of
 311 effective saturation S_e , is given by

$$312 \quad S_e(h) = \frac{\theta(h) - \theta_r}{\theta_s - \theta_r} = \begin{cases} (1 + |\alpha h|^n)^{-m} & , \text{ for } h \leq 0 \\ 1 & , \text{ for } h > 0 \end{cases} \quad (11)$$

313

314 where θ_r and θ_s are the residual and saturated water contents, respectively, and α , m , and
 315 n are empirical shape factors with $m = 1 - 1/n$. The unsaturated hydraulic conductivity is
 316 described by

$$317 \quad K(h) = K_s S_e(h)^{1/2} \left[1 - (1 - S_e(h)^{1/m})^m \right]^2, \quad (12)$$

318 where K_s is the hydraulic conductivity value at full saturation. A total of five parameters
 319 (K_s , θ_r , α , n , and θ_s) therefore describe a soil's hydraulic properties using the VGM model.

320 Equations (10) through (12) provide a link between a set of subsurface VGM parameters
 321 and the corresponding spatiotemporal distribution of water content in response to infiltration.
 322 That is, knowing the distribution of soil VGM parameters along with the boundary and initial
 323 conditions of the infiltration experiment, we can calculate the evolution of water content in the
 324 subsurface. This forward link provides the basis for inverting for the soil hydraulic properties
 325 given a set of dynamic GPR-derived water-content measurements. However, in the context
 326 of stochastic inversion, repeated solution of a fully 3D unsaturated flow model based on (10)
 327 can be extremely computationally demanding. As a result, previous work in this domain has
 328 typically assumed that flow occurs only in the vertical direction (e.g., *Binley and Beven,* 2003;
 329 *Cassiani and Binley,* 2005; *Looms et al.,* 2008; *Scholer et al.,* 2012), such that the following
 330 1D version of Richards' equation can be utilized in the inversion procedure:

$$331 \quad \frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[K(h) \left(\frac{\partial h}{\partial z} + 1 \right) \right]. \quad (13)$$

332 The vertical flow assumption may hold in layered subsurface environments under natural load-
 333 ing conditions (e.g., *Binley and Beven,* 2003), but it will be clearly violated during infiltration
 334 experiments where the area over which loading occurs is spatially restricted and loading rates

335 are significantly higher. This will be particularly the case where there exist large contrasts
336 in subsurface hydraulic properties (e.g., *Looms et al.*, 2008; *Rucker*, 2011). As a result, the
337 1D flow assumption represents a significant source of model error. Although such errors and
338 their potential for posterior parameter bias have been acknowledged in previous research ef-
339 forts (*Scholer et al.*, 2013), they have never before been examined and accounted for in the
340 inversion procedure.

341 **3.2 Infiltration experiment and data**

342 Figure 2 shows the overall setup considered for our synthetic infiltration experiment. Infil-
343 tration at a rate of 2 cm/h is applied to a circular region on the Earth’s surface having a
344 diameter of 3 m. The infiltration is carried out for a period of 11.6 d, during which GPR-
345 derived estimates of horizontally averaged water content are considered to be available every
346 2.8 h. The water-content measurements are considered between boreholes 2-m apart and 8-m
347 deep, with a depth sampling interval of 0.1 m. The subsurface consists of two layers whose
348 VGM parameters are given in Table 1, which texturally describes a sandy soil underlain by a
349 less permeable silt loam. The boundary between the layers is located at 3-m depth.

350 [Figure 2 about here.]

351 [Table 1 about here.]

352 To determine the spatiotemporal distribution of water content corresponding to the ex-
353 perimental setup described above, we used the code VS2D (*Lappala et al.*, 1987) to solve the
354 general 3D Richards’ equation (10) under the assumption of rotational symmetry about the
355 vertical axis, meaning that the model domain was parameterized in terms of radius (r) and
356 depth (z), with $r = 0$ corresponding to the center of the infiltration region. A specified-flux
357 boundary condition was imposed at the Earth’s surface ($z = 0$ m) with no-flow conditions
358 assumed outside of the infiltration region ($r > 1.5$ m). No-flow conditions were also assumed
359 along the outside of the model domain, the latter of which was set at $r = 4$ m. At the bottom
360 of the domain ($z = 10$ m), a fixed-pressure-head value of $h = -0.5$ m was specified in order to
361 simulate the presence of the water table at 10.5-m depth. The initial distribution of soil water

362 content prior to running the infiltration experiment was obtained using a 1D steady-state
363 infiltration code based on the work of *Rockhold et al. (1997)* assuming a constant infiltration
364 rate of 0.036 cm/h.

365 Figure 3 shows snapshots of the modeled subsurface water-content distribution over the
366 course of the infiltration experiment for times $t = 0, 1, 2, 5, 7,$ and 11 d. We see that, once the
367 experiment begins, the infiltration front moves approximately vertically through the sandy
368 soil layer, making its way to the boundary with the silt loam in just under 2 d. From this
369 point onwards, although the front continues to move downwards, a strong lateral component
370 to the flow is observed because of the lesser permeability of the lower layer. Indeed, as the
371 water is not able to infiltrate as quickly into the silt loam, it begins to build up at the interface
372 between the two soils and spread horizontally. Such behaviour cannot be captured using a
373 1D flow model based on equation (13), which is discussed in further detail below.

374 [Figure 3 about here.]

375 We next simulated the GPR-derived water-content measurements acquired during the
376 infiltration experiment, which again represent the data to be inverted for the VGM parameters
377 in each soil layer. To this end, every 2.8 h, the horizontal average of the water-content field
378 between the boreholes was calculated from the VS2D results using a depth discretization
379 interval of 0.1 m. This yielded 81 measurements in depth across 101 GPR acquisition times,
380 to which zero-mean Gaussian random noise with a standard deviation of 0.01 (roughly 5%)
381 was added to simulate the effects of measurement error. It is important to note that, for
382 the sake of simplicity in this example, we did not explicitly model the propagation of GPR
383 energy between the transmitter and receiver antennas in the two boreholes based on the
384 VS2D results, but rather assumed that the ZOP GPR experiment provided a measure of the
385 horizontal average of soil water content as a function of depth. Although, in doing this, we
386 admittedly neglect several aspects of the physics that would be encountered in a field setting
387 such as critical refractions of GPR energy and frequency-dependent resolution limitations
388 (e.g., *Rossi et al., 2012; Rucker and Ferré, 2004*), these aspects were not considered essential
389 for this numerical study into the effects of model error arising from the 1D flow assumption.

390 Figure 4a shows the simulated GPR-derived water-content data, organized into a matrix

391 with depth on the vertical axis and measurement time on the horizontal axis. To gain insight
392 into the importance of model error for this example, Figure 4b shows the corresponding water
393 content calculated as a function of depth and time assuming purely vertical flow, such that the
394 1D Richards' equation (13) could be applied. The results obtained using the 3D and 1D models
395 for the same set of VGM parameters and boundary conditions are clearly and significantly
396 different, most notably with respect to: (i) the speed at which the infiltration front travels
397 through the lower layer, which is greater using the 1D model; and (ii) the evolution of water
398 content in the upper layer after the infiltration front reaches the soil interface, in that the
399 upper layer is seen to “fill up” to full saturation in the 1D case rather than pool and spread
400 laterally. Figure 4c shows the difference between and 1D and 3D simulation results, equal
401 to the sum of the model error and Gaussian measurement uncertainties. Here we see that
402 there are parts of the data space where the magnitude of the error is almost 50%, and that
403 the model error exhibits a high degree of correlation. All of this means that using a 1D flow
404 model to stochastically invert the data in Figure 4a, without accounting for model error, will
405 result in a strong bias in the estimated VGM parameters and unreliable posterior statistics
406 (see Section 3.4). Finally, Figure 4d shows the error image from Figure 4c with the results
407 reorganized such that they are plotted relative to the arrival time of the infiltration front as a
408 function of depth observed in the data (Figure 4a). The importance of this data arrangement
409 step is explained in the following section.

410 [Figure 4 about here.]

411 **3.3 Model-error realizations and analysis**

412 The first step in our approach to dealing with a known source model error in this paper
413 involves generation of a set of stochastic model-error realizations corresponding to parameter
414 sets randomly drawn from the Bayesian prior distribution. Again, this is done so that we
415 can learn about the overall characteristics of the model error, with the goal of using this
416 information to identify the model-error component of the residual during MCMC. Table 2
417 shows the lower and upper bounds of the uniform prior distributions that were assumed for
418 the different VGM parameters in our synthetic study. Note that these distributions are rather

419 broad and encompass a wide range of soil types (e.g., *Carsel and Parrish*, 1988), and that
420 the same priors were assumed for each soil layer. In this way, relatively little information
421 about the hydraulic properties is provided to the inversion procedure and we rely strongly
422 upon the data to resolve them. Also note that the prior bounds for K_s are specified in terms
423 of its logarithm, which is consistent with previous work and reflects the wide range of natural
424 variability of this parameter (e.g., *Scholer et al.*, 2012, 2013).

425 [Table 2 about here.]

426 Each model-error realization was generated by: (i) drawing a random set of VGM parame-
427 ters for each soil layer from the prior distributions in Table 2; (ii) computing the corresponding
428 GPR-derived water-content data as a function of depth and time based on the general 3D
429 Richards' equation (10); (iii) computing the GPR-derived water-content data under the as-
430 sumption of purely vertical flow using the 1D Richards' equation (13); and (iv) calculating
431 the difference between the 3D and 1D simulation results. It is important to reiterate that this
432 part of our model-error approach is easily parallelized in the sense that different model-error
433 realizations can be computed on different processors of a cluster, thereby greatly reducing the
434 time needed to run the relatively large number of expensive 3D unsaturated flow simulations
435 required. In this regard, runs of the 3D solver for our example took approximately 100 s on a
436 standard desktop computer, whereas runs of the 1D solver were over 60 times faster at 1.5 s.

437 Figure 5 shows an example of 18 model-error realizations, each of which has been plotted
438 relative to the arrival time of the infiltration front observed in the 3D simulation results, as
439 was done for Figure 4d. This latter step, whereby the realizations are effectively “aligned”
440 on the curve representing the 3D infiltration-front arrival in depth, is important for this
441 problem because, without it, the realizations would be highly dissimilar in the data space and
442 not amenable to any kind of global analysis. In contrast, after alignment, the model-error
443 realizations are seen to take on a similar form which is described by: (i) a triangular region
444 below 3-m depth that results from the difference in the speed of propagation of the infiltration
445 front in the lower layer between the 3D and 1D simulations; and (ii) another triangular
446 region above 3-m depth that results when the upper layer “fills up” in the 1D simulation for
447 cases where the lower layer is less permeable. Although the widths and amplitudes of these

448 triangular regions are significantly different across the various realizations in Figure 5, the
449 images, due to their similarity in form, are generally well suited to PCA analysis with the aim
450 of generating a compact orthonormal basis for the model error. At the same time, however,
451 it is important to note that the strong variations between the realizations in Figure 5 in
452 terms of width and amplitude mean that the model error is not well described using a simple
453 parametric distribution, and thus not amenable to the global statistical approaches for model
454 error mentioned earlier. Indeed, detailed analysis of the 6500 model-error realizations indicates
455 that the model-error values are highly non-Gaussian-distributed with complex correlation
456 patterns in the data space.

457 [Figure 5 about here.]

458 To construct the model-error basis, a total of 6500 realizations were analyzed using PCA,
459 the results of which showed that only the first 50 principal components (out of 6561) were
460 necessary to capture 98% of the variance of the input. Note that the number of principal
461 components required to capture this percent of variance tends to increase with the number of
462 model-error realizations considered, as smaller sets of realizations will generally exhibit a lesser
463 range of variability that can be represented by a smaller basis (Figure 6). Our choice of 6500
464 realizations represents a point after which this trend stabilizes and the addition of further
465 realizations does not require more principal components to capture 98% of the variance.
466 Figure 7 shows the first 15, and last 3, vectors in the orthonormal model-error basis, ordered
467 with respect to their decreasing contribution to the total variance and plotted as images in
468 the data space. As expected, we see a gradual increase in the spatial frequency content of
469 each vector as its index increases, with the first few vectors tending to capture the overall
470 large-scale trends seen in the realizations in Figure 5 and the higher-order basis elements being
471 necessary to resolve the finer details. Again, under the assumptions of orthogonality stated in
472 Section 2.2, projection of the residual onto this basis during MCMC should adequately identify
473 the model-error component, which can then be removed prior to computing the likelihood.

474 [Figure 6 about here.]

475 [Figure 7 about here.]

476 3.4 Stochastic inversion results

477 We now present the results of three different Bayesian-MCMC inversions to estimate the
478 “true” VGM parameters in Table 1 from the GPR-derived water-content data in Figure 4a,
479 all of which are based on use of a simplified 1D flow model. We begin by presenting the results
480 of inverting using a “standard” Gaussian likelihood given by equation (3), where no correction
481 for model error is considered and the standard deviation of the data errors s_d is artificially
482 inflated in order to compensate for the additional error source. This is followed by inverting
483 using the informal ℓ_2 -norm-based likelihood measure given by equation (9), again with no
484 correction for model error, such that the results obtained using this measure and using the
485 Gaussian likelihood can be directly compared. Finally, we show the posterior results obtained
486 for the case where the ℓ_2 -norm-based likelihood is combined with the correction for model
487 error described in Section 2.2. For each inversion, a uniform MCMC proposal distribution
488 $Q(\mathbf{m}'|\mathbf{m}_i)$, centered on the current state of the Markov chain and whose width was chosen to
489 provide a model acceptance rate of approximately 30% (Gelman *et al.*, 1996), was employed.
490 A total of 800,000 MCMC iterations were run in each case, from which the first 10,000
491 samples were discarded as burn-in. These latter values were deemed appropriate based on
492 visual inspection of each model parameter, along with its mean and variance, as a function of
493 iteration (e.g., Hassan *et al.*, 2009).

494 3.4.1 Gaussian likelihood, no model-error correction

495 Figure 8 shows the marginal posterior histograms obtained for the VGM parameters in each
496 soil layer for the case where the data in Figure 4a were inverted using a standard Gaussian
497 likelihood function. The error standard deviation in equation (3) in this case was arbitrarily
498 set to $s_d = 0.2$, which is 20 times the level of the random noise added to the data, in order
499 to compensate for the model-error contribution to the residual and counteract the strong
500 ranking of models provided by a Gaussian likelihood when the true residual statistics do
501 not agree precisely with those that are assumed. Without such error inflation, the use of
502 equation (3) would result in a highly peaked posterior distribution that could only be sampled
503 with an extremely narrow proposal distribution and unreasonably large number of MCMC

504 iterations. Indeed, *Brynjarsdóttir and O'Hagan (2014)* point out that, when model errors are
505 present and not accounted for in Bayesian inference, the posterior tends to become narrowly
506 focused around the wrong set of model parameters, and this only gets worse as more data are
507 considered. Error inflation permits, at the very least, for the biased parameter set(s) to be
508 identified at the expense of the posterior parameter uncertainties being arbitrary.

509 [Figure 8 about here.]

510 We see in Figure 8 that, because model error is present but has not been accounted for
511 in the inversion procedure, the posterior VGM-parameter histograms are consistently focused
512 on the wrong values. That is, there exists a set of incorrect parameter values whose predicted
513 data, obtained using a 1D flow model, are a better match to the observed data than the
514 true parameters in Table 1. The most significant bias in parameters occurs for the saturated
515 hydraulic conductivity in both layers and the saturated water content of the upper layer, where
516 the true values are seen to fall outside of the limits of the posterior distributions despite that
517 fact that the error inflation imposed in this example is significant. As infiltration occurs
518 significantly more rapidly in a 1D simulation than in 3D for the same set of model parameters
519 (Figure 4), an inversion based on the 1D flow model will tend to select lower values for K_s
520 in both layers in order to best match the observed, 3D-generated data. Further, the 1D flow
521 model predicts a greater accumulation of water at the interface between the two layers, which
522 can be reduced by selecting lower values for θ_s in the upper layer.

523 To gain insight into how such model-error-related biases translate into quantities relevant
524 to flow and transport, Figure 9 shows the water retention and unsaturated hydraulic con-
525 ductivity functions for the two soil layers corresponding to (i) the posterior VGM-parameter
526 sets (color); (ii) the prior parameter ranges (grayscale); and (iii) the true parameter set in
527 Table 1 (blue curve). Here we observe that the true curves often fall either at the limits of the
528 posterior ranges or outside of them, meaning that the posterior parameter sets do not well
529 reflect the soil hydraulic behaviour. Clearly, the model errors arising from the 1D vertical flow
530 assumption cannot be neglected if we wish to have reliable predictions of flow and transport
531 through this system.

532 [Figure 9 about here.]

533 **3.4.2 L2-norm likelihood, no model-error correction**

534 Figure 10 shows the marginal posterior histograms obtained for the case where the data in
535 Figure 4a were inverted using the informal L_2 -norm-based likelihood measure developed in
536 Section 2.3. Again, the advantage of using this measure is that the likelihood is determined
537 based on the expected behaviour of a summary measure of the residual (i.e., its L_2 -norm),
538 rather than on the residual vector itself, thereby avoiding an overly strong preference for model
539 parameter sets whose corresponding residual statistics fit exactly the assumed Gaussian model.
540 As in the Gaussian likelihood case, no attempt was made to remove the effects of model error
541 in this inversion. To account for the increased residual energy due to model error and allow
542 for effective MCMC sampling, a modest amount of error inflation was made by setting the
543 residual standard deviation in equation (9) to lie between $s_{R_1} = 0.01$ and $s_{R_2} = 0.04$.

544 [Figure 10 about here.]

545 We observe in Figure 10 that, as was the case with the standard Gaussian likelihood, a
546 strong bias exists in the posterior results because of the model error coming from the 1D flow
547 assumption. Indeed, the marginal posterior histograms look similar to those in Figure 8, with
548 the true parameter values for K_s and θ_s often falling far outside of the limits of the posterior
549 distributions. In terms of the water retention and unsaturated hydraulic conductivity func-
550 tions, Figure 11 shows results that are almost identical to those in Figure 9. Note, however,
551 that because of the use of the informal likelihood measure, the results presented here were
552 obtained with significantly less error inflation than in the Gaussian likelihood case. That is,
553 in using the L_2 -norm-based likelihood, we greatly increase the probability of acceptance of
554 model parameter sets whose residual norm fits our expectations, but whose residual vector
555 may deviate slightly from Gaussian.

556 [Figure 11 about here.]

557 **3.4.3 L2-norm likelihood, correction for model error**

558 Finally, Figure 12 shows the marginal posterior histograms obtained for the case where the
559 water-content data in Figure 4a were inverted using our informal L_2 -norm-based likelihood

560 measure combined with the proposed correction for model error described in Section 2.2.
561 Only a small amount of error inflation was done in this inversion by setting $s_{R_1} = 0.01$ and
562 $s_{R_2} = 0.015$ in order to account for the fact that, even with the correction, it is unlikely that
563 the model-error component of the residual will be perfectly removed. As a result, the energy
564 in the remainder should be slightly larger than the level of noise added to the data.

565 [Figure 12 about here.]

566 We see in Figure 12 that, as a result identifying and subtracting the model-error component
567 of the residual before evaluation of the likelihood in MCMC, the posterior VGM-parameter
568 histograms are no longer biased, with the true parameter values falling in most cases near
569 the middle of the posterior ranges. With regard to the corresponding hydraulic behaviour,
570 we observe in Figure 13 that the true water retention and unsaturated hydraulic conductivity
571 functions now lie well within the extent of the posterior curves. It is important to point out
572 that, despite the fact that a minimal amount of error inflation was done for this inversion
573 compared to the Gaussian- and informal-likelihood inversions, the posterior distributions are
574 broader, most notably for parameters K_s and θ_s . This results from the fact that (i) a signifi-
575 cant amount of residual energy is removed with our PCA-based correction before calculating
576 the likelihood; and (ii) there exist some incorrect model-parameter sets whose corresponding
577 parameter-error component of the residual will resemble (and will thus be identified as) model
578 error, leading to the parameter sets being accepted in the MCMC inversion procedure. This
579 latter important point is discussed in further detail in the following section.

580 [Figure 13 about here.]

581 3.5 Discussion

582 It is clear from the previous results that, in the context of the considered example problem,
583 our proposed correction for model error offers an effective means of overcoming the posterior
584 parameter bias related to use of a simplified forward model, thereby providing more accurate
585 and useful uncertainty estimates. We now attempt to gain further insight into the reason why,
586 with this correction, particular sets of incorrect model parameters may be accepted in the

587 MCMC procedure, which contributes to the broadening of the obtained posterior distribu-
588 tions. Figure 14 presents the results of an analysis of three different parameter sets, the first
589 row corresponding to the true subsurface VGM parameters (Table 1) and the last two rows
590 corresponding to random “test” sets of VGM parameters drawn from the prior distribution
591 (Table 3). In the columns of the figure we show (i) the predicted GPR-derived water-content
592 data assuming 1D vertical flow; (ii) the residual obtained by subtracting the “observed” data
593 in Figure 4a and expressing the results relative to the arrival time of the infiltration front;
594 (iii) the projection of this residual onto the model-error basis, which represents our estimate
595 of the model-error component of the residual; and (iv) the corresponding remainder, obtained
596 by subtracting the projection from the residual.

597 [Figure 14 about here.]

598 [Table 3 about here.]

599 We see in Figure 14 that, when the true set of VGM parameters is considered and thus
600 when the parameter-error component of the residual is zero (see equation (6)), projection of
601 the residual onto the model-error basis correctly identifies the model-error component, which
602 after subtraction leaves a low-amplitude remainder that is mostly comprised of Gaussian data-
603 measurement uncertainties. As the L_2 -norm of the remainder determines the likelihood, the
604 true parameter set stands a high chance of being accepted in MCMC. For the first (incorrect)
605 set of test model parameters, we observe that the corresponding residual, which now is com-
606 prised of non-zero model- and parameter-error components, closely resembles the model-error
607 realizations presented in Figure 5. Ideally, projection of this residual onto the PCA-derived
608 basis would isolate only the model-error component. However, in this case the entire residual
609 is identified as model error, which again results in a low-amplitude remainder and a corre-
610 spondingly high probability of acceptance. In other words, when the sum of the model- and
611 parameter-error components of the residual tends to look similar to the stochastic model-error
612 realizations, both of these components will be subtracted in our correction procedure, leading
613 to a high likelihood of an incorrect parameter set. Finally, for the last set of test model
614 parameters, we observe the intended functioning of the algorithm; the projection of the resid-

615 ual onto the model-error basis correctly identifies the model-error component, but leaves the
616 parameter-error component which then forms part of the remainder. The high amplitudes
617 observed in the remainder yield a low probability of the parameter set being accepted.

618 The fact that certain sets of incorrect model parameters, whose residuals under the 1D
619 flow assumption appear similar to the stochastic model-error realizations, are given a high
620 likelihood in our modified inversion procedure may be initially disconcerting. However, it must
621 be emphasized that, in any situation where parameter-related errors cannot be distinguished
622 from model errors, the corresponding model-parameter set cannot be rejected as a possibility.
623 Indeed, in this regard, our proposed algorithm should be viewed as a conservative stochastic
624 inversion approach in the presence of model error; if a residual appears to resemble model
625 error based on the generated model-error realizations, then the corresponding parameter set
626 should not be excluded from the Bayesian posterior distributions. The strong advantage of
627 our approach compared to not accounting for model error is that bias is strongly reduced and
628 the true parameter set becomes well represented by these distributions.

629 4 Conclusions

630 Building on the recent work of *Köpke et al.* (2018), we have presented in this paper a method-
631 ology for accounting for model errors in Bayesian-MCMC inversions that is geared towards
632 the common case where such errors arise from the use of an computationally efficient simpli-
633 fied forward model in place of a more accurate but computationally burdensome numerical
634 solution. Our approach is based on the analysis of a suite stochastic model-error realizations,
635 created before the MCMC iterations by running the simplified and full forward solvers to-
636 gether for randomly drawn model-parameter sets from the prior distribution, which leads to
637 the development of an orthonormal basis for the model error. Under the assumption that
638 the model errors for the considered problem can be well described by this basis and that
639 the model-error component of the residual lies orthogonal to the parameter-error and data-
640 measurement-error components, projection of the residual onto the basis identifies the model
641 error, which is then subtracted from the residual before evaluating the likelihood.

642 We saw through the considered example problem that application of our model-error cor-

643 rection, combined with an informal likelihood measure based on the expected behaviour of
644 the L_2 -norm, leads to a strong reduction in bias and notably better characterization of pos-
645 terior uncertainties. This comes at the cost of needing to perform a number of full forward
646 model runs (in our case a few thousand) to generate the model-error basis prior to MCMC.
647 Note again, however, that these full numerical simulations can be conducted in parallel. Our
648 approach represents a remarkable computational savings when compared to MCMC based
649 entirely on the full forward solver, in which hundreds of thousands of expensive model eval-
650 uations, conducted in series, would be necessary. For the specific example presented in this
651 paper involving 800,000 Metropolis iterations, use of the fully 3D Richards' equation solver
652 within MCMC would require over 900 days on a standard desktop computer. In contrast,
653 running our algorithm based on the 1D forward solver with model-error correction took less
654 that two weeks.

655 A critical assumption in our proposed approach is that of orthogonality between the
656 model- and parameter-error components of the residual. As much as our experience until
657 now suggests that this will be approximately true in many cases, hence explaining the success
658 of our method, it cannot be proven and we observed that some incorrect model-parameter
659 sets may produce a residual that looks like model error. In the latter cases, the model- and
660 parameter-error components of the residual cannot be distinguished by projecting onto the
661 basis and the parameter sets will stand a good chance of being accepted. In our view, this is
662 not a concern as it simply means that the posterior parameter distributions will be broadened
663 to include such parameters; i.e., our approach will conservatively include the parameters as
664 possibilities. However, if this behaviour is undesirable, a two-stage MCMC algorithm could
665 be proposed in which our approach would be used in a first accept/reject phase to effectively
666 filter out unreasonable parameter sets from being tested with the full numerical solution,
667 albeit at greatly increased computational cost.

668 It must be emphasized that the approach described herein is only intended for known
669 sources of model error, for which random realizations of the error can be generated and used
670 to help identify the model-error component of the residual. Although this will often be the
671 major source of bias for inverse problems in geophysics and hydrology, there are situations

672 where even our best forward solution will not provide a good enough description of the physical
673 process involved. In the case of such unknown or unspecified model errors, our methodology
674 can still be expected to effectively deal with the model errors for which it was intended,
675 thereby providing more reliable posterior uncertainty estimates. Another related issue is the
676 fact that, for many problems, particularly those of high dimension with spatially distributed
677 parameters, the nature of the model errors may change significantly over the model parameter
678 space and it may not be possible to effectively describe them using a single global basis. In this
679 case, the work of *Köpke et al.* (2018) shows that a KNN dictionary-based approach to model-
680 error identification, whereby the basis is constructed locally at each MCMC iteration, can be
681 a highly effective means of obtaining reliable posterior parameter distributions when using an
682 approximate forward solver. It is also likely that the computational efficiency of the approach
683 of *Köpke et al.* (2018) can be further improved by using parallel computation within the
684 MCMC procedure to generate local model-error realizations simultaneously. Finally, future
685 work should investigate whether the approach proposed in this paper might be adapted for
686 use with gradient-based MCMC methods employing an adjoint solver based on the simplified
687 forward model.

688 **Acknowledgments**

689 This work was supported by a grant to J. Irving from the Swiss National Science Foundation,
690 grant number 200021-140864. The authors also wish to thank Richard Healey from the
691 U.S. Geological Survey for support with the VS2D software during the initial stages of this
692 research project.

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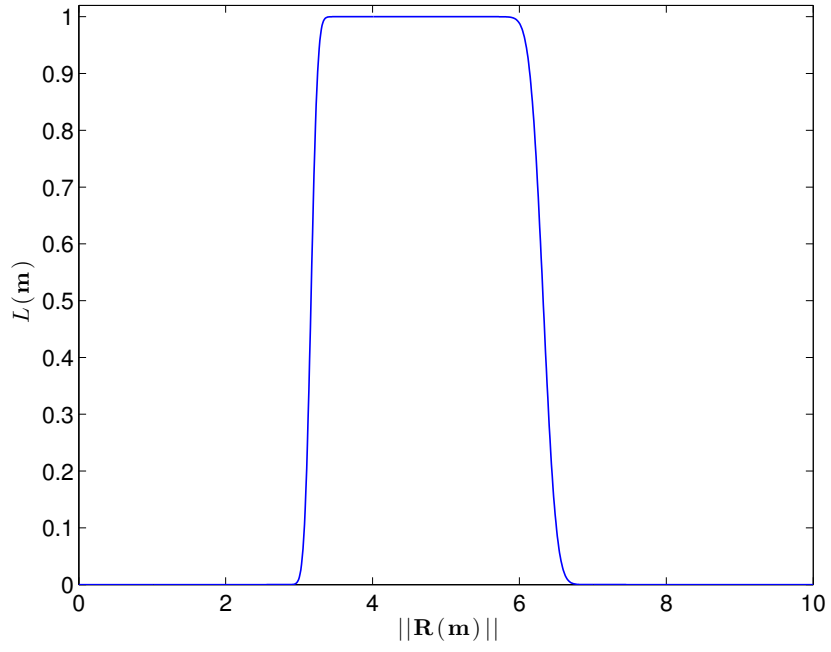


Figure 1: Normalized ℓ_2 -norm likelihood given by equation (9) as a function of $\|\mathbf{R}(\mathbf{m})\|$ for $N = 1000$ with $s_{R_1} = 0.1$ and $s_{R_2} = 0.2$.

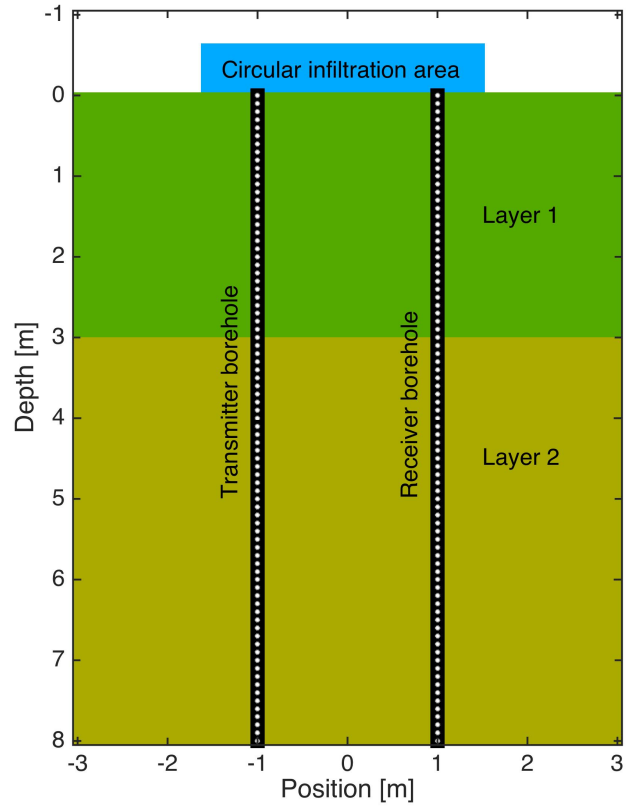


Figure 2: Setup for the synthetic infiltration experiment considered in this study. The white dots represent transmitter and receiver antenna positions for the ZOP GPR measurements.

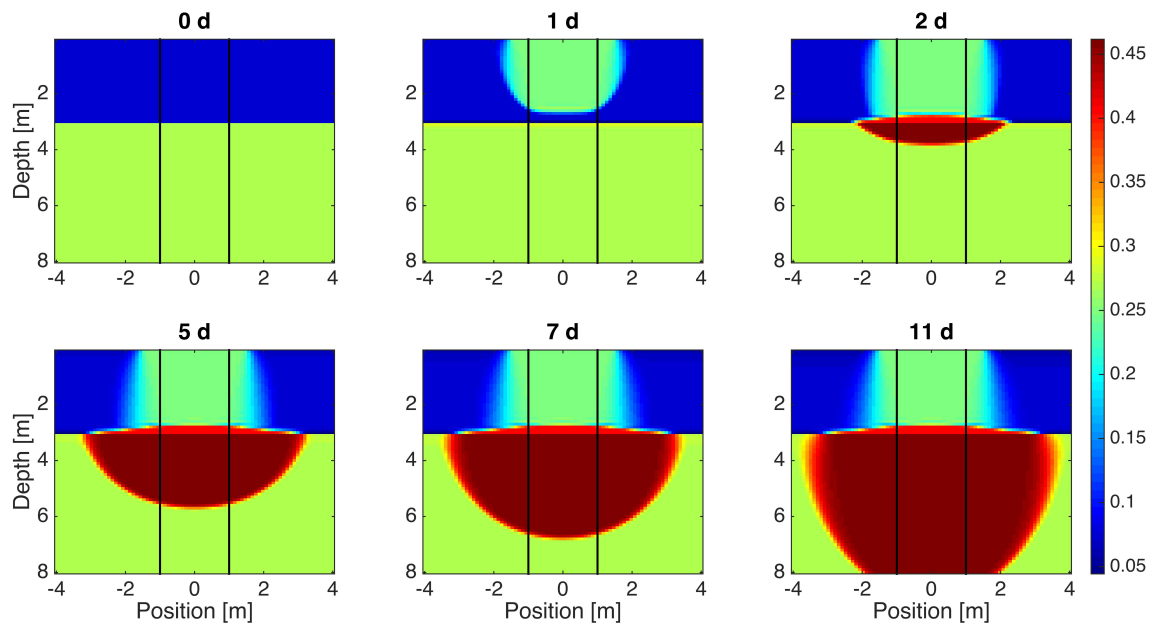


Figure 3: Spatial distribution of water content in the subsurface at various times throughout the infiltration experiment. The GPR boreholes are shown for reference.

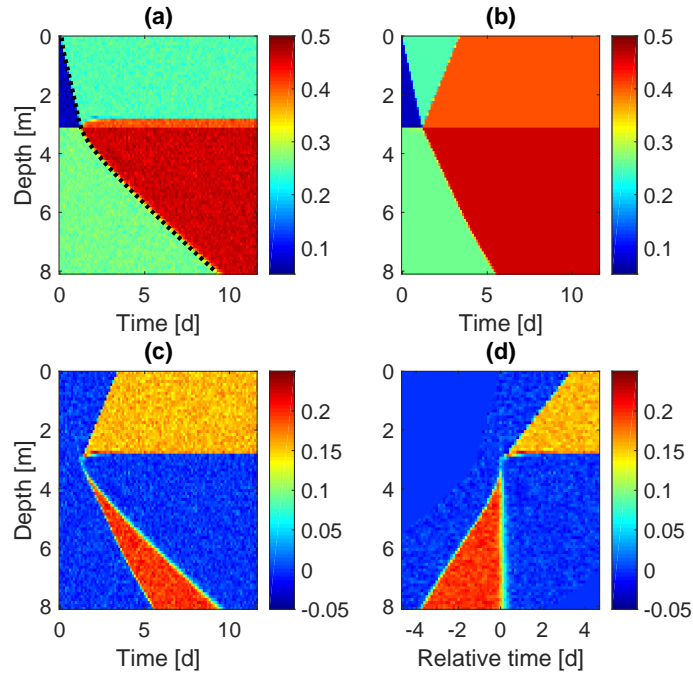


Figure 4: (a) Average soil water content between the boreholes as a function of depth and measurement time, computed using a 3D infiltration model with the addition of Gaussian measurement noise, representing the synthetic data to be inverted for the VGM parameters in Table 1. The arrival time of the infiltration front as a function of depth is indicated with a black dashed line. (b) Corresponding water-content distribution obtained assuming purely vertical (1D) flow. (c) Difference (b)-(a), which is equal to the sum of the model error and measurement uncertainties. (d) Error image from (c) expressed relative to the arrival time of the infiltration front in (a).

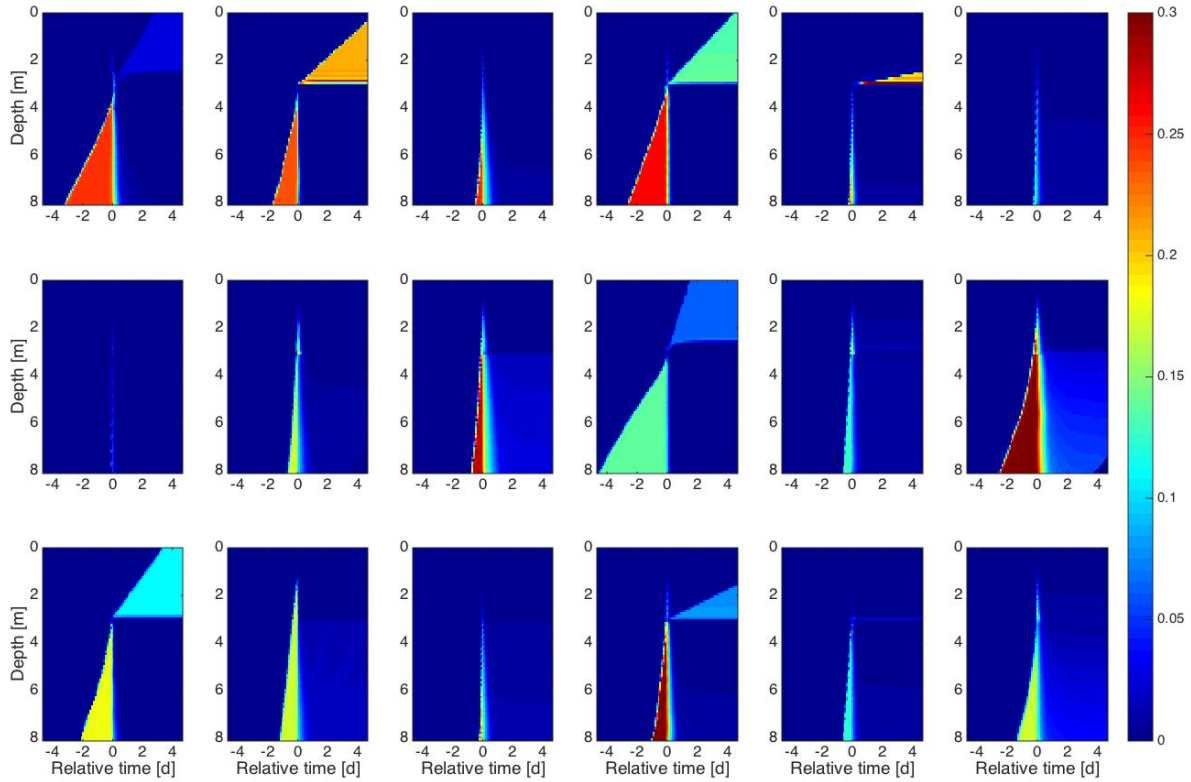


Figure 5: Example stochastic realizations of the model error corresponding to random sets of VGM parameters drawn from the prior distributions in Table 2. For greater coherency between the images, each has been expressed relative to the arrival time of the infiltration front in depth as observed in the 3D flow simulation. A total of 6500 realizations were generated to construct the model-error basis.

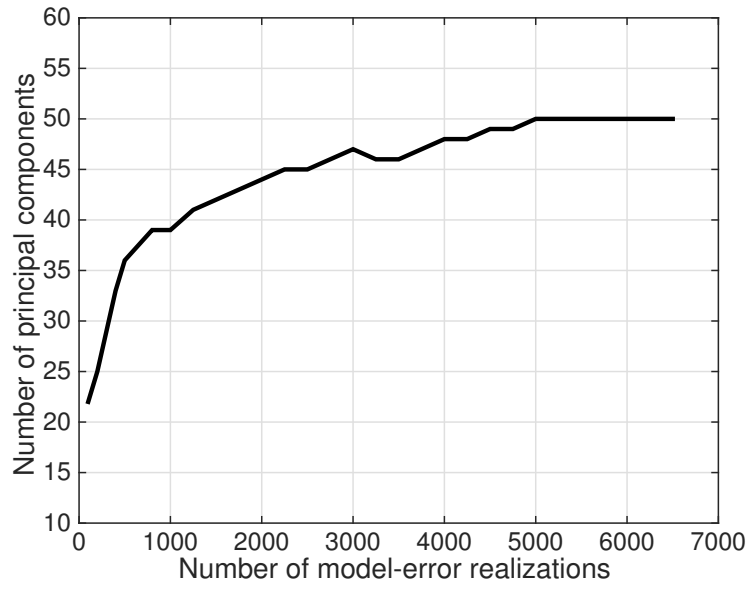


Figure 6: Number of principal components needed to capture 98% of the variance of the model-error realizations as a function of the number of realizations considered.

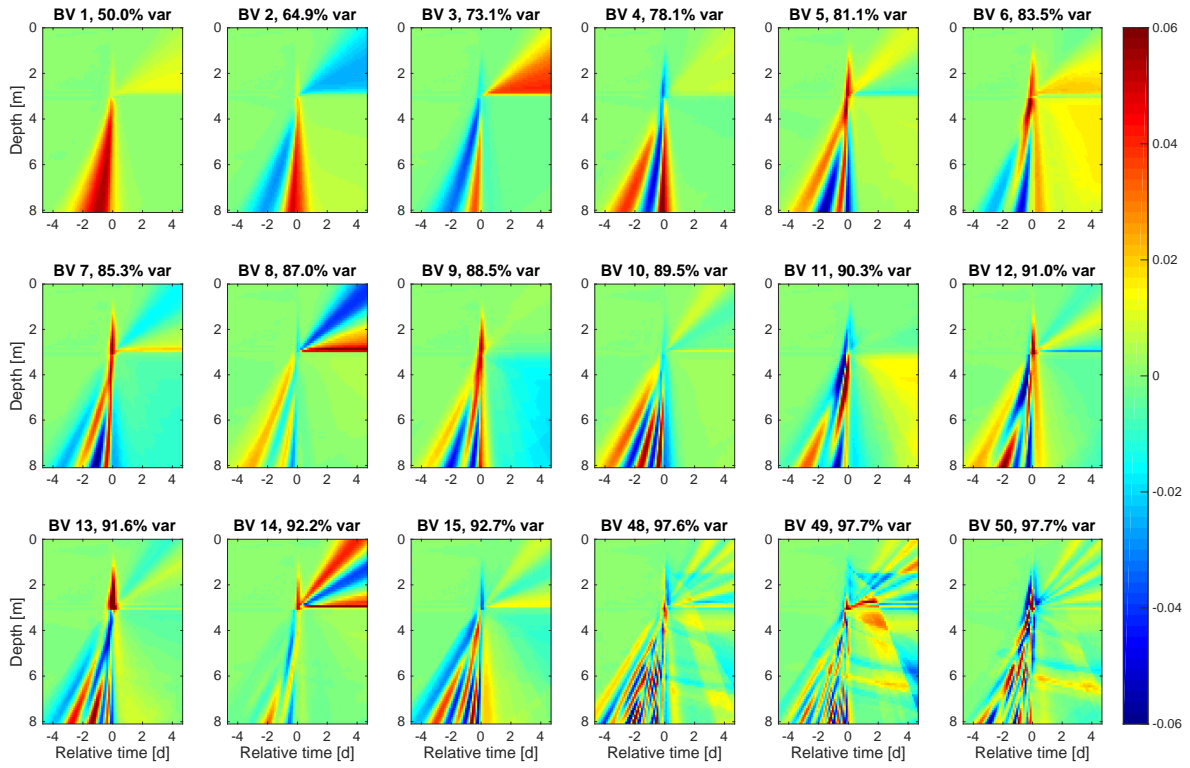


Figure 7: The first 15, and the last 3, of 50 model-error basis vectors, arranged in decreasing order with respect to their contribution of the total variance. The vectors were obtained by performing PCA on the set of 6500 stochastic model-error realizations. Each vector is plotted as an image with the cumulative contribution to the variance noted in the title.

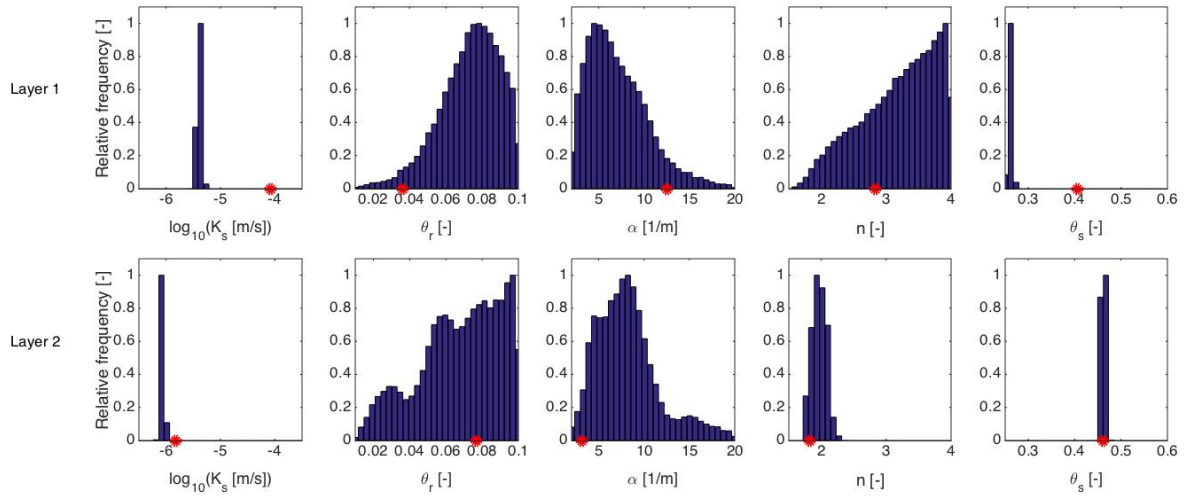


Figure 8: Marginal posterior histograms for the VGM parameters in each soil layer, obtained through MCMC sampling using an inflated Gaussian likelihood function for the residuals with no model-error correction. The red dots indicate the true parameter values. The limits of the horizontal axis on each plot represent the prior uniform parameter bounds.

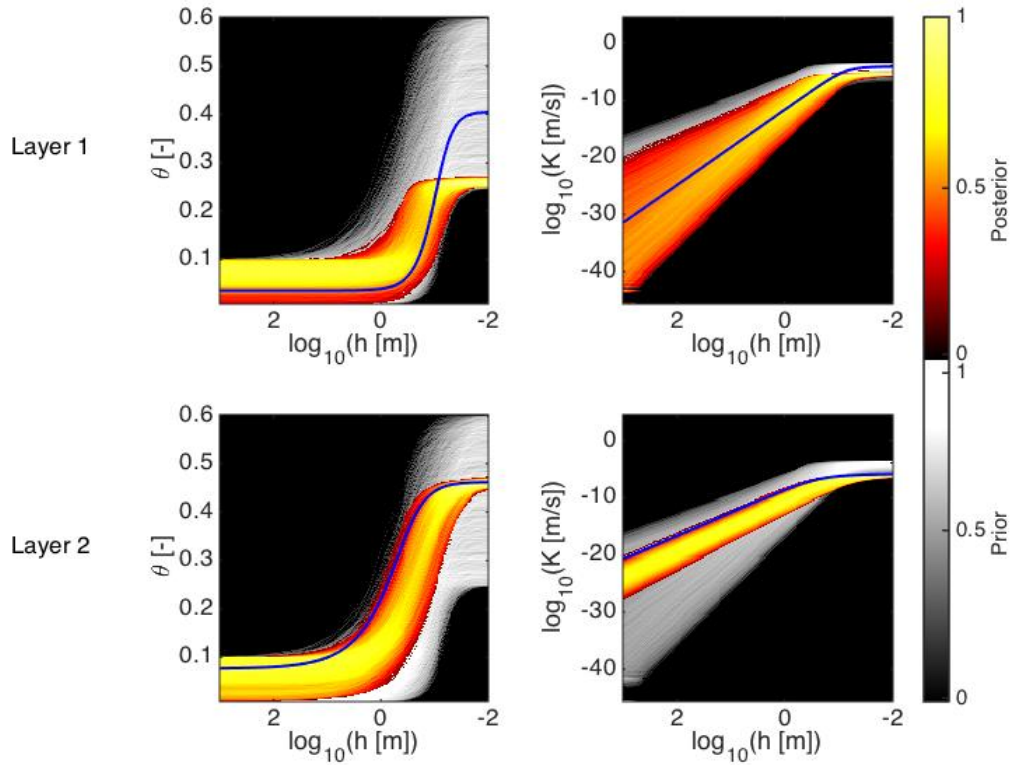


Figure 9: Water retention (left) and unsaturated hydraulic conductivity (right) functions for each soil layer corresponding to the prior distribution (gray; Table 2) and the posterior distribution obtained using an inflated Gaussian likelihood function for the residuals with no model-error correction (color; Figure 8). The blue lines represent the curves corresponding to the true parameter set in Table 1. The prior and posterior results are expressed in terms of curve densities.

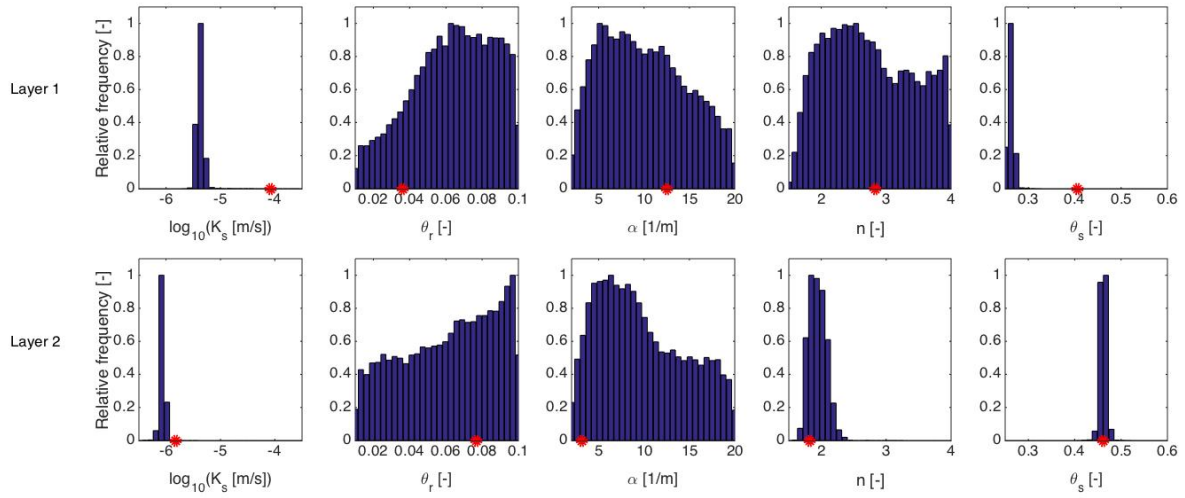


Figure 10: Marginal posterior histograms for the VGM parameters in each soil layer, obtained through MCMC sampling using an L_2 -norm-based likelihood measure for the residuals with no model-error correction (see text for details). The red dots indicate the true parameter values. The limits of the horizontal axis on each plot represent the prior uniform parameter bounds.

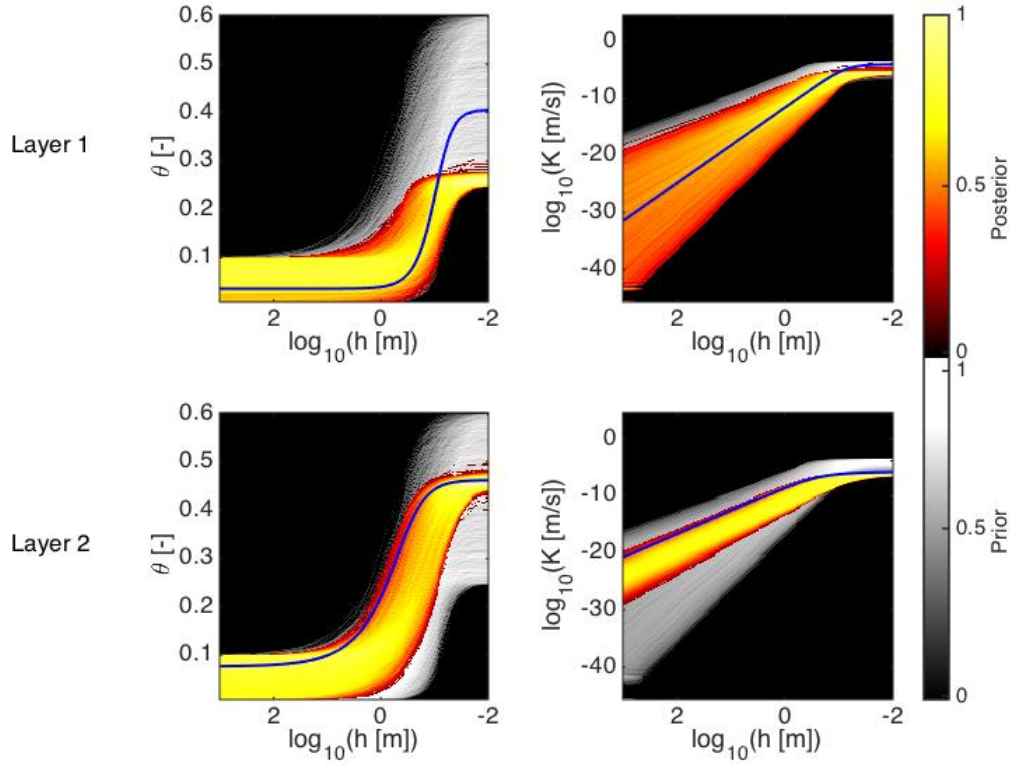


Figure 11: Water retention (left) and unsaturated hydraulic conductivity (right) functions for each soil layer corresponding to the prior distribution (gray; Table 2) and the posterior distribution obtained using an L_2 -norm-based likelihood measure for the residuals with no model-error correction (color; Figure 10). The blue lines represent the curves corresponding to the true parameter set in Table 1. The prior and posterior results are expressed in terms of curve densities.

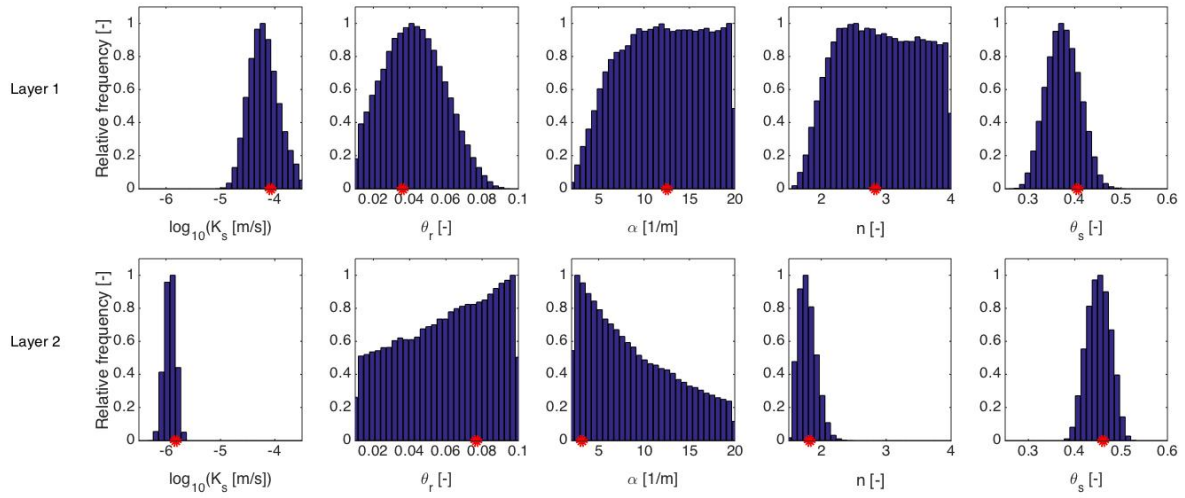


Figure 12: Marginal posterior histograms for the VGM parameters in each soil layer, obtained through MCMC sampling using an L_2 -norm-based likelihood measure for the residuals after correcting for model error (see text for details). The red dots indicate the true parameter values. The limits of the horizontal axis on each plot represent the prior uniform parameter bounds.

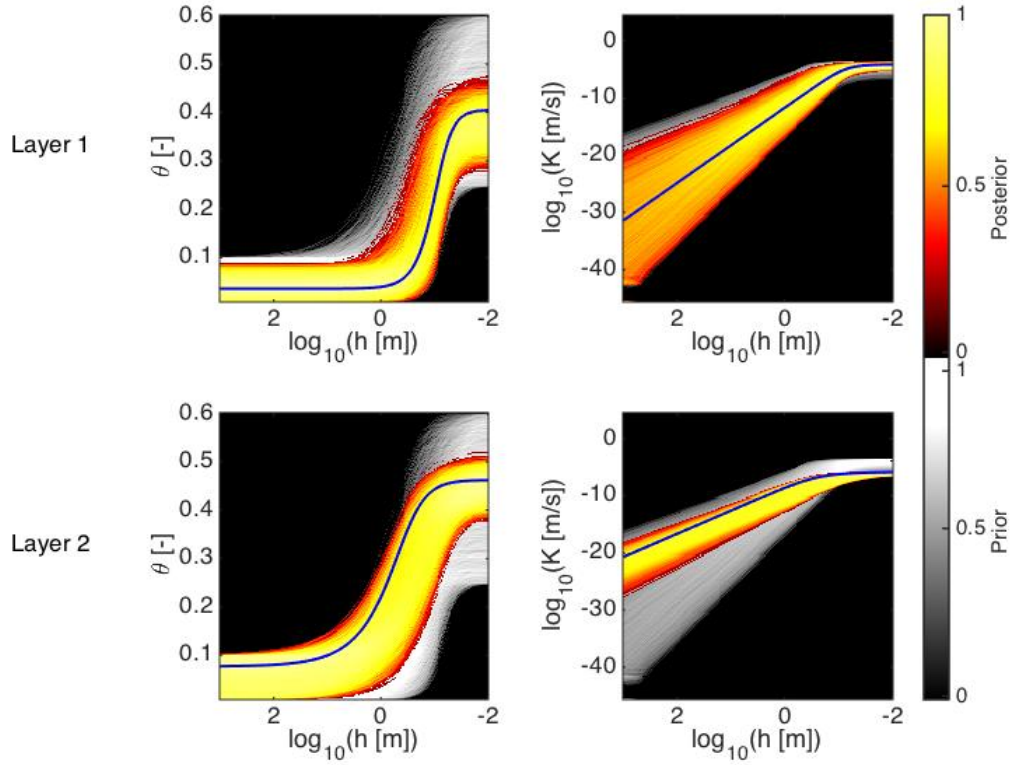


Figure 13: Water retention (left) and unsaturated hydraulic conductivity (right) functions for each soil layer corresponding to the prior distribution (gray; Table 2) and the posterior distribution obtained using an L_2 -norm-based likelihood measure for the residuals after correcting for model error (color; Figure 12). The blue lines represent the curves corresponding to the true parameter set in Table 1. The prior and posterior results are expressed in terms of curve densities.

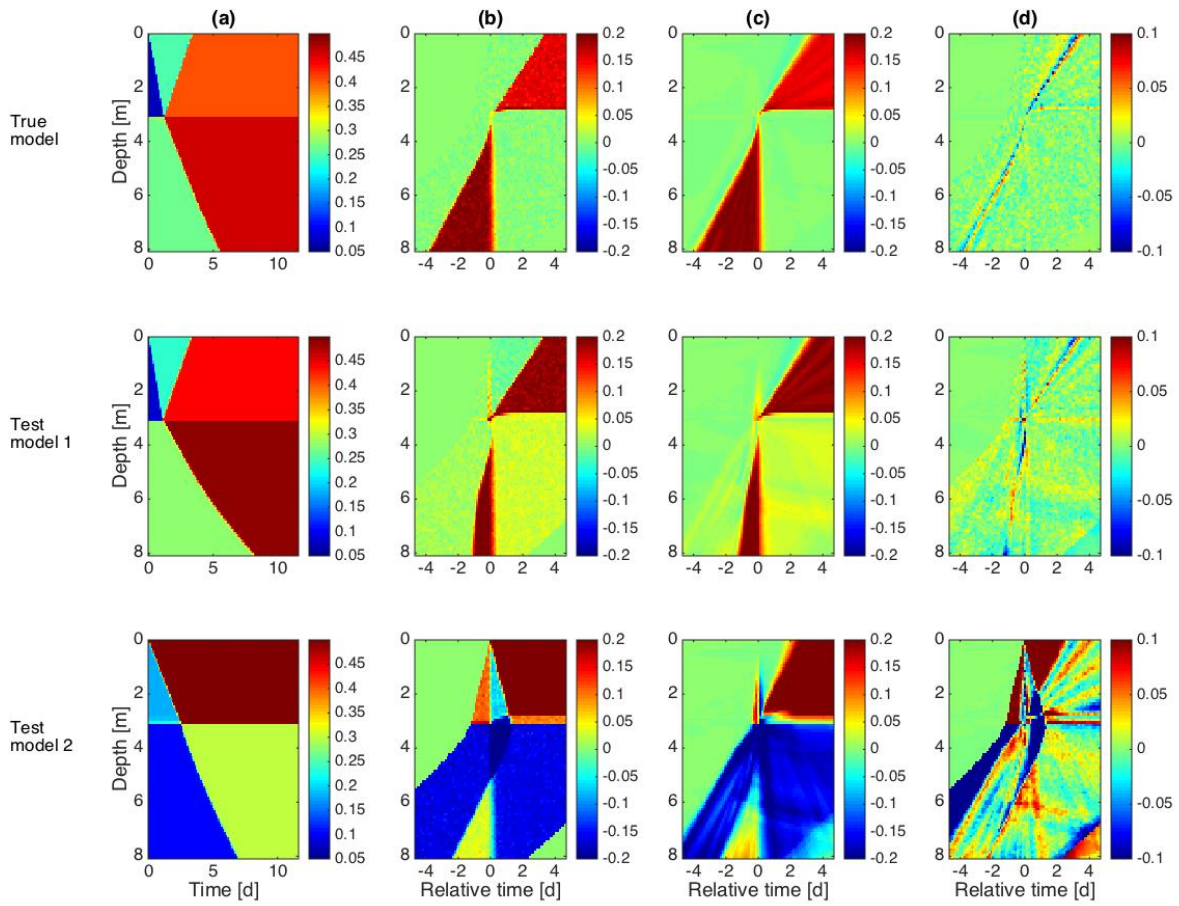


Figure 14: For the true set of VGM parameters (Table 1) and two sets of incorrect “test” model parameters (Table 3): (a) Predicted water content assuming 1D vertical flow; (b) Residual obtained by subtracting the synthetic data in Figure 4a from the results in (a) and expressing relative to the arrival time of the infiltration front observed in the data; (c) Projection of the residual in (b) onto the model-error basis; (d) Corresponding remainder (b)-(c).

	$\log_{10}(K_s \text{ [m/s]})$	$\theta_r \text{ [-]}$	$\alpha \text{ [1/m]}$	$n \text{ [-]}$	$\theta_s \text{ [-]}$
Layer 1	-4.074	0.036	12.552	2.830	0.405
Layer 2	-5.826	0.077	3.165	1.819	0.462

Table 1: VGM parameters considered for the 2-layer synthetic example.

	$\log_{10}(K_s \text{ [m/s]})$	$\theta_r \text{ [-]}$	$\alpha \text{ [1/m]}$	$n \text{ [-]}$	$\theta_s \text{ [-]}$
Lower bound	-6.500	0.010	2.000	1.500	0.250
Upper bound	-3.500	0.100	20.000	4.000	0.600

Table 2: Lower and upper bounds of the uniform Bayesian prior distributions assumed for the VGM parameters in each layer.

		$\log_{10}(K_s \text{ [m/s]})$	$\theta_r \text{ [-]}$	$\alpha \text{ [1/m]}$	$n \text{ [-]}$	$\theta_s \text{ [-]}$
Test model 1	Layer 1	-3.950	0.050	5.600	3.500	0.440
	Layer 2	-6.030	0.060	4.100	1.900	0.490
Test model 2	Layer 1	-5.300	0.080	7.000	2.600	0.500
	Layer 2	-5.700	0.030	10.000	3.000	0.300

Table 3: VGM parameters corresponding to the two test models considered in Figure 14.