Hydrologic Process Parameterization of Electrical Resistivity Imaging of Solute Plumes Using POD McMC

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ABSTRACT

Markov chain Monte Carlo (McMC) techniques are widely used in geophysics due to their ability to recover multiple probable outcomes that enable uncertainty assessment. Standard McMC methods, however, become computationally intractable in high dimensionality spaces. We present a McMC approach based on a sparse proper orthogonal decomposition (POD) model parameterization that implicitly incorporates the physics of the underlying process.

First, we construct POD bases that are tuned to the hydrologic process of interest. A small number of basis vectors can represent most of the variability in the target process, leading to dimensionality reduction with estimation of small number of POD coefficients compared to the size of the full dimensionality space.

We demonstrate the performance of the algorithm with synthetic electrical resistivity imaging of unimodal and bimodal solute plumes. The unimodal plume is consistent with the hypothesis underlying the generation of the POD bases whereas bimodality in plume morphology was not theorized. The same set of basis vectors were, however, employed in both reconstructions. We show that McMC can proceed in the reduced dimensionality space while accounting for the physics of the underlying process.

INTRODUCTION

- Geophysical estimation of mass and solute plume morphologies is becoming increasing popular for numerous hydrogeological investigations including optimal design of contaminant remediation schemes and estimation of transport parameters.
- Geophysical estimation involves inherent uncertain inputs due to limited noisy measurements with incomplete understanding of subsurface processes.
- Markov chain Monte Carlo (McMC) methods enable uncertainty assessment of geophysical estimation in light of the inherent uncertain inputs.

THE PROBLEM

Standard McMC become computationally intractable in high dimensional problems, such as in spatially distributed large 2D and 3D systems.

- This research presents an McMC version of the Proper Orthogonal Decomposition (POD)-based inversion algorithm (*Oware et al.*, 2013; *Oware and Moysey*, 2014).
- The POD-based inversion parameterizes the problem in the reduced dimensionality space using small number of optimal basis vectors tuned to the target process as projection vectors.
- Hence, a small number of inversion parameters are estimated, making McMC in high dimensionality spaces feasible while accounting for the physics of the underlying process.

METHODS

REFERENCE SIMULATION

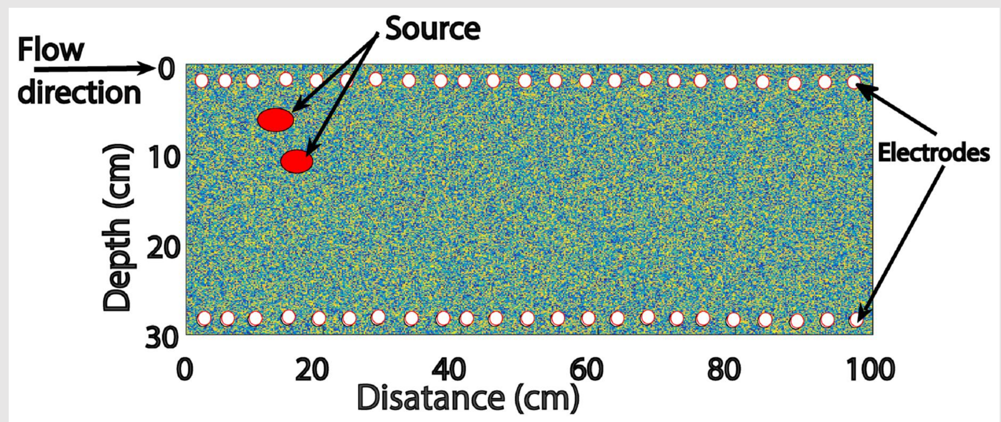


Figure 1: Schematic illustration of the experimental setup of the 2-D flow and transport in a random field. The synthetic reference simulation was inspired by a corresponding lab-scale setup (lab-scale results not presented here). The horizontal borehole orientation was used to provide good aspect ratio for the resistivity survey while enabling a long horizontal tracer migration field.

- Flow and transport simulated using a code written in MATLAB.
- A single and double sources were used to simulate unimodal and bimodal target plume morphologies, respectively (Fig. 2).

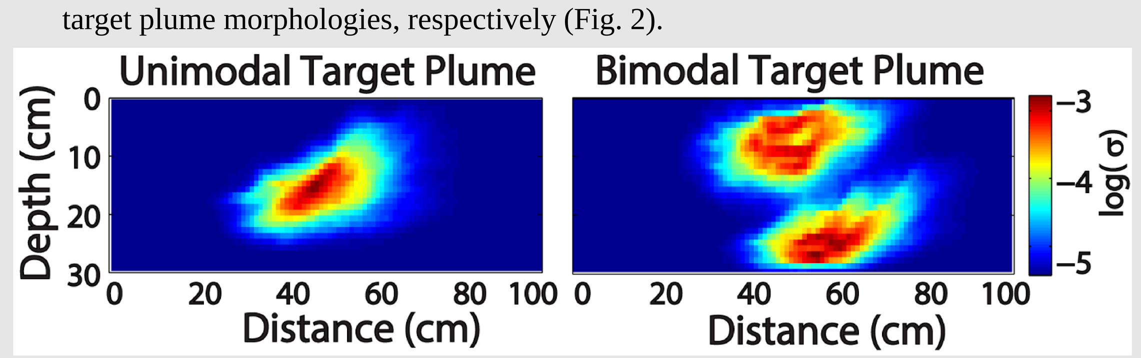


Figure 2: Unimodal and bimodal target plume.

- Circulating dipole-dipole was employed to acquire 1788 quadruples. The data were corrupted with uncorrelated Gaussian noise with standard deviation proportional to 3% of the data values.
- FW2_5D [*Pidlisecky and Knight*, 2008] was used for the resistivity forward simulations.

DETAILS OF THE POD McMC ALGORITHM

- Fig. 3 presents the workflow for the proposed POD McMC algorithm.
- The POD plumes (Fig. 4) are constructed from POD decomposition of training images (TIs) that mimic a single solute source transport process in a random field.
- A projection of the TIs into the reduced optimal basis space produces $\mathbf{c}_{prior}$ from which prior standard deviations (or variances) for each coefficient are estimated. For instance, 400 TIs will result in 400 realizations of each coefficient, producing prior distributions for each coefficient (Fig. 5).
- The starting or reference coefficient ($\mathbf{c}_0$) structure is obtained from a projection of a homogenous background model into the basis space.
- The Gaussian nature of the histograms in Fig. 5 supports the assumption of a prior Gaussian model, N(0,1), for the coefficient re-simulation.
- A sampling window is employed to re-simulate a subset of the total coefficients at each iteration. The sampling window grows at a specified rate to incorporate more information as iteration progresses starting from the coefficients of the low-order bases to those of the least informative bases.
- Posterior samples are obtained only after the window grows fully and all the coefficients are resampled jointly.

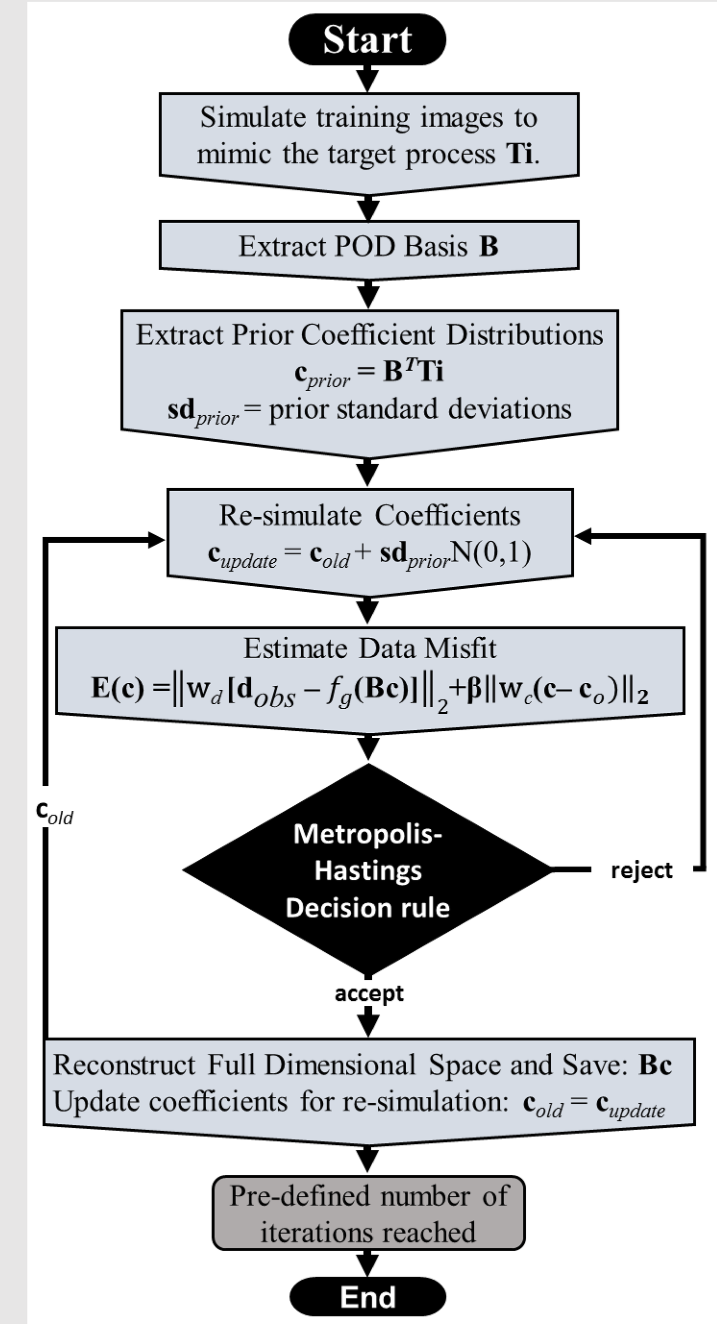


Figure 3: Flow chart of the POD Monte Carlo Method

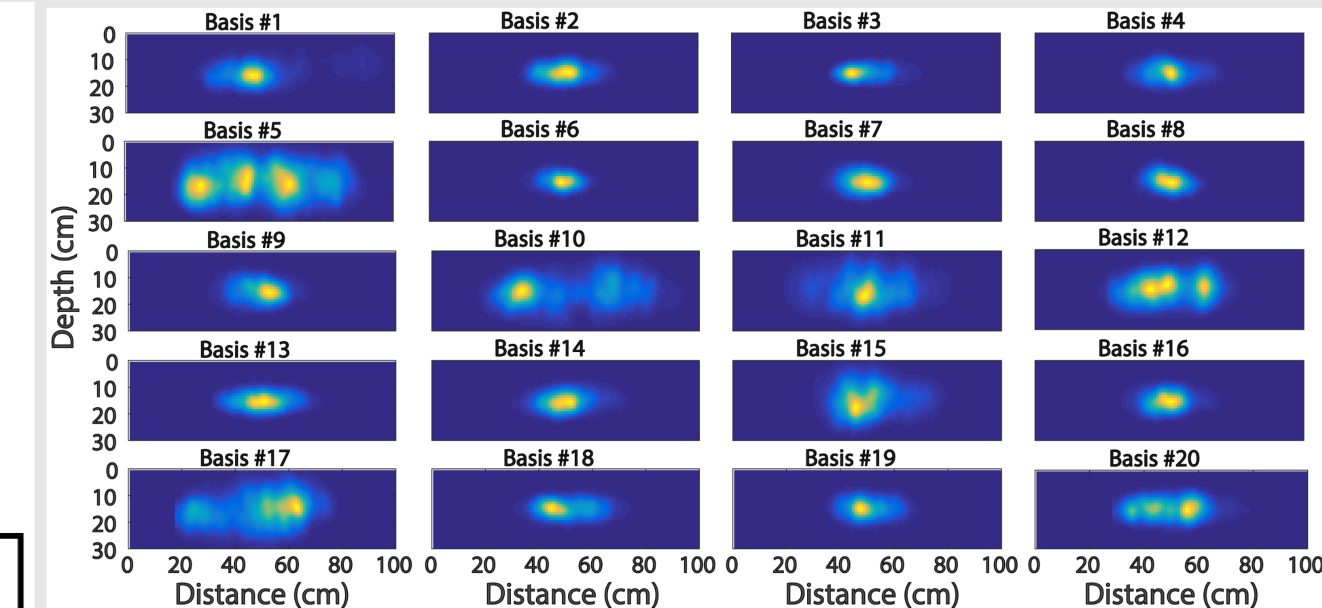


Figure 4: The first 20 principal POD basis (POD plumes) constructed from training images under the assumption of a single source transport process.

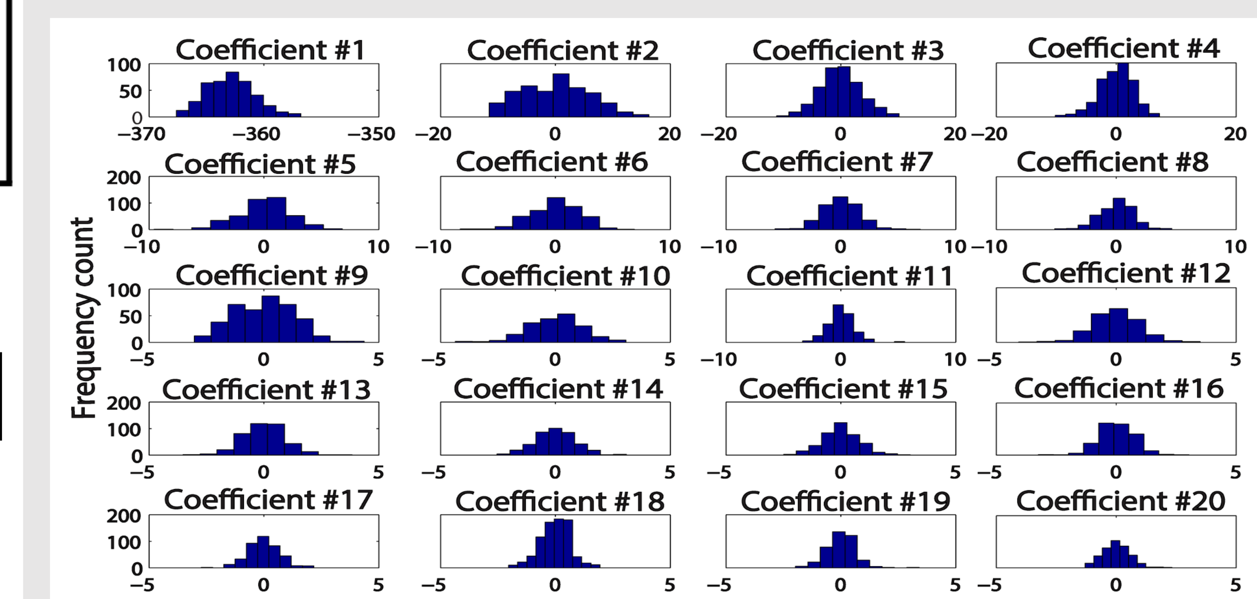


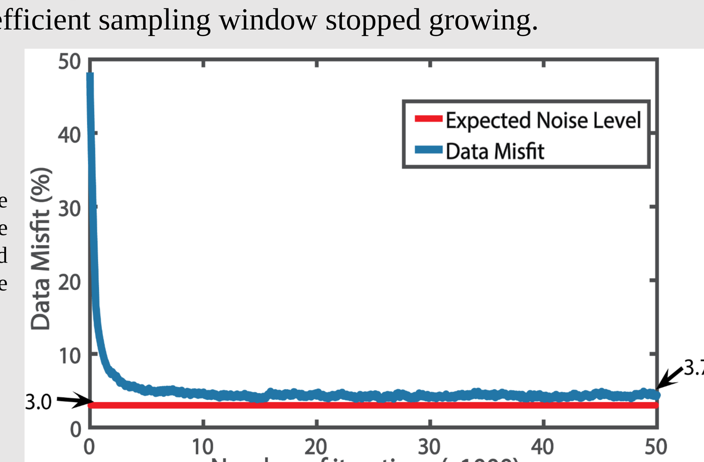
Figure 5: Histogram plots of prior coefficients ($\mathbf{c}_{prior}$) corresponding to the 20 principal POD plumes in Fig. 4.

RESULTS

INVERSION RESULTS FOR THE UNIMODAL TARGET PLUME WITH ACCURATE PRIOR ASSUMPTIONS

- The algorithm was ran for 50,000 iterations and seems to burn-in rapidly (Fig. 6). The starting data misfit was around 50% which reduced to a stationary level of about 3.7% compared to the expected error level of 3%.
- The posterior samples were considered from 30,000 to 50,000 when the coefficient sampling window stopped growing.

Figure 6: A plot of the sampling path of the data misfit compared to the expected noise level.



- Qualitative comparison of the posterior mean and the realizations suggest the target plume was accurately estimated with minimal plume smearing (Fig. 7).
- The consistency of the prior assumption in the unimodal test case is captured in the estimated seemingly low standard deviations.

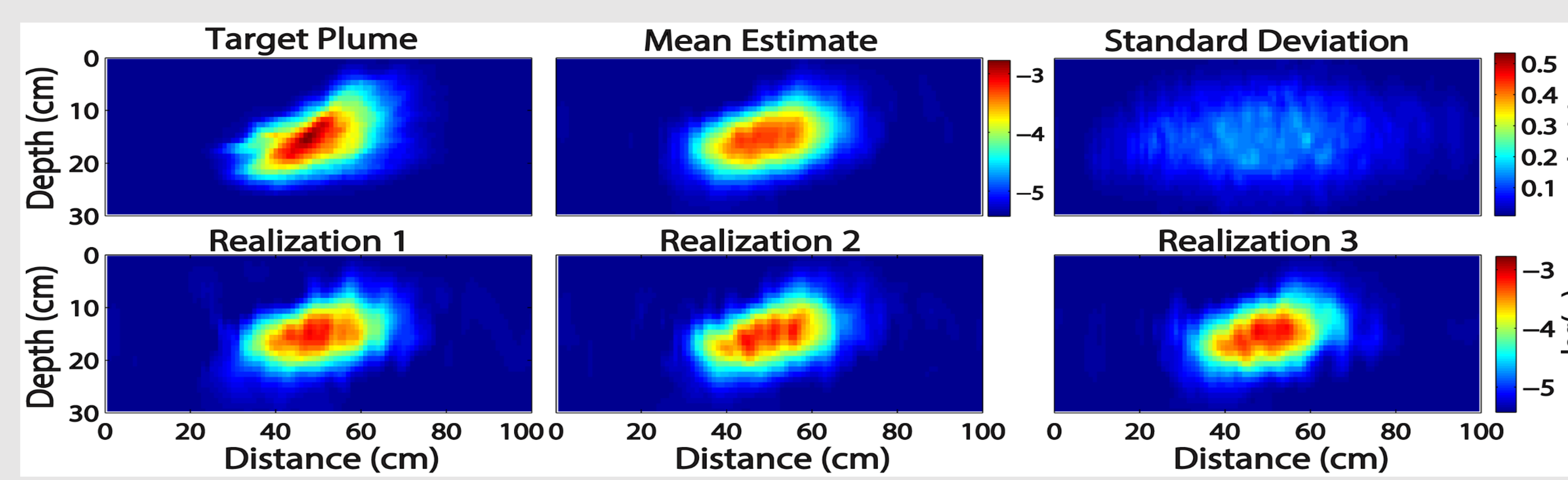
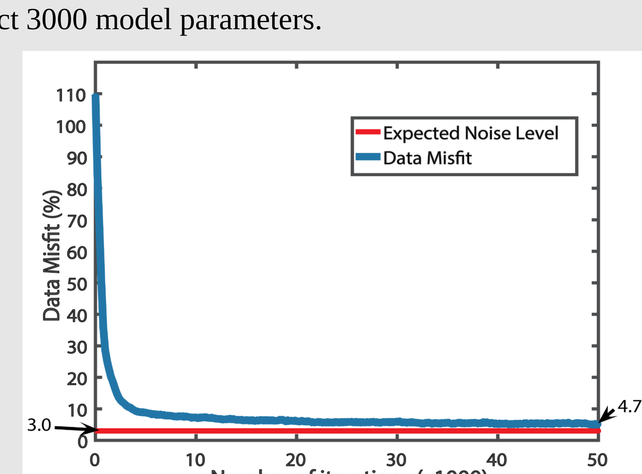


Figure 7: Inversion results for the unimodal plume test case in which the prior information is consistent with the conceptual model.

INVERSION RESULTS FOR THE BIMODAL TARGET PLUME WITH INACCURATE PRIOR ASSUMPTIONS

- The starting data misfit was around 110% which reduced to an asymptotic level of about 4.7% compared to the expected error level of 3% (Fig. 8). The high starting misfit and the high equilibrium error level compared to those of the unimodal case are attributable to the inaccurate prior hypothesis in the bimodal test case.
- The algorithm required less than 2 hours of computational time to complete the 50,000 iterations, estimating 300 coefficients to reconstruct 3000 model parameters.

Figure 8: A plot of the sampling path of the data misfit compared to the expected noise level.



- Although bimodality was not conceptualized, the algorithm was able to recombine the basis vectors in a manner that captured the bimodality in the target to fit the resistivity measurements (Figs. 8 and 9).
- Qualitative comparison of the posterior mean and the realizations with the target plume reveal the background region in between the two plumes were not properly resolved, which is reflected as high uncertainty region in the standard deviation estimation.
- The overall high uncertainty associated with the reconstruction of the bimodal plume compared to that of the unimodal plume (Figs. 7 and 9) is plausibly due to the inaccuracy of the prior assumption in the bimodal test case.

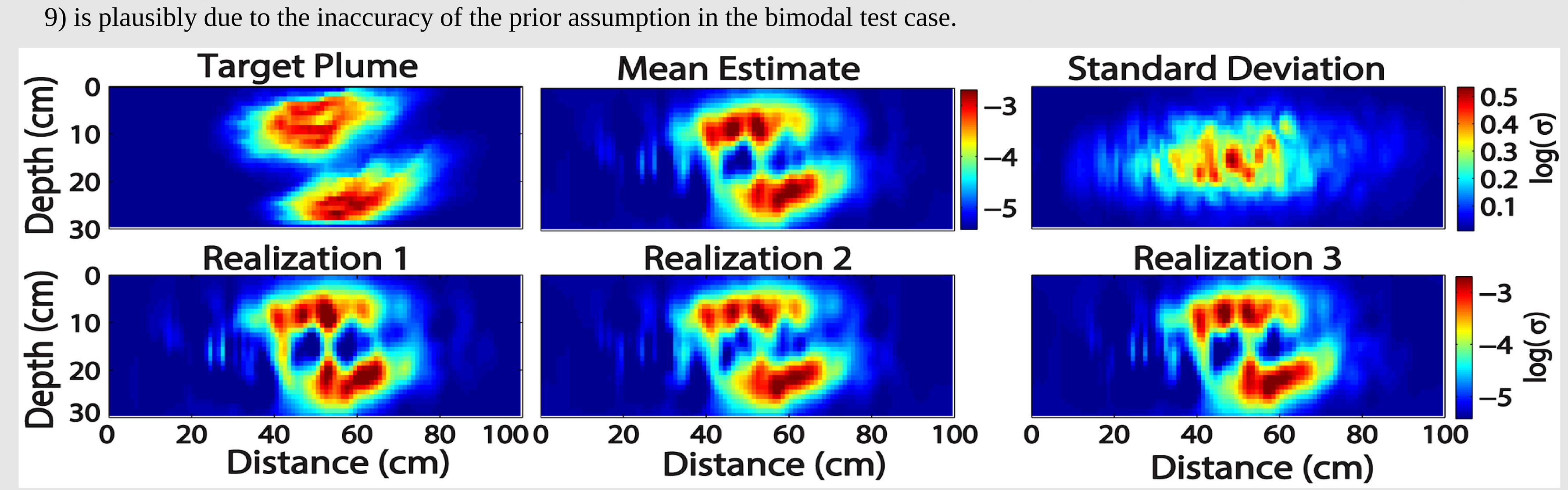


Figure 9: Inversion results for the bimodal plume test case in which the prior information is inconsistent with the conceptual model.

CONCLUSIONS

- We have demonstrated that McMC can be parameterized in the reduced dimensionality space while accounting for the physics of the underlying process.
- We were able to accurately capture plume morphology even if the conceptual model is not completely accurate or fully developed. Nevertheless, accurate prior information reduces uncertainty in the estimation.
- The algorithm was found to be computationally efficient, operating at 90% truncation in the dimensionality of the problem, i.e., 300 coefficients were estimated to reconstruct 3000 full dimensionality space.

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Pidlisecky, A., and R.J. Knight (2008), FW2_5D: A MATLAB 2.5-D electrical resistivity modeling code. *Computers & Geosciences*, 34(12), 1645-1654.