U.S. Department of Energy Office of Science

Environmental Remediation Sciences Program

INTEGRATED FIELD RESEARCH CHALLENGE SITE
Hanford 300 Area

Data Assimilation for Saturated Zone Hydraulic Conductivity Model and Future Plans

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Background

Our team focuses on development of the hydrologic model of the site through assimilating of the various types of data collected at the site, including data from boreholes and from a variety of tests and surveys.

Our efforts proceed along two complimentary lines of research. The first line is the development of a new approach for data inversion and assimilation called Method of Anchored Distributions (MAD, Rubin et al., 2009) and the numerical code needed for its implementation. The MAD framework is presented in Box 2.

The second line is the implementation of MAD to the Hanford IFRC site, which is a unique research site for studying and developing state-of-the-art inverse models because of the diversity of data types being acquired and the multiple experiments being conducted at the site. These two elements combined offer unprecedented opportunities for testing and improving MAD and answering fundamental questions related to 3D hydrogeological and geochemical characterization.

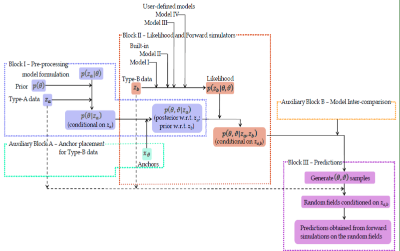
Our implementation efforts thus far focused on assimilating data from (1) the constant-rate injection tests, (2) the electromagnetic borehole flow meter (EBF) data, and (3) the March 2009 tracer test. Results from this effort are presented in Box 3. The implementation effort included linking MAD with the flow and transport code PFLOTRAN.

Theoretical Development

Our primary achievement on the theoretical side is the development and implementation of a new theory for stochastic inverse modeling and uncertainty quantification – MAD. MAD is built to assimilate multiple types of data that are collected at multiple observation scales, and that are related directly or indirectly to the target variables (e.g., conductivity, porosity). The data are assimilated using a Bayesian framework, and the end product is a series of 3D realizations of the conductivity field.

The significant points of departure of MAD from the current concepts are as follows:

1. It employs a theoretically sound method for moving information across multiple scales of observations and for reducing the dimensionality of the inverse model.
2. It does not require limiting assumptions (e.g., Gaussianity) with regard to the statistical distributions of parameters.
3. It does not rely on mathematical constraints (e.g., regularization or optimization) to ensure the stability of the inverse problem. Consequently, it provides an unbiased estimate of the uncertainty.
4. It is modular, which means that it is not linked to any forward modeling tool. MAD's modular structure is summarized in the diagram.

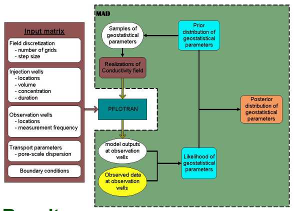


Assimilation of Experimental data at the IFRC Site

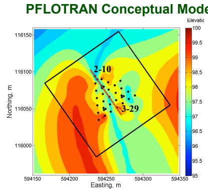
Data Assimilated:

- Constant-rate injection tests and EBF data (the posterior distribution obtained serves as prior to the tracer test)
- Tracer experiment data conducted in March of 2009 (it produces posterior distributions in results)

PFLOTRAN Integrated into MAD



PFLOTRAN Conceptual Model



Domain: 120m×120m×10m

Grid Size: 2m×2m×0.5m

Max Time Step: 1 hour

Simulation Time: 250 hours

Boundary Conditions: Transient fluctuating head

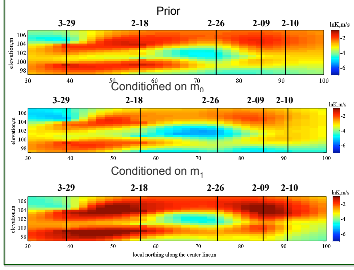
Wallclock Time: ~40min for 1 realization on a single processor core

Simulations were performed using the massively parallel reactive flow and transport code PFLOTRAN developed under the SciDAC-2 program. The code was run on LBNL's Franklin Cray XT4 supercomputer at the NERSC facility making use of PFLOTRAN's unique multi-realization simulation capability for running multiple simultaneous simulations utilizing multiple processor cores per realization.

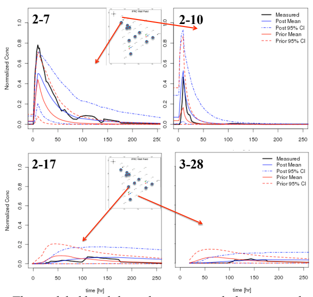
Results

Conditional Hydraulic Conductivity Fields

- Demonstrates high-low-high vertical profile along the center of the well field
- This profile is enhanced after tracer data is assimilated



Tracer Breakthrough Curves



- The modeled breakthrough curves match the measured ones better after assimilating the tracer data

Technical Challenges and Near-Term Plans

Technical issues:

- Accurate specification of boundary conditions (e.g. interpolation between wells)
- Coupled modeling of saturated and unsaturated zones.
- Accurate modeling of vertical flows in wells.

Near-term plans:

- Assess optimal strategies for the likelihood function (e.g. which temporal moment or combination of moments of the breakthrough curves to use? OR time-series representation?)
- Add porosity to the list of target variables.
- Incorporate lithology information into MAD, possibly through the use of soft conditioning.

Future Research

We plan to pursue research questions related to 3D hydrogeological and geochemical characterization:

- How to improve site characterization using data from tracer experiments? Specifically, how to benefit from concentration measurements, as opposed to relying on aggregate measures of spatial spread?
- How to improve site characterization using data from geophysical surveys? Specifically, how to benefit from coupling data from resistivity surveys with hydrologic data in light of the large uncertainty associated with petrophysical models and the difficulty in scaling them from the lab to the field?
- How to quantify uncertainty accurately, and how much uncertainty can be tolerated such that the research hypotheses of this project could be accepted with confidence?
- Given the high computational cost of 3D data interpretation, can we develop and implement a method for continuous updating of parameter estimates and uncertainty, building upon previous updates, as increasing amount of information become available?

References

Rubin Y., X. Chen, H. Murakami, M. Hahn, "A Bayesian approach for inverse modeling, data assimilation and conditional simulation of spatial random fields." submitted to Water Resources Research.

Murakami, H., X. Chen, M.S. Hahn, M.L. Rockhold, V.R. Vermeul, Y. Rubin, "Bayesian Approach for Three-dimensional Aquifer Characterization at the Hanford 300 Area", submitted to Hydrology and Earth Science Systems.

Acknowledgment

This work is supported by the U.S. Department of Energy under contract DE-AC05-76RL01830. This work used the resources of the National Energy Research Scientific Computing Center, which is supported by the DOE Office of Science under Contract No. DE-AC02-05CH11231. The field generation code is provided by Wolfgang Nowak.

PNNL-SA-71875