

# **DATA WORTH AND OPTIMAL SAMPLING ANALYSES TO REDUCE MODEL PREDICTION UNCERTAINTY FOR GROUNDWATER TRANSPORT**

**Hongkyu Yoon**, Sandia National Laboratories, 505-284-3609, [hyoon@sandia.gov](mailto:hyoon@sandia.gov)

1. Hongkyu Yoon, Geoscience Research and Applications, Sandia National Laboratories, Albuquerque, NM 87185, USA
2. Yonas K. Demissie, Environmental Science Division, Argonne National Laboratory, Argonne, IL, USA
3. Sean A. McKenna, Geoscience Research and Applications, Sandia National Laboratories, Albuquerque, NM 87185, USA
4. Albert J. Valocchi, Civil and Environmental Engineering, University of Illinois at Urbana-Champaign, Urbana, IL 61801, USA
5. Charles J. Werth, Civil and Environmental Engineering, University of Illinois at Urbana-Champaign, Urbana, IL 61801, USA

In natural subsurface systems, expensive data collection limits the amount of information obtained to properly characterize the subsurface system and develop a reliable groundwater model. Data worth analysis combined with optimal design of monitoring networks can be used to provide the necessary information to define the optimal placement for subsurface sampling under constraints of limited characterization. In this work, we utilize the concept of data worth and sampling optimization techniques to reduce groundwater model prediction uncertainty. We develop two sampling optimization methods using a model prediction covariance resulting from inverse parameter estimation and newly emerging schemes such as Ant Colony optimization. In addition to direct evaluation of the uncertainty reduction, Mutual Information (MI) criteria are used to quantify the information content of the collected data with the underlying assumption that data with higher MI will play a bigger role in reducing the uncertainty in the model prediction. The analysis is conducted using a unique experimental dataset which includes concentration breakthrough curves at a 0.25 cm grid scale in each dimension over a 13 x 8 x 8 cm<sup>3</sup> heterogeneous sand-box (~53,000 measurement locations) obtained using magnetic resonance imaging. The model prediction uncertainty of the mean arrival times and second central moments averaged at different scales (e.g., 0.25cm, and 1 cm cubes, as well as vertical columns) can provide guidance for new data collection efforts during monitoring network design. We employ a highly parameterized groundwater transport model and data worth analysis to evaluate the reduction of model predictive uncertainty at different scales and locations as a result of newly collected data. The effect of structural uncertainty on model prediction and data sampling will be explored by evaluating their relationship with the variogram model parameters.

This material is based upon work supported as part of the Center for Frontiers of Subsurface Energy Security, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0001114. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.