Quantifying Vadose Zone Flow and Transport Uncertainties Using a Unified, Hierarchical Approach

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Research Objective

The objective of this research is to develop and demonstrate a general approach for modeling flow and transport in the heterogeneous vadose zone. The approach uses similar media scaling, geostatistics, and conditional simulation methods to estimate soil hydraulic parameters at unsampled locations from field-measured water content data and scale-mean hydraulic parameters determined from available site characterization data. Neural network methods are being developed to estimate soil hydraulic parameters from more easily measured physical property data such as bulk density, organic matter content, and percentages of sand, silt, and clay (or particle-size distributions). Field water content distributions are being estimated using various geophysical methods including neutron moderation, ground-penetrating radar, and electrical resistance tomography. One of the primary goals of this research is to determine relationships between the type of data used in model parameterization, the quantity of data available, the scale of the measurement, and the uncertainty in predictions of flow and transport using these methods. Evaluation of the relationships between available data, scale, and uncertainty are using data from a large-scale, controlled field experiment.

Research Progress and Implications

This report summarizes work completed after 2.5 years of a 3-year project. A large-scale injection experiment was conducted in summer 2000 as part of the Hanford Science and Technology (S&T) program at a location on the Hanford Site where a previous injection experiment had been conducted in 1982. The site was instrumented in 1982 with thirty-two, 18-m-deep wells arranged radially around a central injection well. Additional instruments installed as part of the S&T project included polyvinyl chloride access tubes to provide access for cross-borehole ground-penetrating radar and electrical resistance tomography. Five injections of water were made during the S&T experiment over the course of a month with periodic monitoring via the boreholes.

Core samples were collected from three additional boreholes at the site as part of this EMSP project. Approximately 56 of these cores were subsampled for measurements of bulk density, porosity, particle-size distribution, water retention, and hydraulic conductivity. Hydraulic property model parameters have been estimated from the core data. Neural network analysis has been used with the core data to develop pedotransfer functions for the site that relate the more easily determined physical property data to the measured hydraulic properties at the site. Scaling analysis also has been carried out on the core data to estimate scale-mean hydraulic parameters, which are being used to estimate model parameter values at unmeasured locations.

Geostatistical analysis of the site has been carried out using wet bulk density data collected in 1995 at 2.5-cm depth intervals in all of the boreholes and neutron probe data collected in 2000 at

30-cm depth intervals. In this analysis, the wet bulk density distribution was simulated first at 2.5-cm resolution using sequential indicator simulation. These results then were used as soft data to constrain the sequential gaussian simulations of water content, with the neutron probe moisture data spaced at 30 cm used as the hard data. Porosity was calculated from the wet bulk density and the water content using an average particle density. The geostatistical analysis revealed vertical and horizontal anisotropy in the water content and wet bulk density data. The anisotropy in the horizontal directions is mostly due to non-stationarity of the data, with the correlograms suggesting the presence of a trend. The apparent trend appears to be due to greater variability in the sediment layers in the direction parallel to NNW-SSE than there is in the perpendicular direction, i.e., some of the layers appear to pinch out more rapidly in that direction. This causes an increase in the difference in moisture or bulk density values as separation increases along the NNW-SSE axis.

The generated parameter fields span a domain 20 m wide on each side and 12 m deep. Parameters have been generated on this domain at a resolution of 25 cm horizontally and 2.5 cm vertically (approximately 3 million nodes). The parameterization routines, including an upscaling procedure based on volumetric averaging, have been generalized for easy application to other sites. Currently, we are running simulations at a resolution of 50 cm horizontally and 2.5 cm vertically (approximately 1 million nodes). E-type averages of porosity and water content were used to generate the parameters for this simulation.

Planned Activities

The high-resolution model results will be used as a reference for comparison with results obtained using upscaled model parameters and alternative parameterizations based on the neural network analyses and geophysical data. Uncertainties will be evaluated by comparing simulations using different input data and by simulating on different parameter sets generated from alternative geostatistical realizations.

Information Access

Details regarding the field experiment and geophysical data used for model parameterization and testing can be found at http://vadose.pnl.gov/. The hydraulic property data gathered by this project are available from the principal investigator.