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Incorporating layer- and local-scale heterogeneities in numerical simulation of unsaturated flow and tracer transport

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ABSTRACT

This study characterizes layer- and local-scale heterogeneities in hydraulic parameters (i.e., matrix permeability and porosity) and investigates the relative effect of layer- and local-scale heterogeneities on the uncertainty assessment of unsaturated flow and tracer transport in the unsaturated zone of Yucca Mountain, USA. The layer-scale heterogeneity is specific to hydrogeologic layers with layerwise properties, while the local-scale heterogeneity refers to the spatial variation of hydraulic properties within a layer. A Monte Carlo method is used to estimate mean, variance, and 5th, and 95th percentiles for the quantities of interest (e.g., matrix saturation and normalized cumulative mass arrival). Model simulations of unsaturated flow are evaluated by comparing the simulated and observed matrix saturations. Local-scale heterogeneity is examined by comparing the results of this study with those of the previous study that only considers layer-scale heterogeneity. We find that local-scale heterogeneity significantly increases predictive uncertainty in the percolation fluxes and tracer plumes, whereas the mean predictions are only slightly affected by the local-scale heterogeneity. The mean travel time of the conservative and reactive tracers to the water table in the early stage increases significantly due to the local-scale heterogeneity, while the influence of local-scale heterogeneity on travel time gradually decreases over time. Layer-scale heterogeneity is more important than local-scale heterogeneity for simulating overall tracer travel time, suggesting that it would be more cost-effective to reduce the layer-scale parameter uncertainty in order to reduce predictive uncertainty in tracer transport.

1. Introduction

Hydrogeologic environments consist of natural soils and rocks that exhibit multi-scale spatial variability, or heterogeneity, in hydraulic and transport parameters from core samples to layer structures and lithofacies. Although the parameters are intrinsically deterministic (i.e., they exist and are potentially measurable at all scales), knowledge of these parameters usually is limited, especially at field scales. Parameter uncertainty thus arises and renders the predictions of contaminant transport uncertain. Quantification of parameter uncertainty and its propagation in hydrogeological models has been studied for decades using stochastic methods, as reviewed in several books (e.g., Gelhar, 1989; Dagan, 1989; Dagan and Neuman, 1997; Zhang, 2002; Rubin, 2003). Quantifying uncertainty at the field scale is of particular importance because decisions are often based on the field-scale predictions. However, field-scale models for representing complex hydrogeologic environments are complicated, making it difficult to evaluate the propagation of parameter uncertainty through the complicated models.

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In field-scale modeling, it is common practice to separate a large field domain into hydrogeologic layers (or lithofacies and hydrofacies) based on available data such as site geology, hydrogeology, and geophysics. Hydraulic and transport parameters of each layer often are treated as homogeneous variables and are calibrated to match the field observations of state variables. Layer-scale heterogeneity, especially after layerwise parameters are calibrated, is important in simulating the overall flow and transport trend and pattern. While local-scale heterogeneity within the layers is important in predicting flow path, velocity, and travel time of contaminants, it is often neglected in modeling practices. This study aims to characterize both layer- and local-scale heterogeneities and evaluate their relative effect on the predictive uncertainty in unsaturated flow and contaminant transport.

Our study site is the unsaturated zone (UZ) of Yucca Mountain (YM), which has been recommended by the U.S. Department of Energy (USDOE) as the nation's first permanent geologic repository for spent nuclear fuel and high-level radioactive waste. Since the UZ will host the potential repository and act as an important natural barrier in delaying potential arrival of radionuclides at the water table, it is important to understand how much and how fast water and radionuclides travel through the UZ to the groundwater. The UZ consists of various complex hydrogeologic units, and spatial variability of hydraulic properties in each unit can be viewed as deterministic and/or random processes of multiple scales. Yet, only limited data are available to characterize multi-scale heterogeneities, which results in uncertainty in model parameters and, subsequently, model predictions.

Heterogeneities in the hydraulic properties at the UZ have been investigated by many researchers. Based on the degree of welding, rock properties, and hydraulic properties, the UZ is separated into 5 major geologic units and 33 hydrogeologic layers (Flint, 1998, 2003; BSC, 2003b; Flint et al., 2006). Zhou et al. (2003) categorized the heterogeneity for site, layer, and local scales. Typically, in studies of YM, *site scale* refers to the UZ model domain of numerical modeling studies; *layer scale* refers to the hydrogeologic layers with layerwise average properties; and *local scale* refers to the spatial variation in hydraulic properties within a layer. In the last decade, layer-scale heterogeneity has been characterized and incorporated into the three-dimensional (3-D) site-scale numerical model (e.g., Wu et al., 1999, 2004; BSC, 2004a; Wu et al., 2007). Parameter uncertainty and sensitivity analysis for tracer or radionuclide transport in the YM UZ has been conducted mainly at the layer scale (Nichols and Freshley, 1993; Illman and Hughson, 2005; Zhang et al., 2006; Ye et al., 2007). Local-scale heterogeneity in the model parameters within a layer is also important since it affects the flow path, velocity, and travel time of tracers or radionuclides (Bodvarsson et al., 2001; Haukwa et al., 2003; Zhou et al., 2003; Viswanathan et al., 2003; Illman and Hughson, 2005; Zhang et al., 2006). This study incorporates the layer- and local-scale heterogeneities and conducts a Monte Carlo simulation to investigate their relative importance to the propagation of parameter uncertainty. Based on a-priori knowledge of the UZ described in the Appendix A, the model parameters of particular importance in our local-scale heterogeneity characterizations include matrix permeability and porosity. Since the uncertainty of these two parameters has been characterized at the layer scale in Ye et al. (2007), selecting them for the uncertainty analysis enables us to distinguish between the effects of local-scale and layer-scale heterogeneities on predictive uncertainty of unsaturated flow and tracer transport.

This study is focused on examining the relative effect of layer- and local-scale heterogeneities on predictive uncertainty, but not on jointly assessing the predictive uncertainty due to heterogeneities of the two scales. However, this study can be extended for a joint assessment of multi-scale heterogeneity using, for example, the Random Domain Decomposition (RDD) approach (Winter and Tartakovsky, 2000, 2002; Winter et al., 2002, 2003; Guadagnini et al., 2004; Xiu and Tartakovsky, 2004; Winter et al., 2006). The RDD also separates a field-scale geologic system into a number of geologic units (e.g., hydrogeologic layers and lithofacies), but treats boundaries of the geologic units as uncertain (the units being random composites). The key input of the RDD is the probability of boundary locations, used for averaging local-scale uncertainty to incorporate uncertainty of the unit boundaries. While estimating the probability is still in its development stage (Winter et al., 2006), the problem may be resolved using geostatistical methods (e.g., Guadagnini et al., 2004). When the boundary locations are fixed (e.g., Winter et al., 2006), some results of the RDD can also be obtained by conventional stochastic methods as observed in this study. In terms of separating a highly heterogeneous domain into less heterogeneous hydrogeologic layers, this study is conceptually analogous to the RDD. If uncertainty in the layer boundary locations can be statistically quantified for the UZ, which will be very difficult for the complicated geological system with limited characterization data, this study can be extended to incorporate this uncertainty using the RDD.

2. Characterization of parameter heterogeneity

Fig. 1 presents a typical geological profile along a vertical east–west transect of borehole UZ-14 (shown in Fig. 2) at YM, illustrating a conceptual model currently used to analyze UZ flow patterns and explaining the possible effect of faults and perched water on the UZ system. Details of the conceptual and numerical models for simulating the unsaturated flow and tracer transport are given in the Appendix A. Primarily based on the degree of formation welding, the geologic formations have been organized into five major hydrogeologic units (Montazer and Wilson, 1984): Tiva Canyon welded (TCw) unit, Paintbrush nonwelded (PTn) unit, Topopah Spring welded (TSw) unit, Calico Hills nonwelded (CHn) unit, and Crater Flat undifferentiated (CFu) unit. Due to the intensive characterization of the YM UZ that already has been performed, we consider that boundaries of the units have been delineated with a reasonable degree of accuracy. Each major unit is further divided into several subunits referred to as the hydrogeologic layers.

There are two types of available data for matrix permeability and porosity: core measurements at the local scale and calibrated values at the layer scale. From 33 boreholes, 5320 rock core samples were collected (Flint, 1998, 2003; BSC, 2003b) yielding 546 measurements of saturated hydraulic conductivity (which can be converted to permeability in our simulations) and 5257 measurements of porosity. Particularly,