US Department of Energy, Office of Science
Office of Biological and Environmental Research (BER)
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FY10 First Quarter Performance Measure

The first FY10 ERSD overall Performance Assessment Rating Tool (PART) measure for Pacific Northwest National Laboratory is to '*Provide a report that describes how physical heterogeneities can be represented for the field site in a 3D context*'. The field site refers to the Integrated Field Research Challenge (IFRC) site, located in the 300 Area of Hanford Site in southeastern Washington State. In this, the first of four quarterly PART reports, we describe how physical heterogeneities have been characterized and used for parameterizing numerical flow and transport models of the field site. These models are currently being used in conjunction with a series of well-controlled laboratory and field experiments to evaluate our hypothesis-driven research on uranium mass transfer and reactive transport processes at the site.

1. Introduction

Physical and geochemical heterogeneities have long been recognized as having a dominant influence on flow and transport of contaminants in the subsurface. Characterization of physical heterogeneities is extremely important since physical heterogeneity arguably exerts the most significant influence on flow and transport behavior in most natural groundwater systems. Geochemical reactions, sorption, and mass transfer processes are inextricably linked to physical properties of the porous media (e.g. via variations in grain size, sorting, and surface area), so robust characterization of physical properties and their heterogeneity provides a foundation upon which mechanistic representations of reaction and mass transfer processes can be based.

The multi-scale nature of subsurface heterogeneity suggests that multiple methods with different volumes of interrogation be used for subsurface characterization. Point measurements of physical, hydraulic, and geochemical properties on core samples seldom provide sufficient information for effective characterization of subsurface properties for application to field scales. Therefore core-based and smaller scale measurements are typically correlated with other types of data, such as borehole geophysical logs, and used in conjunction with geostatistical methods as conditioning data. Larger-scale field characterization methods such as pump tests provide a means for characterization of the bulk hydraulic conductivity at field-relevant scales, but the volumes of interrogation of such field tests are usually unknown and variable, owing to physical heterogeneity.

Within the past decade or so, more emphasis has been placed on the use of non-invasive and multi-scale geophysical methods for subsurface characterization (Hubbard et al. 2001), and in integrating or assimilating such data with more traditional core, borehole geophysical log, and field pump test data using Markov Chain Monte Carlo and Bayesian methods (Rubin and Hubbard, 2005). Some of the geophysical methods of interest for hydrologic applications include surface and cross-hole electrical resistivity and ground-penetrating radar, and shallow seismic reflection and refraction. These methods all have different, but complementary scales of resolution and volumes of interrogation (Hubbard et al. 2001).

Recent emphasis has also been placed on combining different types of geophysical data noted above with field tracer test data, and using numerical simulations for joint inversion and optimization of model parameters (Chen et al. 2009). These inversion and optimization approaches provide a means for 1) honoring all available data such that the parameters used for modeling flow and transport at a site are all consistent with the observed data, and for 2) quantifying the uncertainty in flow and transport predictions while accounting for uncertainty in both the transport observations and in the field and laboratory characterization data.

The Hanford IFRC site exists within a groundwater uranium plume that has persisted, largely unchanged in area and concentration levels, in spite of the cessation of all waste discharges in the early 1990's and excavation of known source areas immediately underlying the former waste disposal ponds and trenches. This site is particularly challenging to characterize and accurately model owing to: 1.) the very coarse and heterogeneous nature of the sediments, which creates difficulties in obtaining representative intact core samples, 2.) its proximity to the Columbia River whose highly dynamic flow conditions create strong interactions and mixing of river and ground waters with different aqueous chemistries that affect uranium surface complexation and sorption processes in the sediments, and 3.) uncertainties in the inventory and spatial distribution of contaminant uranium.

Multi-scale mass transfer and geochemical reaction processes and a continuing source of uranium in the vadose zone have been posited as possible mechanisms responsible for uranium plume persistence at the site (Peterson et al. 2008; McKinley et al. 2009). Hypotheses related to these mechanisms are being evaluated using a series of well-controlled laboratory and field experiments and numerical modeling (Rockhold et al. 2009; Zachara, 2009a; 2009b; Zheng et al. 2009). Parameterization of the flow and transport models that are being applied to the site requires many different types of characterization data. The remainder of this report describes some of the measurements that have been performed to characterize physical heterogeneities at the site and associated modeling activities. Subsequent quarterly reports in this PART series for the Hanford 300 Area IFRC site will focus on geochemical aspects of the problem and the development of a field-scale reactive transport model for uranium.

2. Characterization of the Field Site

The Hanford IFRC well-field was installed within the groundwater uranium plume in summer 2008 (Bjornstad et al. 2009). The triangular well field (Figure 1.) is 60 m on a side and located within the footprint of the former South Process Pond that received uranium-bearing wastes from reactor fuel fabrication from 1943 to 1975. The field site is located approximately 250 m from the Columbia River (see inset map on Figure 1). The nominal spacing between most wells is 10 m, to facilitate the use of cross-hole geophysical measurements. The average depth to groundwater at the site is ~10 m, but

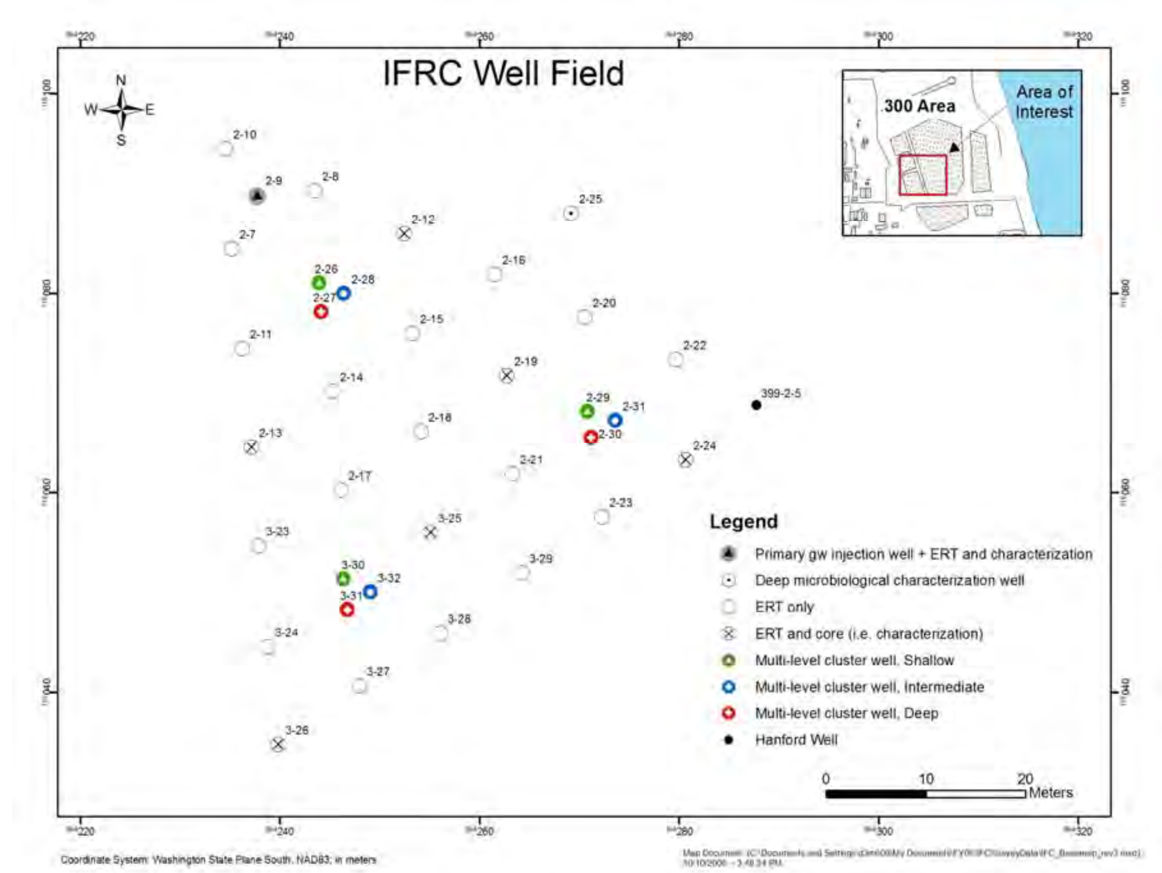

Figure 1. Plan view of the Hanford 300 Area IFRC well field. The predominant groundwater flow direction is the southeast.

the water table elevation can vary by 2-3 m or more annually and by 1 m or more daily (Williams et al. 2008).

Borehole geophysical logging was performed with total gamma, spectral gamma, and neutron-moisture logging tools for most of the IFRC well locations in the temporary 6 7/8-in-ID carbon steel casing prior to well completion. Total gamma, electrical conductivity, acoustic televiewer, and borehole deviation logging was also performed after completion of the 4-in-ID PVC-cased wells. Zero-offset cross-borehole ground-penetrating radar (GPR) measurements were also made between selected well pairs using a Sensors & Software PulseEKKO Pro with 100MHz antennas and 1000V high power transmitter. Figure 2 shows an example of the travel time data between two IFRC wells that was produced by this system.

Geologic and geophysical logs and grab samples from the IFRC well drilling were used to determine the elevation of the interface between the gravel- and cobble-dominated Hanford Fm and the underlying finer-grained silty-sand subunit of the Ringold Fm at each well location. These so-called unit "picks" have been combined with the picks for other far-field well locations to update an earlier EarthVision™ model representation of

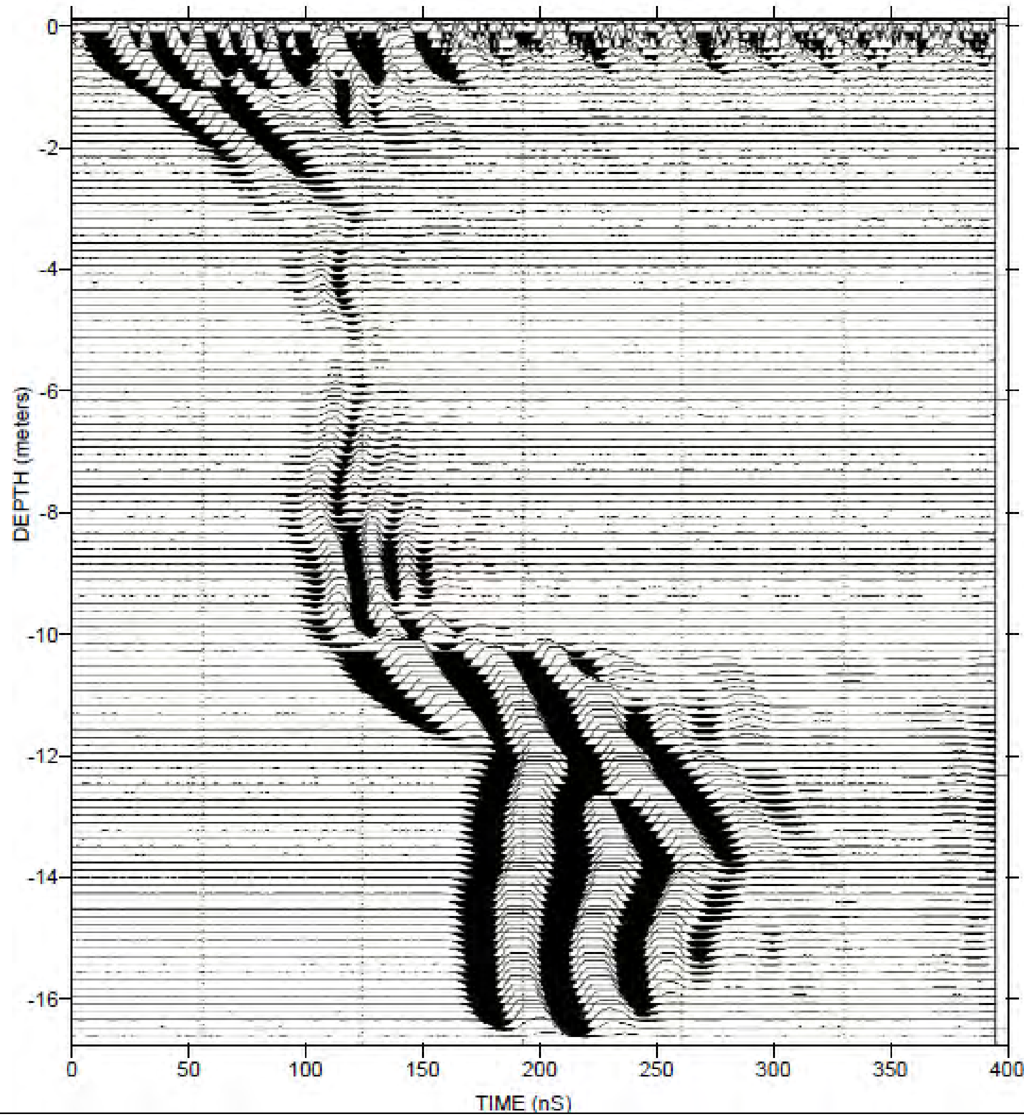

Figure 2. Travel-time data produced from zero-offset cross-hole ground-penetrating radar between wells 2-8 and 2-12 (10-m spacing) at the IFRC well field. Data from Golder Associates, Inc., Redmond, Washington.

the Hanford/Ringold Fm contact in the 300 Area (Williams et al. 2008). A map showing the elevations of this contact in the vicinity of the IFRC well field is shown in Figure 3.

This Hanford-Ringold Fm interface map is currently being used by all modelers of Hanford 300 Area IFRC field experiments. Note that the average elevation of the ground surface at the IFRC site is ~114.9 m and the average depth to the Hanford-Ringold Fm contact is ~18 m below ground surface.

Most of the IFRC wells are instrumented with two (upper and lower) strings of stainless steel electrodes for electrical resistivity tomography (ERT) and thermistors for monitoring temperature (Johnson et al. 2009; Ward et al. 2009). The upper string exists within the vadose zone and the lower string in the saturated zone. Both the electrodes and thermistors are spaced 60 cm (2 ft) apart. The upper ERT and thermistor strings were strapped onto the outside of the PVC casing prior to well completion and are thus permanently installed within the sand pack. The lower ERT and thermistor strings hang inside the well casing and are removable.

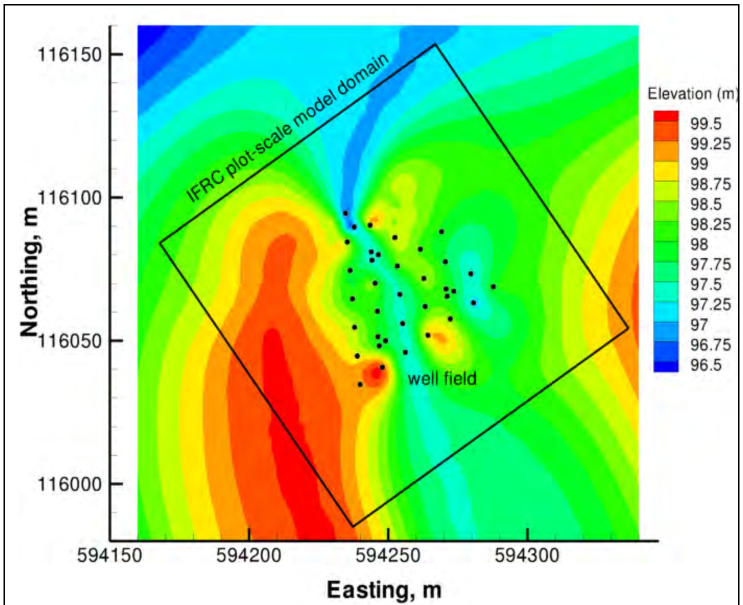

Figure 3. Map showing interpreted elevation of surface of Hanford-Ringold Fm contact in vicinity of Hanford 300 Area IFRC site. Black dots show well locations and black square shows approximate plan-view extent and orientation of numerical flow and transport models being applied to evaluate field experiments. Note apparent channel feature extending through center of well field.

An 8-channel Multi-phase Technologies, LLC, MPT-DAS-1 electrical impedence tomography system is currently being used for ERT data acquisition at the IFRC site. The inverted ERT data have been used in conjunction with electrical conductivity logs collected in the completed PVC wells to develop a 3D map of the conductivity distribution at the site (Figure 4). Electrical conductivity is a function of several variables, including porosity, moisture content, grain-size distribution, mineralogy, and fluid composition (Lesmes and Friedman, 2005). Quantitative use of electrical conductivity data for inferring other physico-chemical properties thus requires concomitant measurement of, or assumptions about some or all of these other variables, and the development of petrophysical relationships that relate them to one another. Such relationships are being developed for 300 Area sediments and the IFRC site through one of PNNL's SFA tasks.

Intact core samples were collected in Lexan™ liners with a split-spoon sampler during drilling of seven of the IFRC wells (locations shown in Figure 1). Depth-discrete grab samples were also collected in plastic sleeves from the other wells. Some of the intact cores have been used for uranium desorption/sorption and mass transfer experiments (to be described in a subsequent PART report), and for measurement of bulk and particle densities, grain size distributions and mineralogy, porosity, saturated hydraulic conductivity, and pressure-saturation-permeability (k-S-P) relations. The k-S-P data will be used to estimate hydraulic parameters for modeling vadose zone infiltration experiments (currently planned for FY11), and for investigating possible relationships between uranium concentrations and different pore-size classes. Grab samples (approximately 175 from over 500) have been used for measurements of grain size distributions, total and extractable uranium, surface area, and extractable Fe(III) forms for petrophysical correlations. Gamma energy analyses (GEA) have also been performed on different size fractions of these samples. The GEA results are being used to develop property transfer functions that relate spectral gamma log data (^{40}K, ^{238}U, ^{232}Th) to grain size distribution metrics (Draper et al. 2009). This GEA work, which is being performed under a PNNL SFA task, will potentially allow the borehole spectral gamma log data to be used directly for estimating grain size distribution metrics, porosity, and other parameters of interest. Similar relationships have been developed and applied previously to 300 Area sediments by Williams et al. (2008).

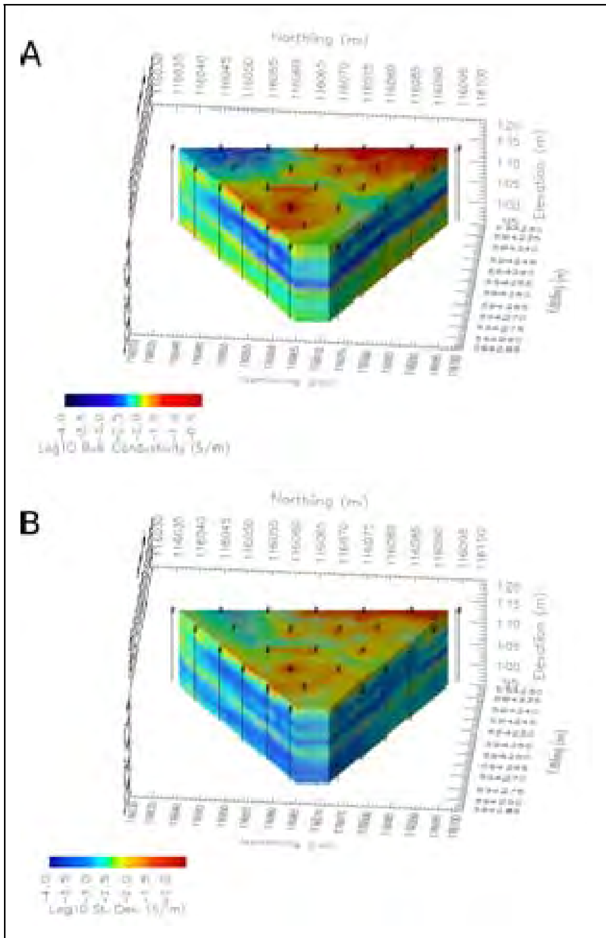

Figure 4. Mean and standard deviation of bulk electrical conductivity distribution (6 realizations). A) mean bulk electrical conductivity. B) standard deviation.

Figure 5 shows split-core photographs of samples collected during drilling of well 399-3-18 in the 300 Area. This well is located approximately 200 m due east of the IFRC well field, near the Columbia River shoreline. Figure 5 clearly illustrates the influence of sediment texture and associated mineralogy on gamma and spectral gamma log responses, providing more evidence to support the development of petrophysical relationships that link these variables. The split-core photograph shows a sharp break between the Hanford and Ringold Fm sediments while the gamma log response varies smoothly across this interface. This is a direct result of the volume of interrogation of the gamma probe, which Rider (1996) estimates is ~40 cm in the vertical direction (~20 cm above and below the detector) and ~10 cm into the formation. This type of smoothing effect should be considered when using any kind of surrogate data, such as geophysical logs or cross-hole GPR that have different volumes of interrogation, to infer values of physico-chemical properties at other scales. Note that the Ringold Fm subunit shown in Figure 5 is the same subunit that underlies the IFRC site.

The largest scales of interrogation used thus far for characterization at the IFRC site stem from short-duration, constant rate injection tests that were performed in fourteen of the IFRC wells to estimate bulk Hanford Fm hydraulic conductivity (K). Electromagnetic borehole flowmeter (EBF) testing was also performed in twenty-six of the wells, at 30- to 60-cm (1-2 ft) spacing. These combined data sets have been used for developing 3D distributions of hydraulic conductivity at the field site, assuming that the bulk hydraulic conductivity values represent weighted arithmetic averages of the local K values along the screened intervals of each tested well. Figure 6 shows examples of the EBF data that have been produced for the IFRC site.

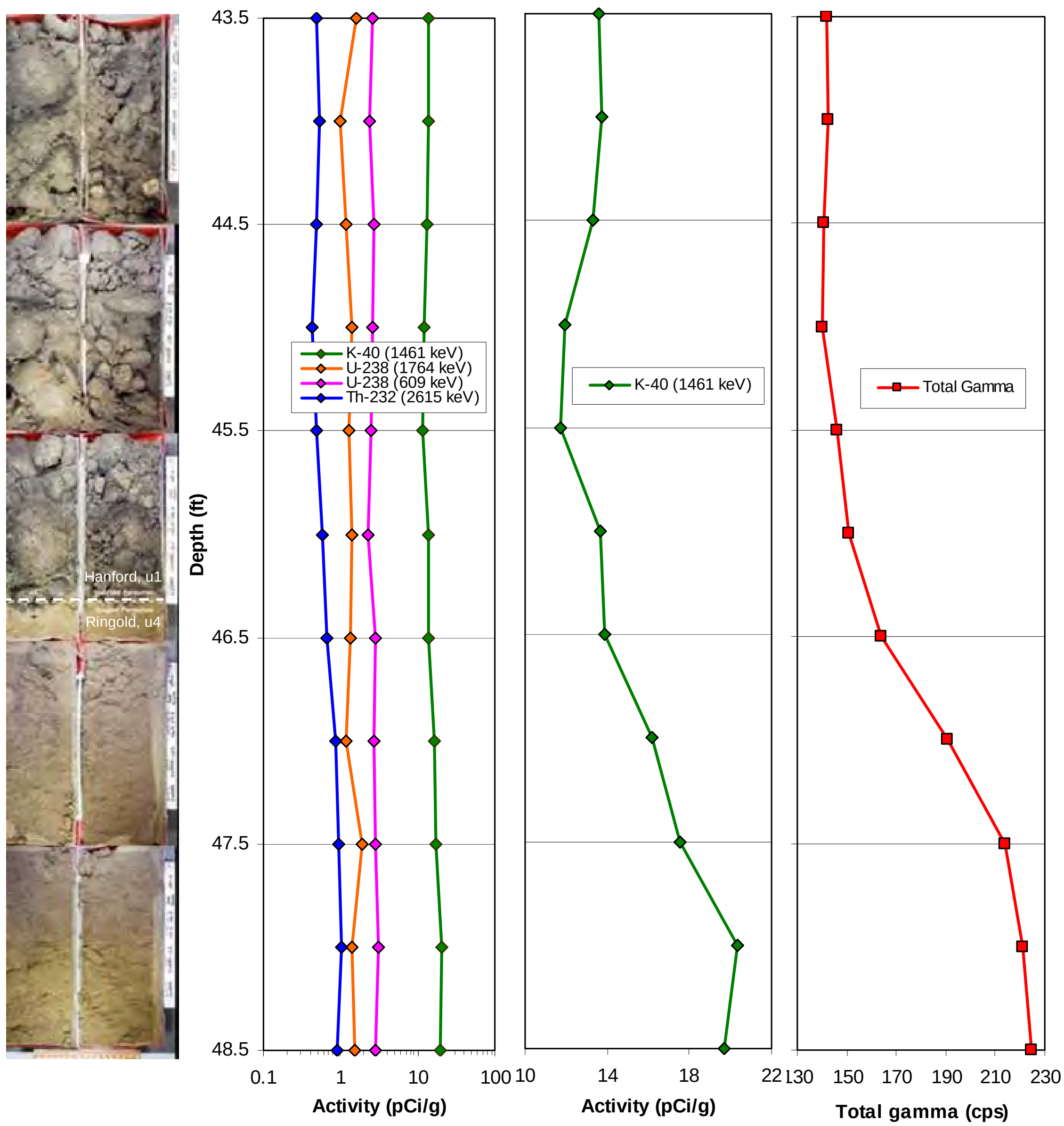

Figure 5. Split-core photographs of sediment samples from both the Hanford (upper 2 cores) and Ringold (lower 2 cores) Fm collected during drilling of well 399-3-18 (located ~200 m east of the IFRC well field), and spectral gamma and total gamma log readings for the same depth interval (from Williams et al, 2008). Note the differences in texture between the Hanford and Ringold Fm sediments, the sharp break between them, and the corresponding smoothly varying responses from the gamma logs across this interface.

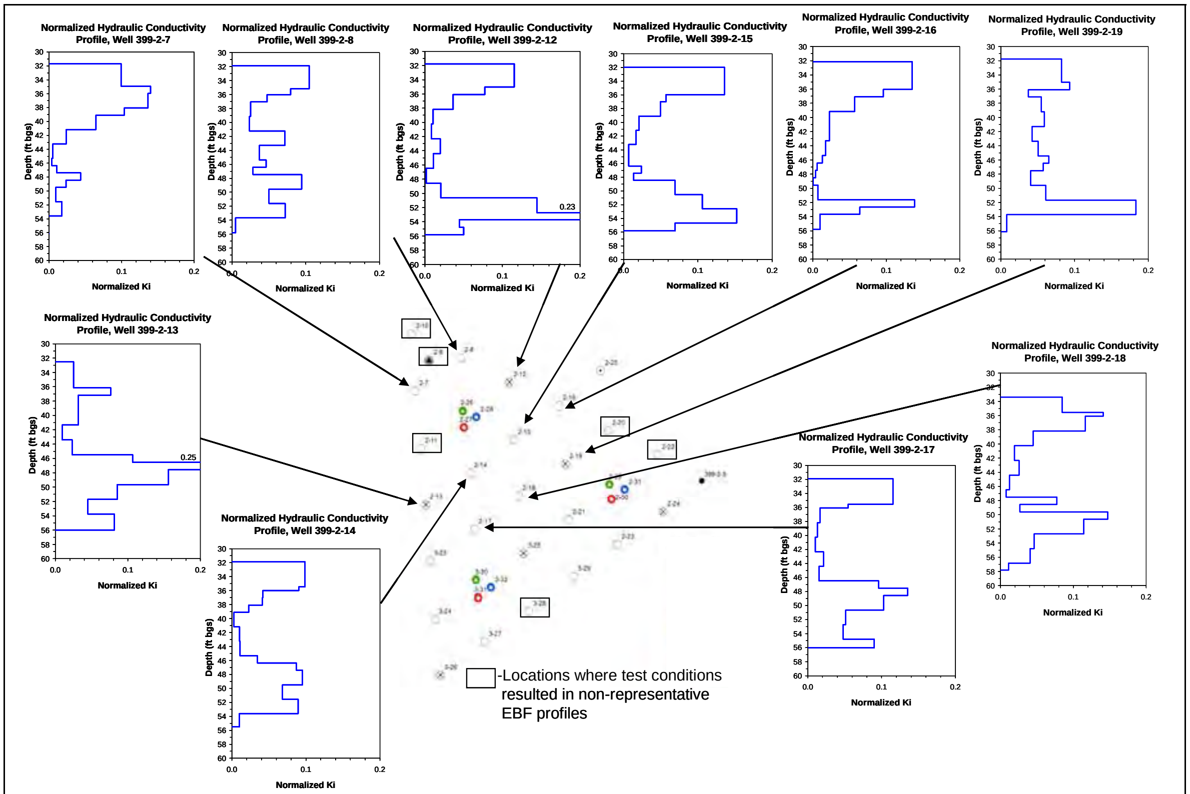

Figure 6. Normalized hydraulic conductivity profiles at selected Hanford 300 Area IFRC wells based on electromagnetic borehole flow meter testing.

In general, the EBF profiles of the saturated zone indicate that the upper and lower sections of the Hanford Fm have significantly higher permeabilities than the middle section at this site. The depth and positioning of the lower hydraulic conductivity (K) zone displays significant variability across the site.

3. Flow and Transport Modeling and Parameterization

Fluctuations in Columbia River stage have a dramatic affect on flow and transport behavior at the 300 Area IFRC field site. Figure 7 shows how the measured groundwater levels and the computed gradients and flow directions varied during the first two tracer tests performed at the site, in November 2008 and March 2009. During the November 2008 experiment, water levels at the field site varied by more than 0.3 m, head gradients ranged from about 1.5e-4 to 8.5e-4, and the azimuth of the flow vector ranged from about 30 to 220 degrees. Although the ranges of variability were similar, flow conditions were more stable in March 2009, with water levels at the site varying by ~0.2 m. The head gradients during the March 2009 experiment ranged from about 1.5e-4 to 6.5e-4 and the azimuth of the flow vector ranged from about 20 to 220 degrees. In both the November 2008 and March 2009 tracer tests, the average trajectory of the plumes was more or less down the center of the well field, as anticipated. Water level data from the IFRC site and

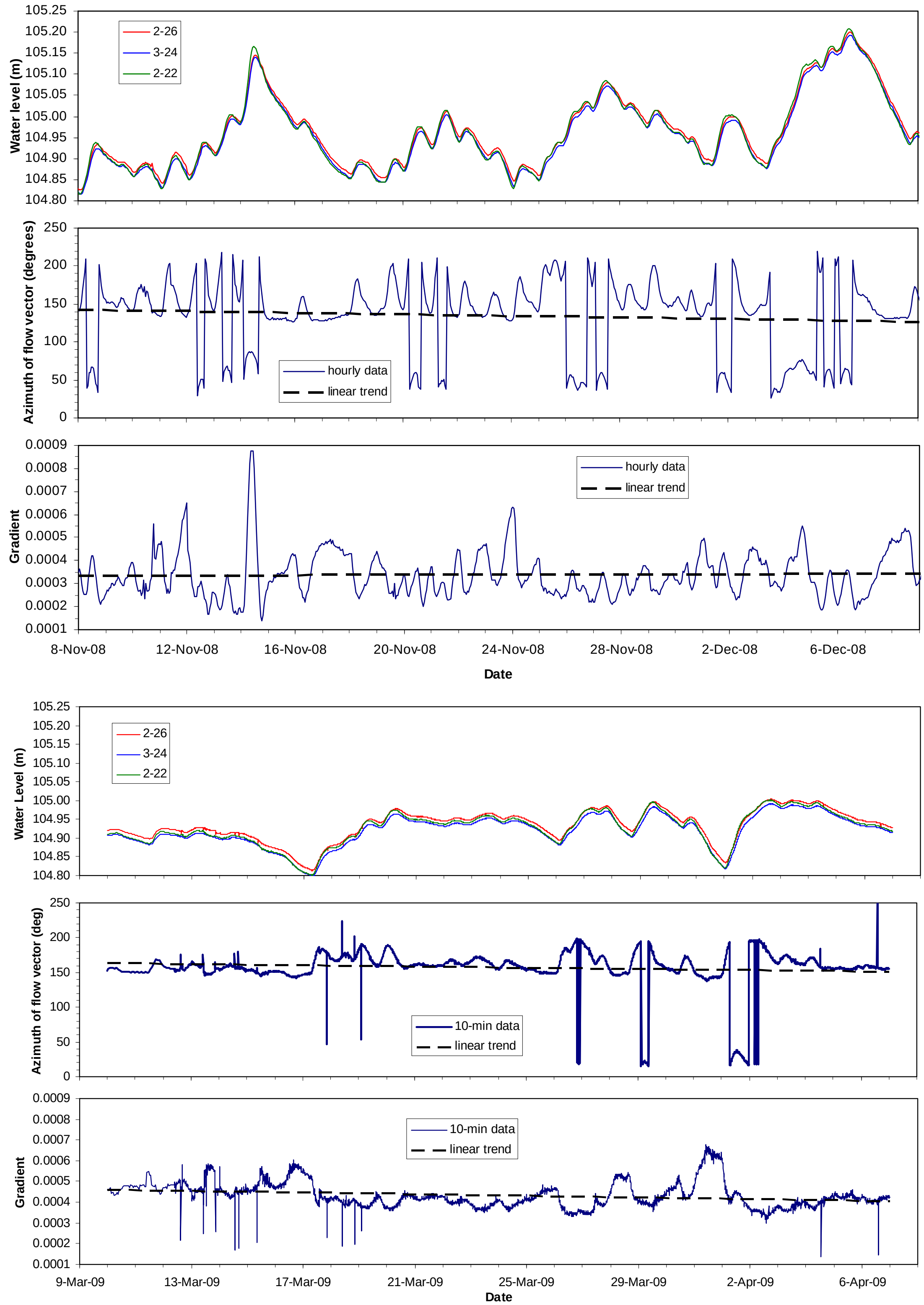

Figure 7. Observed water levels and computed flow directions and gradients during the November 2008 (top 3 panels) and March 2009 tracer tests (bottom 3 panels) at the Hanford 300 Area IFRC site. Note that the flow conditions were much more stable during the March 2009 test.

a surrounding far-field well network have been used to estimate boundary conditions for numerical simulation of the November 2008 and March 2009 tracer tests.

The short-duration constant rate injection and electromagnetic borehole flowmeter (EBF) data have been combined to estimate absolute values of hydraulic conductivity at the locations were these data were available. Variography has been performed to estimate the spatial autocorrelation structure and anisotropy of hydraulic conductivity at the site.
Various methods for spatial interpolation and stochastic simulation (e.g. kriging, co-kriging, inverse-distance interpolation, and sequential Gaussian simulation) have been used for generating spatially distributed K values representing the IFRC well field and its surroundings (Rockhold et al. 2009; Zheng et al. 2009; Chen et al. 2009). Figure 8 shows cutaway views of estimated 3D hydraulic conductivity distributions at the IFRC site. The constant rate injection test and EBF data have also been reanalyzed and alternative representations of the 3D K distribution have been generated using a Bayesian method (Murakami et al. 2009).

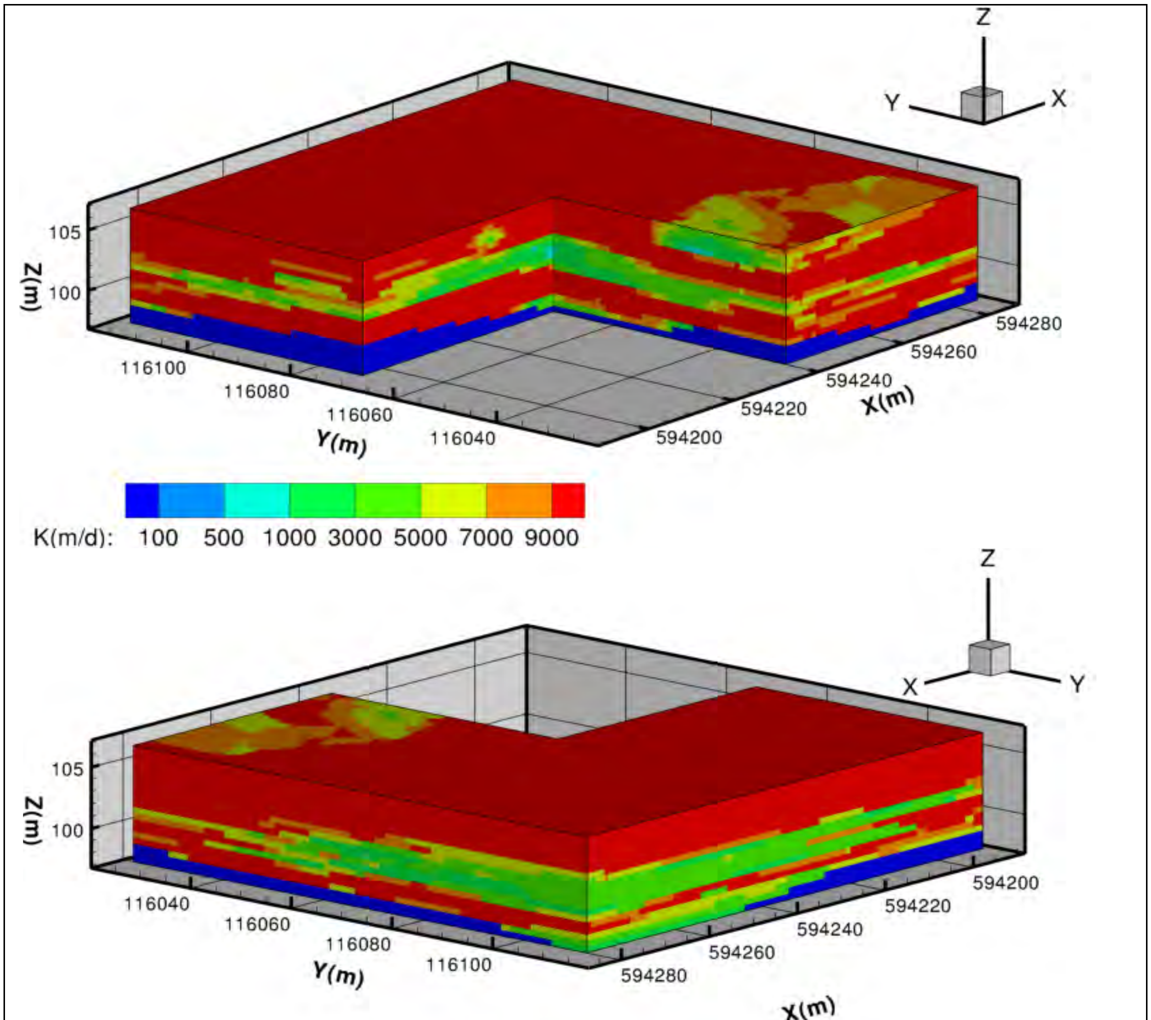

Figure 8. Cutaway views of an estimated hydraulic conductivity distribution at the Hanford 300 Area IFRC well field.

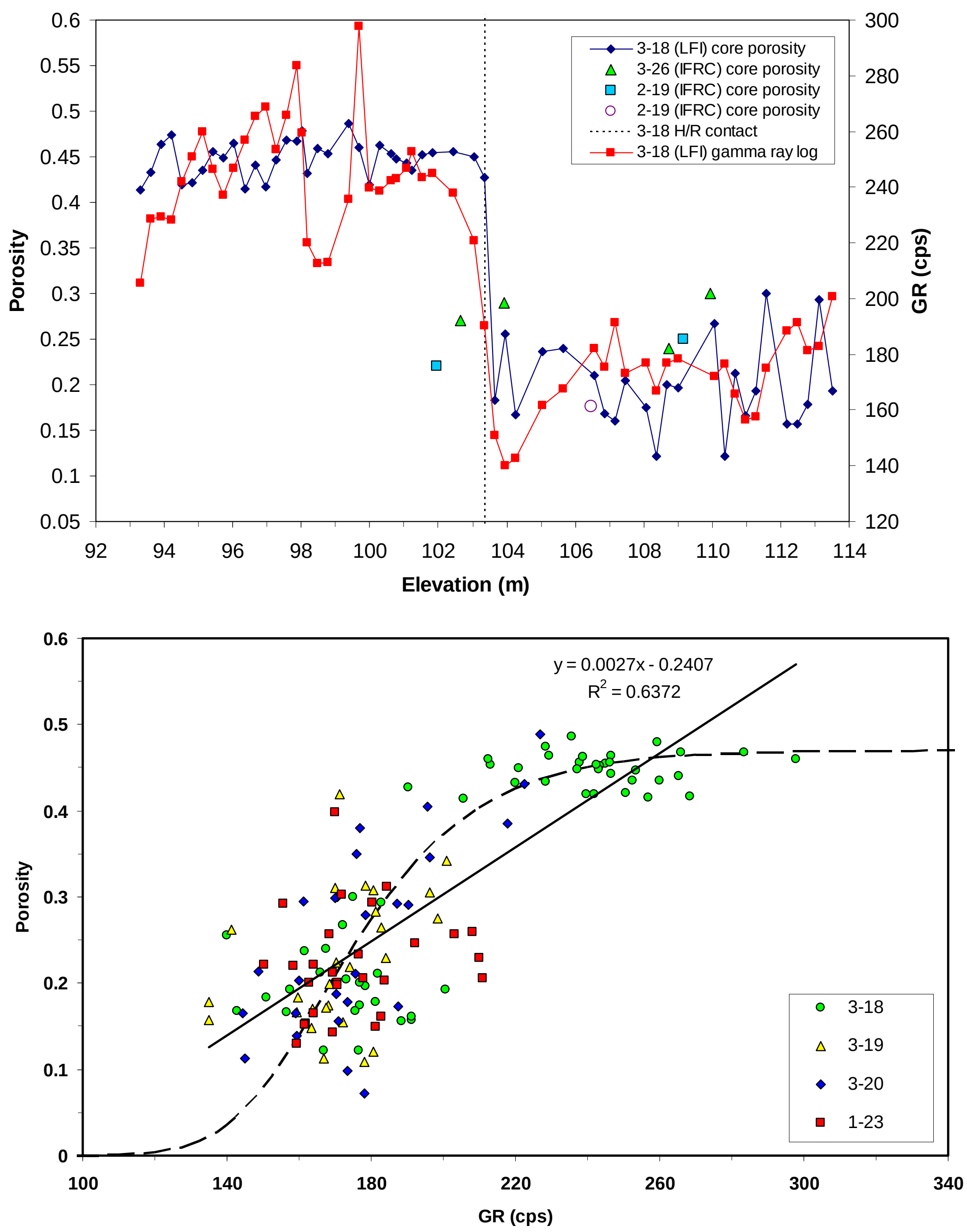

Figure 9. Correspondence between core porosity and gamma log values for a 300 Area well (top plot) and correlations between gamma log and core porosity data (bottom plot).

Relatively few intact core samples from the IFRC site have been analyzed so far to determine porosities, but analyses of data from previous 300 Area investigations have shown relatively strong correlations between core porosities and gamma log readings

(Figure 9). As noted previously, correlations have also been developed for different grain size distribution metrics and spectral gamma log data (Williams et al. 2008; Draper et al. 2009). Borehole gamma and spectral gamma log data are currently being evaluated for use in conjunction with core data to estimate porosity and other properties at the site using various methods including co-kriging and petrophysical relationships.

The hydraulic conductivity and other property distributions described above are being used for modeling the first two tracer experiments that were performed at the IFRC site. These efforts include inverse modeling and parameter optimization using Bayesian methods, the pilot-point method, and others. These modeling efforts are the subject of a series of papers that are in preparation by the Hanford 300 Area IFRC science team and collaborators.

4. Summary

This report, the first of four quarterly reports, describes the characterization of subsurface hydro-geologic properties and parameterization of field-scale models of flow and non-reactive tracer transport at the Hanford 300 Area IFRC site. A variety of methods have been used to characterize the heterogeneity of physical properties at the site, and the analysis of these data sets is ongoing. These methods include core-based measurements of porosity, permeability, pressure-saturation-permeability relations, and sorption and mass transfer characteristics on intact core samples. Field hydraulic characterization has included short-duration constant rate injection tests, depth-discrete electromagnetic borehole flow-meter measurements, and non-reactive tracer injections. These data sets have been combined to provide an initial estimate of the 3D distribution of hydraulic conductivity at the field site. More refined geostatistical models of hydraulic conductivity will result following integration of the geophysical data. This will be enabled by the development of petrophysical relationships that relate variables such as electrical conductivity and spectral gamma ray counts to physico-chemical properties measured on grab samples.

The results of many of the efforts described above were presented recently at the annual meeting of the American Geophysical Union in San Francisco California. Much of this work is also the subject of manuscripts that are in preparation for submission early in 2010. The references section of this report lists selected presentations and publications that have resulted from Hanford IFRC research, and additional references that have been cited in this first quarterly PART report.

Authors

This report was developed by Mark Rockhold (PNNL) with contributions from Chris Strickland (PNNL), Tim Johnson (INL), and Roelof Versteeg (INL). John Zachara (PNNL) is the project P.I.

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