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under Contract DE-AC05-76RL01830

A Long-Term Strategic Plan for Hanford Sediment Physical Property and Vadose Zone Hydraulic Parameter Databases

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LA Middleton

September 2009

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Richland, Washington 99352

Abstract

Physical property data and unsaturated hydraulic parameters are critical input for analytic and numerical models used to predict transport and fate of contaminants in variably saturated porous media and to assess and execute remediation alternatives. The Remediation Decision Support (RDS) project, managed by the Pacific Northwest National Laboratory (PNNL) for the U.S. Department of Energy (DOE) and the CH2M Hill Plateau Remediation Company (CHPRC), has been compiling physical and hydraulic property data and parameters to support risk analyses and waste management decisions at Hanford. Efforts have been initiated to transfer sediment physical property data and vadose zone hydraulic parameters to CHPRC for inclusion in HEIS-Geo, a new instance of the Hanford Environmental Information System database that is being developed for borehole geologic data. This report describes these efforts and a strategic plan for continued updating and improvement of these datasets.

Acknowledgments

We thank Bruce Williams and William D. Webber of CHPRC for providing oversight for the RDS project and review comment on this and related works.

Acronyms and Abbreviations

CHPRC	CH2M Hill Plateau Remediation Company
DOE	U.S. Department of Energy
EDM	Environmental Data Manager
EMSL	Environmental Molecular Sciences Laboratory
HEIS	Hanford Environmental Information System
HTAG	Hanford Technical Advisory Group
PNNL	Pacific Northwest National Laboratory
PSD	particle size distribution
RDS	Remediation Decision Support
SFTEL	Subsurface Flow and Transport Experimental Laboratory

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1.0 Introduction

There are a number of different physicochemical and hydraulic properties and parameters that are required for simulating fluid flow and heat and mass transfer in porous media. Some of these properties, listed in Rockhold (2008), include grain-size distributions, bulk and particle densities, water retention characteristics, saturated hydraulic conductivity, and thermal conductivity. These properties are needed for simulating fluid flow, solute transport, and thermal effects associated with some remediation methods (e.g. soil dessication) that are being used at Hanford. Numerical simulation of these processes is required to predict the transport and fate of contaminants in the subsurface, to quantify the uncertainty in model predictions, and to evaluate, design, and operate different remediation alternatives.

The Remediation Decision Support (RDS) project, managed by Pacific Northwest National Laboratory (PNNL) for the U.S. Department of Energy (DOE) and the CH2M Hill Plateau Remediation Company (CHPRC), has been developing databases of physical and geochemical properties, and hydraulic and transport or sorption parameters, to support site assessments at Hanford (Last et al. 2009). One of the goals of this project is to compile high-quality and traceable datasets, parameters, and parameter distributions that can be used by operable unit managers to support remedial decisions. Efforts have also been initiated to transfer some of the datasets and parameters to CHPRC for inclusion in the Hanford Environmental Information System (HEIS) or equivalent databases. Making these data and parameter estimates available to anyone with access to HEIS should allow for maximum beneficial use of this information.

Efforts to compile physical and hydraulic property databases have been ongoing for quite awhile. The Physical and Hydraulic Properties Database began as a collection of data compiled into Microsoft Excel worksheets as documented by Freeman and Last (2003). This informal database brought together to a single location various Hanford data sets, but the database was not all inclusive, and lacked querying, visualization, and export capabilities. Under the Characterization of Systems (now RDS) project the data in the Freeman and Last (2003) database was imported into a software program called SoilVision® (http://www.soilvision.com/), a commercial geotechnical software package designed for storing and analyzing soils data. Licensing and use restrictions have limited the use of this software package and associated databases for Hanford sediments to PNNL staff. One of the goals of the RDS project is to make these data more widely accessible.

Although the process of compiling physical property data and hydraulic and transport or sorption parameters would seem to be straightforward, it has in fact been very convoluted and difficult for a number of reasons. The data and parameters of interest have been collected over many (>20) years and have involved many different site contractors and individuals. The traceability of the data and the analysis methods is often poor, particularly for some of the older datasets. Some of the efforts to establish data traceability and to check quality, consistency, and parameter reproducibility prior to transferring data to HEIS are described by Rockhold and Middleton (2009) and Rockhold et al. (2009).

Experimental methods have also evolved over time so that new and improved methods and experimental apparatus are now available. Mixing of the older and newer datasets potentially results in variable data quality associated with different experimental methods and procedures. There are also numerous experts on site who specialize in characterization and modeling of flow and transport in the vadose zone. Each has their own particular biases about how various analyses (e.g. gravel corrections) should be performed and about how hydraulic parameters should be estimated (e.g. fixing or fitting θ_s). Parameter estimation procedures have been applied inconsistently so that when parameters from different sources are pooled to estimate distributions (e.g. means and variances) the resulting variability includes both real differences, attributable to actual sediment characteristics, and apparent differences that can be attributed to inconsistent analysis procedures. This report describes some of these issues and our efforts towards identifying robust data and parameter sets that can be incorporated into HEIS.

This report is organized as follows. Section 2 discusses the primary physical properties and hydraulic parameters of interest for transferring to HEIS in the short term (1-2 years), and illustrates some of the hydraulic parameter estimation issues noted above. Section 3 outlines the steps that will be needed to accomplish the transfer of physical property data and hydraulic parameters to HEIS. Section 4 presents a long-term strategic plan for continued updating, improvement, and expansion of the physical and hydraulic property databases. Sections 5 and 6 present conclusions and references, respectively.

2.0 Physical Properties and Hydraulic Parameters

The two types of information that are of primary interest for transferring to HEIS in the short term (1-2 years) are physical properties, including bulk and particle densities and grain-size distributions, and hydraulic parameters. Additional properties and associated parameters of interest include geochemical properties (e.g. mineralogy), thermal and electrical properties, and transport-related parameters. These other properties and parameters are not currently as prevalent or used as much as the physical properties and hydraulic parameters, so our focus will be on the latter. We anticipate that at some point in the future some of these other properties and parameters will also be included in HEIS or an equivalent database.

2.1 Physical properties

Figure 2.1 shows an example of grain size data generated using both wet sieve and hydrometer methods for a sediment sample from Hanford's 300 Area. Although there can be exceptions, grain size data are typically limited to less that 30 data pairs, each representing the mass fraction of the sediment that is less than a given diameter. These data can be interpolated from, or continuous functions can be fit to the data as shown by the pink curve in Figure 2.1, to estimate various size grain or particle size distribution (PSD) metrics. Since the number of size metrics that may be of interest could be close to or even exceed the number of actual grain-size distribution data points, it makes more sense to put the fractions passing the different sizes into HEIS rather than the size metrics. This will allow for maximum flexibility is using the data.

Note that the fitted function shown as the pink curve in Figure 2.1 and the various grain size distribution metrics that are reported in the figure were generated using Excel™ with its Solver add-in and custom-built, Visual Basic for Applications macros. Additional sorption and transport-related properties such as the geometric surface area can also be easily calculated. This type of curve fitting and estimation of grain size distribution metrics can also be performed using commercial software packages such as SoilVision™. The types of grain-size distribution metrics shown in Figure 2.1 have proven to be useful for estimating both hydraulic and sorption parameters using empirical correlation functions (Oostrom et al. 2005, Ward et al. 2006, Williams et al. 2008).

2.2 Hydraulic parameters

The governing equations for water or multi-fluid flow in variably saturated porous media require the use of constitutive functions that relate the relative permeability or unsaturated hydraulic conductivity to fluid saturations or water contents and pressures. Although multi-fluid flow is of concern at Hanford (owing to the release of carbon tetrachloride and co-contaminants), our primary interest here is in water flow and associated solute transport. Readers interested in constitutive relative permeability, saturation, and capillary pressure (k-S-p) relations for multi-fluid flow problems, and in particular carbon tetrachloride, are referred to Oostrom et al. (2006).

Grain size data for Hanford 300 Area, Well 399-1-23, Sample C5000-39D (24.5-25.5 ft bgs).

wt	%<	size(μm)	fraction<	size(mm)	size(phi)	pred frac<	resid^2	PSD metric	value
1	100.00		1.00000	127.0000	-6.9887	0.99997	0.00000	d5(phi)	5.99
1	100.00		1.00000	75.0000	-6.2288	0.99019	0.00010	d10(phi)	2.84
1	82.29		0.82289	50.0000	-5.6439	0.83024	0.00005	d16(phi)	1.08
1	65.89		0.65893	37.5000	-5.2288	0.65001	0.00008	d25(phi)	-0.44
1	49.75		0.49747	25.0000	-4.6439	0.49169	0.00003	d50(phi)	-4.69
1	41.64		0.41645	19.0000	-4.2479	0.42935	0.00017	d75(phi)	-5.47
1	36.88		0.36875	12.5000	-3.6439	0.37132	0.00001	d84(phi)	-5.66
1	35.11		0.35115	9.5000	-3.2479	0.34762	0.00001	d90(phi)	-5.80
1	31.60		0.31599	4.7500	-2.2479	0.31342	0.00001	d95(phi)	-5.95
1	30.29		0.30290	3.3500	-1.7442	0.30298	0.00000	σ_{IG}(phi)	3.49
1	29.63		0.29633	2.8000	-1.4854	0.29754	0.00000		
1	28.28		0.28285	2.0000	-1.0000	0.28225	0.00000	d5(mm)	0.02
1	23.78		0.23778	1.0000	0.0000	0.22042	0.00030	d10(mm)	0.14
1	14.23		0.14233	0.5000	1.0000	0.16361	0.00045	d16(mm)	0.47
1	11.05		0.11045	0.2500	2.0000	0.12405	0.00018	d25(mm)	1.35
1	9.28		0.09281	0.1060	3.2379	0.09082	0.00000	d50(mm)	25.74
1	8.78		0.08778	0.0750	3.7370	0.08077	0.00005	d75(mm)	44.38
1	8.39		0.08390	0.0530	4.2379	0.07210	0.00014	d84(mm)	50.73
1	8.15		0.08151	0.0869	3.5249	0.08485	0.00001	d90(mm)	55.82
1	7.19		0.07192	0.0609	4.0369	0.07543	0.00001	d95(mm)	62.03
1	6.23		0.06233	0.0349	4.8415	0.06323	0.00000	d_{geom}(mm)	6.85
1	5.75		0.05753	0.0190	5.7162	0.05276	0.00002	σ_{geom}(mm)	15.39
1	5.03		0.05034	0.0109	6.5180	0.04509	0.00003		
1	4.31		0.04315	0.0077	7.0275	0.04096	0.00000	USDA texture system	
1	3.93		0.03931	0.0062	7.3251	0.03879	0.00000	% coarse	71.78
1	3.88		0.03883	0.0054	7.5339	0.03735	0.00000	% sand	21.15
1	2.45		0.02445	0.0015	9.3459	0.02740	0.00001	% silt	4.16
								% clay	2.92
						weighted SSR =	0.00168		

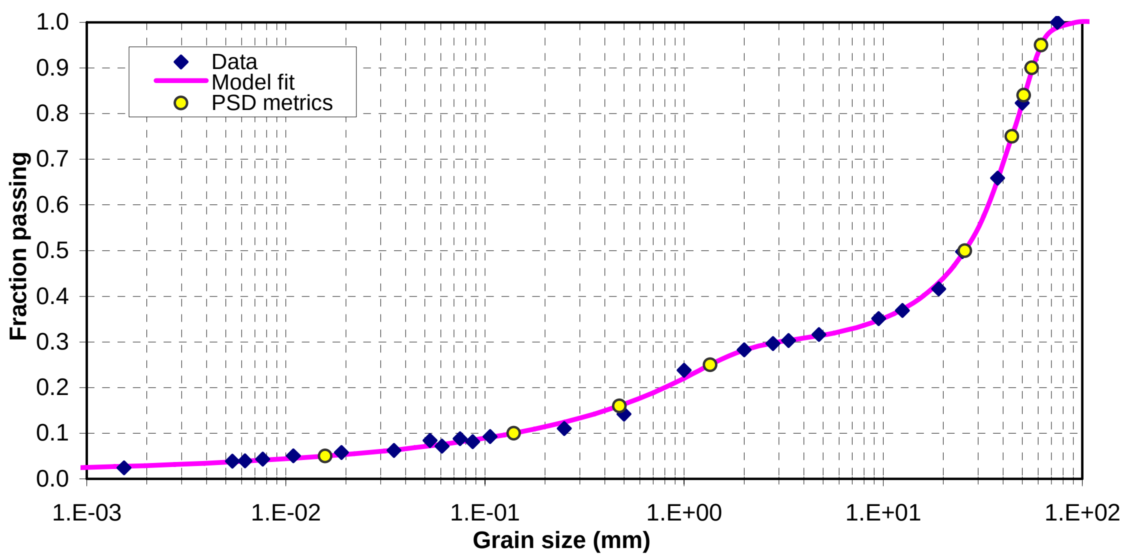

Figure 2.1. Example of Grain-Size Distribution Data and Metrics for a Sediment Sample from the 300 Area

Water retention characteristics represent the volumes of water held in the porous medium by capillary and adsorptive forces at given energy states or pressures. The unsaturated hydraulic conductivity is the rate at which the porous medium will transmit water for a given saturation and hydraulic gradient. The hydraulic properties of variably saturated porous media are hysteretic, or non-unique, and depend on the wetting and drying history. Hysteresis in these properties is potentially important but is typically neglected because modeling hysteresis requires additional characterization data that is not typically available, and significantly more computational effort in subsurface flow and transport simulators.

Various functions have been developed to represent water retention and unsaturated hydraulic conductivity relationships. For example, the van Genuchten (1980) water retention function can be written as

$$S_e(h) = \left[1 + (\alpha h)^n\right]^{-m} \tag{2.1}$$

where:

S_e = effective saturation = $\dfrac{\theta - \theta_r}{\theta_s - \theta_r}$, $0 \le S_e \le 1$
h = soil-moisture tension [L]
θ = volumetric water content [-]
α = curve-fitting parameter related to the air-entry pressure [L^{-1}]
n, m = curve-fitting parameters related to pore size distribution; the relationship m = 1-1/n is often assumed [-]
θ_r = residual water content [-]
θ_s = saturated water content [-].

The van Genuchten hydraulic conductivity relationship, based on the Mualem (1976) hydraulic conductivity model, can be written as

$$K(S_e) = K_s S_e^{\ell}\left[1 - \left(1 - S_e^{1/m}\right)^m\right]^2 \tag{2.2}$$

where K_s is the saturated hydraulic conductivity and ℓ is a pore-interaction term that is equal to 1/2 for the Mualem model with m =1 - 1/n. The Brooks and Corey (1964) water retention relationship can be written as

$$S_e(h) = \left(\frac{h_b}{h}\right)^{\lambda} \text{ for } h \ge h_b \tag{2.3}$$

$$S_e(h) = 1 \text{ otherwise}$$

where h_b is the air-entry pressure and λ is a pore-size distribution index.

The Brooks-Corey function can be combined with the Burdine (1953) or Mualem (1976) relative permeability models to yield

$$K(S_e) = K_s S_e^{2+\ell+2/\lambda} \tag{2.4}$$

where ℓ = 1/2 for the Mualem model and ℓ = 1 for the Burdine model.

The Campbell (1974) water retention function is written as

$$\frac{\theta}{\theta_s} = \left(\frac{h_b}{h}\right)^{1/b} \quad \text{for } h \geq h_b \tag{2.5}$$

$$\frac{\theta}{\theta_s} = 1 \text{ otherwise}$$

where b is also a pore-size distribution index. The corresponding hydraulic conductivity relationship for the Campbell (1974) model is

$$K(\theta) = K_s\left(\frac{\theta}{\theta_s}\right)^{2b+3} \tag{2.6}$$

Note that all of the single-valued water retention and hydraulic conductivity relationships given above assume that hysteresis is not important.

Using the so-called Mualem-based restriction, $m = 1\text{-}1/n$, the van Genuchten water retention function plots as an S-shaped curve that is symmetric in the dry and wet ends (van Genuchten, 1980). If m and n are both allowed to be free parameters, such that $m \neq 1 - 1/n$, the curve can be asymmetric and even mimic the shape of a Brooks-Corey or Campbell type water retention function that has a sharp air-entry pressure. However, in this case the unsaturated hydraulic conductivity function becomes more complicated than that given by Eq. (2.2) and requires the use of complete and incomplete beta functions that have to be evaluated numerically.

For the Campbell and Brooks-Corey water retention models, $\lambda=1/b$, and the two models are equivalent when $\theta_r = 0$. In this case the Campbell hydraulic conductivity function is also equivalent to the combined Brooks-Corey and Burdine models, with $\ell = 1.0$. Although the exponent ℓ representing pore-interaction terms in Eq. (2.2) and (2.4) takes on certain values for specific models, it can also be treated as an unknown parameter to be estimated. Data for estimating parameters such as ℓ usually come from so-called multistep outflow experiments (Tuli et al. 2001).

Because of their additional parameters, the van Genuchten and Brooks-Corey models usually fit water retention data somewhat better than the Campbell model. The Campbell functions are included here primarily because they are used in the RESRAD model (Yu et al. 1993) that is used for some risk assessments at Hanford and elsewhere. The RESRAD manual contains a list of default values of the b parameter for different soil types. These default parameters (from Clapp and Hornberger, 1978) are applicable to soil types that have much finer textures than are typical for Hanford sediments. The default RESRAD b values are generally larger than what should be expected for most Hanford sediments.

Meyer et al. (1997) derived an expression for b in terms of θ_s, θ_r, and λ, assuming that the Brooks-Corey and Campbell models predict the same hydraulic conductivity for a given value of water content. The water content used is that corresponding to an effective saturation of 0.5. This yields the following equation that can be solved for b.

$$b = 0.5\left\{ \frac{\ln(0.5)(3 + 2/\lambda)}{\ln[0.5(1 + \theta_r/\theta_s)]} - 3 \right\} \tag{2.7}$$

If Brooks-Corey model parameters are available but the water retention data are not, Eq. (2.7) can be used to estimate the *b* parameter. Another alternative for estimating the Campbell *b* parameter that was used by Last et al. (2009) is to use van Genuchten or Brooks-Corey model parameters to generate discrete water retention data points and then to fit these generated values using the Campbell model.

Figure 2.2 shows water retention data for a sample collected from the so-called Sisson and Lu Site in the 200 East Area of the Hanford Site, generated from a multistep outflow experiment. The methods used for measuring physical properties and estimating hydraulic parameter for samples from this site are described by Schaap et al. (2003). The general procedures for performing multistep outflow experiments and for estimating hydraulic parameters using inverse modeling are described by Tuli et al. (2001). The fits of various water retention functions to the data using different procedures are also shown.

Figure 2.2 illustrates some interesting points. The porosity of each of the samples described by Schaap et al. (2003) was calculated in the conventional way from

$$\phi = 1 - \frac{\rho_b}{\rho_s} \tag{2.8}$$

where ρ_b and ρ_s are the measured bulk density and the assumed particle density (2.65 g cm^{-3}), respectively.

The multistep outflow experiments that were performed on these samples started with an equivalent tension of 12.5 cm of water. Given the relatively coarse nature of these sediments, this tension resulted in nearly 30% of the available water in the sample draining during the first pressure step. For hydraulic parameter estimation Schaap et al. (2003) report that the θ_s values were fit using an optimization procedure and the calculated values of porosity were simply used as upper bound constraints on the fitted values of θ_s. Consequently, almost all of the fitted values of θ_s are significantly lower than the calculated values of porosity, as shown in Figure 2.2. This result is in part a consequence of the first pressure step being too large relative to the texture of the porous media such that too much water drained from the sample leaving no data points to represent the wet end of the water retention curves.

The fitting approach used by Schaap et al (2003) is problematic from the standpoint that in previous analyses of samples from other sites by other analysts, θ_s has been assumed to be equivalent to porosity and was treated as a fixed parameter rather than being fitted.

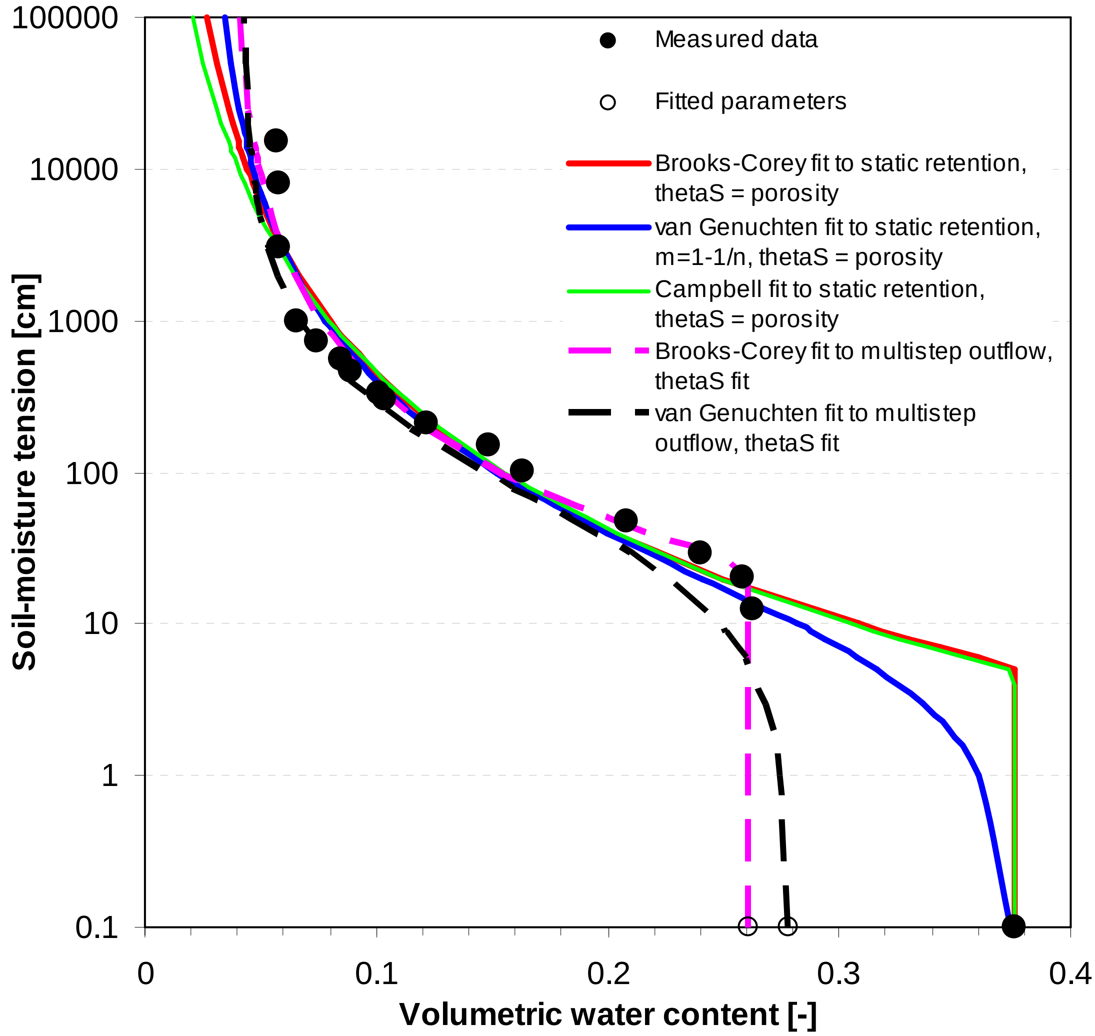

Figure 2.2. Measured and Fitted Water Retention Characteristics for Sample S1-24 from the Sisson and Lu Site (data and inverse model fits from Schaap et al. 2003)

When groups of parameters that have been estimated in different ways like this are combined to estimate statistical distributions, the apparent variability reflects a combination of real differences due to actual physical characteristics and spatial variability, as well as apparent differences arising from inconsistencies in analysis procedures. As clearly shown in Figure 2.2, measured or calculated values of porosity and fitted values of θ_s can be significantly different.

Figure 2.3 shows the unsaturated hydraulic conductivity functions corresponding to the water retention functions shown in Figure 2.2. Similar to their treatment of θ_s, Schaap et al. (2003) also fitted values of the apparent saturated hydraulic conductivities, K_o, and used the measured values of K_s as upper bound constraints on the fitted values.

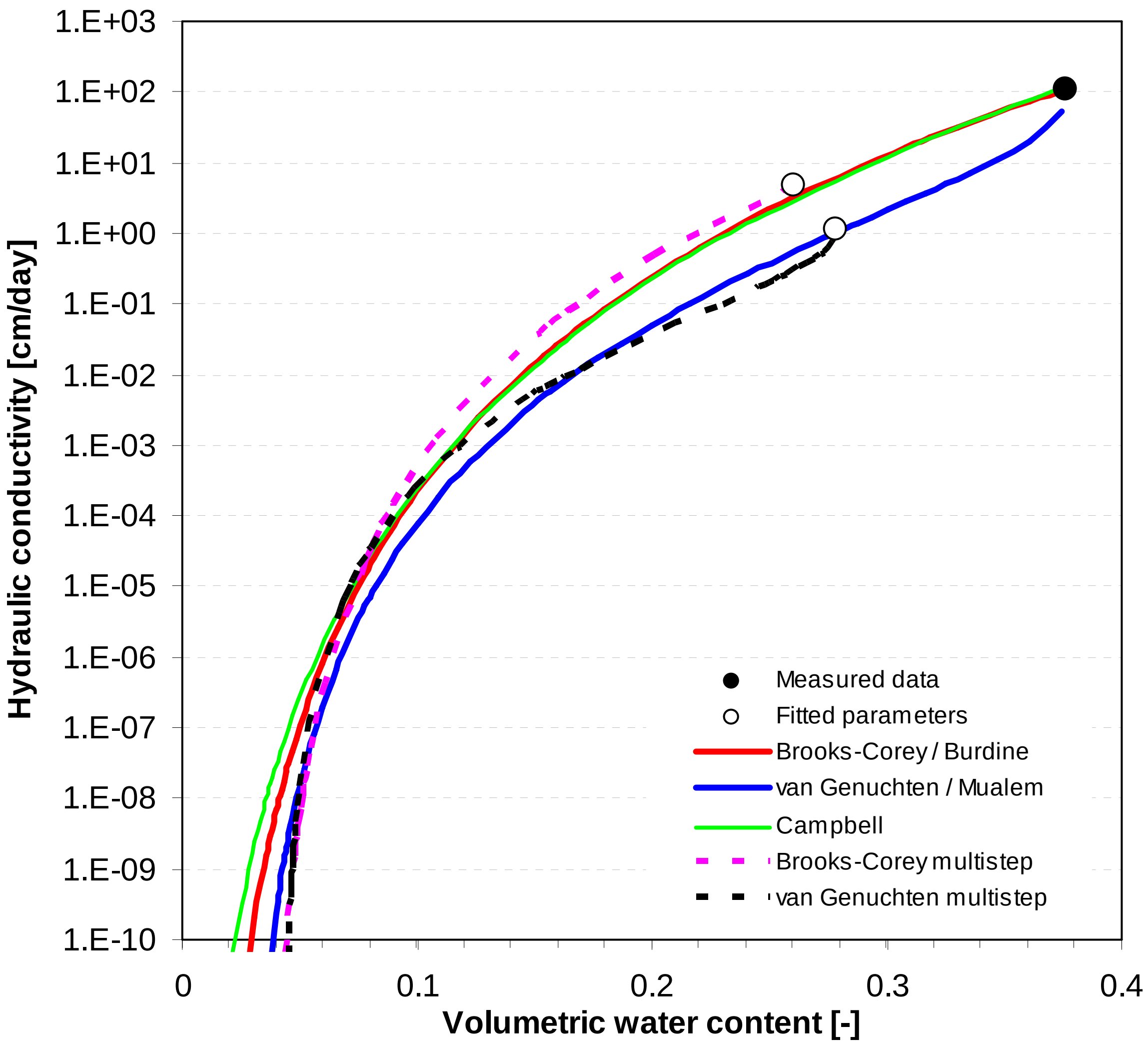

Figure 2.3. Unsaturated Hydraulic Conductivity Functions for Sample S1-24 from the Sisson and Lu Site (data and inverse model fits from Schaap et al. 2003)

Consequently the fitted values of K_o, which have been used as surrogates for the actual saturated hydraulic conductivity, are up to 2 orders of magnitude lower than the measured value of K_s for this particular sample. A difference in the fitted K_o values also occurs due to the use of different hydraulic functions, but this difference is less than one order of magnitude. Similar to θ_s and porosity, when fitted parameters such as K_o are mixed with measured values of K_s, the apparent variability is not due solely to real differences in actual sediment properties arising from spatial variability between different sample locations, but is also due in part to inconsistencies in the analysis procedures.

Similar effects can be seen in parameters reported by Khaleel et al. (2000; 2001; 2002), summarized in Last et al., Appendix A (2009), in which measured values of unsaturated hydraulic conductivity were used as match points and apparent values of the saturated hydraulic conductivity were fitted rather than being fixed at their measured values. In this case they assumed fixed values for the ℓ parameter (which was implicit in their choice of hydraulic functions) and allowed K_o to be fitted in order to get their chosen unsaturated hydraulic conductivity function to pass through the measured unsaturated K match points. However, if they had allowed values of ℓ to be fit, they could have fixed K_s at the measured values and still had their functions pass through their match points. Their chosen fitting process resulted in fitted values of the saturated hydraulic conductivity of very dissimilar geologic units, such as the fine-grained and semi-consolidated Plio-Pleistocene silts and caliche units and the much coarser overlying Hanford Fm sand and gravel units, having fitted values of saturated hydraulic conductivity that are very similar (within a factor of 3) when they should actually differ by orders of magnitude. These authors did not anticipate that their fitted parameters would be combined with other parameter sets to estimate statistical distributions, but this is in fact what has happened. Issues like this are pervasive in the hydraulic parameter datasets that have been compiled for Hanford sediments.

We propose that a systematic approach be taken to develop a more consistent and reliable set of physical properties and hydraulic parameters and their distributions using both old and new data, starting with the data (~60 samples) from Schaap et al. (2003) as a prototype dataset. The static water retention data will be refit for all samples using the van Genuchten, Brooks-Corey, and Campbell water retention models, as shown by the first three curves shown in Figure 2.2. Values of θ_s will be fixed at the measured or calculated values of porosity, rather than being fitted. In our opinion, this is the best and most consistent approach for estimating water retention parameters from laboratory measurements on sediment samples that have been completely saturated and then subjected to drying. For the van Genuchten model, the Mualem-based restriction (m=1-1/n) will be used to avoid the later use of complete and incomplete beta functions for numerical evaluation of the unsaturated hydraulic conductivity function. Measured values of K_s will be used to represent the saturated hydraulic conductivity rather than fitted values of K_o.

The purpose of the proposed reanalysis is to develop a set of hydraulic parameters that have been generated in a consistent manner so that more reliable statistical distributions of the parameters can be obtained. In the past hydraulic parameters have also been developed from field experiments (Rockhold et al. 1988), and from laboratory experiments in which samples were rewet following drainage. The data from these other types of experiments represent conditions that are distinctly different from the drainage data depicted in Figure 2.2, and involve the effects of both hysteresis and entrapped or encapsulated air. Therefore the parameters obtained from these different types of laboratory and field experiments should not be mixed.

Additional datasets will be reanalyzed as described above, and data will be refit where appropriate, to ensure that parameter estimation is performed in a consistent manner. The various hydraulic parameter datasets that have been evaluated and reanalyzed will then be transmitted to CHPRC in batches for inclusion in HEIS-Geo.

3.0 Prototype Datasets and Data Fields for HEIS-Geo

The prototype datasets for grain-size distribution data and vadose zone hydraulic parameters that have been identified for transmittal to CHPRC represent the core samples collected from three boreholes (referred to as S-1, S-2, and S-3) at the so-called Sisson and Lu site, located in the 200 East Area of the Hanford Site. As noted previously, the drilling of these boreholes and core sampling is described by Last and Caldwell (2001). Measurements of physical properties, including bulk density and grain size distributions, and previous estimates of hydraulic parameters are described by Schapp et al. (2005).

The suggested data fields for physical and hydraulic parameters to be initially added to HEIS-Geo are listed in Table 3.1. HEIS-Geo is a new instance of HEIS that is being created to better accommodate borehole geologic data. The suggested fields in Table 3.1 are preliminary and subject to revision pending review by HTAG, the HEIS Environmental Data Manager (EDM), and other interested parties.

It should be noted that measurements of soil or sediment hydraulic properties in the laboratory are usually performed on vertically-oriented core samples. Zhang et al. (2003) and Raats et al. (2004) have shown that in a multi-dimensional context, the ℓ parameter (Equations 2 and 4) can be directionally-dependent such that $\ell_x \neq \ell_y \neq \ell_z$. Since actual measurements of unsaturated hydraulic properties in different directions on the same samples usually do not exist, the tensorial nature of these pore-interaction terms has to be determined by inverse modeling or by some other means, such as using particle-packing models and pore-scale modeling. However, in spite of the lack of direct measurements, comparisons of observed and simulated results for field-scale experiments suggest that tensorial pore-interaction terms are appropriate and necessary to yield improved representations of the anisotropy in simulations of water flow under unsaturated conditions. Therefore the recommended data fields for hydraulic parameters in HEIS will also include tensorial pore-interaction terms. We don't expect these directional pore-interaction parameters to be available in the short term, but methods may be developed in the near future to estimate them more effectively so we have included them in the recommended data fields.

Suggested data fields for grain size distribution data are listed in Table 3.2. The data fields given in Tables 3.1 and 3.2 could conceivably be combined, but are listed separately here, because hydraulic properties may not have been measured on the same samples that grain size distributions were measured on. This is particularly true for some of the older data (e.g. ROCSAN sieve data).

Table 3.1. Suggested Data Fields for Physical and Hydraulic Parameters to be added to HEIS-Geo

Data Field	Description
Site_ID	Identifier for the site (eg. operable unit designation, Tank Farm, experimental field site name, etc.)
Site_ID_Qual	B, W, or E (for borehole, well, or excavation)
Borehole_ID	Temporary identification number for borehole (e.g. C6186)
Well_ID	Well identification number (e.g. 399-2-9)
Easting	Easting coordinate
Northing	Northing coordinate
HorizCoord_units	[L]
HorizCoord_Ref	Reference for horizontal coordinates (e.g. NAD29 or NAD83)
Samp_ID	Identifier for sample
SampDepth_Top	Depth to top of sample

SampDepth_Bot	Depth to bottom of sample
Surface_Elev	[L]
VertCoord_Ref	Reference for vertical coordinates (e.g. NAVD88)
Depth_unit	[L]
BulkDen	Bulk density
BulkDen_units	[M L^{-3}]
BulkDen_Meth	Reference for method used to determine bulk density
PartDen	Particle (aka. grain) density
PartDen_units	[M L^{-3}]
PartDen_Meth	Reference for method used to determine bulk density
Ks_x	Saturated hydraulic conductivity in x (horizontal)-direction
Ks_y	Saturated hydraulic conductivity in y-direction (typically assume Ksat_x = Ksat_y)
Ks_z	Saturated hydraulic conductivity in z (vertical)-direction
Ks_unit	
Ks_Meth	Reference for method used to determine Ks
Porosity	
Theta_S	Saturated water content [dimensionless]; could be equal to porosity
Theta_R	Residual or irreducible water content [dimensionless]
vG_alp	vanGenuchten model alpha parameter
vG_alp_units	[L^{-1}]
vG_n	vanGenuchten model n parameter [dimensionless]
vG_m	vanGenuchten model m parameter, default m=1-1/n [dimensionless]
Ks_fitted_vG	Fitted Ks value generated using vG retention model
Mual_lx_vG	Mualem model pore interaction term, x-direction, when used with vG retention model [dimensionless]
Mual_ly_vG	Mualem model pore interaction term, y-direction, when used with vG retention model [dimensionless]
Mual_lz_vG	Mualem model pore interaction term, z-direction, when used with vG retention model [dimensionless]
BC_hd	Brooks-Corey model air-entry pressure
BC_hd_unit	[L]
BC_lam	Brooks-Corey model lambda parameter [dimensionless]
Ks_fitted_BC	Fitted Ks value generated using BC retention model
Mual_lx_BC	Mualem model pore interaction term, x-direction [dimensionless]
Mual_ly_BC	Mualem model pore interaction term, y-direction [dimensionless]
Mual_lz_BC	Mualem model pore interaction term, z-direction [dimensionless]
Camp_hd	Campbell model air-entry pressure
Camp_hd_units	[L]
Camp_b	Campbell model b parameter (dimensionless)
MRC_Meth	Reference for method used to measure moisture retention characteristics
Ref_Info	General reference information for publication in which data and procedures are described in more detail.

Table 3.2. Suggested Data Fields for Grain Size Data to be added to HEIS-Geo

Data Field	Description
Site_ID	Identifier for the site (eg. operable unit designation, Tank Farm, experimental field site name, etc.)
Site_ID_Qual	B, W, or E (for borehole, well, or excavation)
Borehole_ID	Temporary identification number for borehole (eg. C6186)
Well_ID	Well identification number (eg. 399-2-9)
Easting	Easting coordinate
Northing	Northing coordinate
HorizCoord_units	[L]
HorizCoord_Ref	Reference for horizontal coordinates (eg. NAD29 or NAD83)
Samp_ID	Identifier for sample
SampDepth_Top	Depth to top of sample
SampDepth_Bot	Depth to bottom of sample
Surface_Elev	[L]
VertCoord_Ref	Reference for vertical coordinates (eg. NAVD88)
Depth_unit	[L]
PSD_Methods	Reference to methods used for grain size analyses
Ref_Info	General reference information for publication in which data and procedures are described in more detail.
N_PSD_tuples	Number of grain size - fraction passing tuples (data pairs)
GrainSize_units	[L]
GrainSize_01	[L]
GrainSize_02	[L]
GrainSize_03	[L]
…	[L]
GrainSize_N	[L]
FracPass_01	Real number <= 1.0
FracPass_02	Real number <= 1.0
FracPass_03	Real number <= 1.0
…	Real number <= 1.0
FracPass_N	Real number <= 1.0

4.0 Long-Term Strategic Plan

Development of a long-term strategic plan for continual improvement and updating of the physical properties and hydraulic parameter datasets for the Hanford Site that will eventually be contained in HEIS database is contingent upon first approving and then implementing new data schemas in HEIS. The approval process requires the involvement of HTAG, currently managed by JoAnne Rieger (CHPRC), who is responsible for reviewing and approving of any changes to HEIS. Implementation of new data schemas in HEIS is the responsibility of the Hanford Environmental Data Manager, who is currently Bill Webber (CHPRC). Mark Rockhold (PNNL) met with CHPRC staff in FY09 (Bill Webber in July 2009 and Bill Webber and JoAnne Rieger in early September 2009) to discuss the current structure of HEIS, plans for HEIS-Geo, and new data schemas for sediment physical properties and hydraulic parameters. It was decided that two new data schemas would be needed initially, one for grain size data and one for physical properties and hydraulic parameters, such as depicted in Tables 3.1 and 3.2.

The second new data schema for grain-size distribution data would be somewhat more straightforward than the physical and hydraulic property data schema. In the past, sieve data representing the fraction passing or retained by a given sieve size from the ROCSAN database have been incorporated into the Virtual Library. Laboratory analyses of grain-size distributions typically include the coarser fractions, determined by either wet or dry sieve methods and the finer (silt and clay) fractions that are determined by sedimentation using hydrometer or laser diffusion spectrometry methods. Therefore the data schema for grain size will need to include metadata fields that allow for documentation of the methods used for analysis of both the coarser (wet or dry sieve) and finer size (hydrometer or laser diffraction) fractions.

After the prototype datasets have been successfully loaded into HEIS-Geo or an equivalent repository, we envision that existing physical property data and hydraulic parameters that are currently maintained by PNNL will be transferred in batches to CHPRC in a standardized format (e.g., CSV, or Excel spreadsheets). Periodic transfer of these datasets will continue until all of the desired datasets have been incorporated into HEIS-Geo. New datasets will be documented and then transferred in the same way.

New measurements of physical and hydraulic properties and estimation of hydraulic parameters are ongoing and we expect the data and associated parameter for these new datasets to also be added to HEIS-Geo. For example, multistep outflow experiments have recently been performed on a number of intact core samples from both the 300 Area and the 100-N Area at Hanford. Figure 4.1 shows a photograph of the experimental apparatus that is being used for these multistep outflow experiments. These experiments are being performed in the Subsurface Flow and Transport Experimental Laboratory (SFTEL) housed in PNNL's Environmental Molecular Sciences Laboratory (EMSL).

Figure 4.1. Apparatus for Automated, Laboratory Measurement of Sediment Hydraulic Properties (k-S-p relations) in EMSL (SFTEL)

Determination of unsaturated hydraulic properties and parameters using the multistep outflow experiment (Tuli, 2001) involves the measurement of thousands or even tens of thousands of voltages from multiple (typically 3) pressure transducers. The transducer voltages are converted to pressures and outflow volumes using calibration equations. The pressure and outflow data are then used with a flow simulator that is coupled with an inverse parameter estimation algorithm to optimize hydraulic parameters such that the differences between observed and simulated pressures and outflow volumes are minimized. Figure 4.2 shows an example of some the raw data that are generated during these experiments, and simulation results obtained using the STOMP (White and Oostrom, 2006) simulator for hydraulic parameters that were optimized using PPEST (Doherty, 2001).

Storing thousands or tens of thousands of voltage or pressure and outflow volume data points for a single sample would not be a good use of HEIS. Storing of 15-20 fitted hydraulic parameters, representing three or more different hydraulic property functions (described in Section 2), appears to be a good solution, as long as sufficient metadata is also provided that contains information on reference documents in which the data have been published (e.g. laboratory record book numbers, technical reports, and journal articles), the methods or procedures that were used (e.g. multi-step outflow versus hanging water column and pressure-plate extraction), and other pertinent information about parameter estimation from which the raw data could potentially be obtained if needed. Methods used for measuring saturated hydraulic conductivity in the SFTEL are described by Wiestsma et al. (2009).

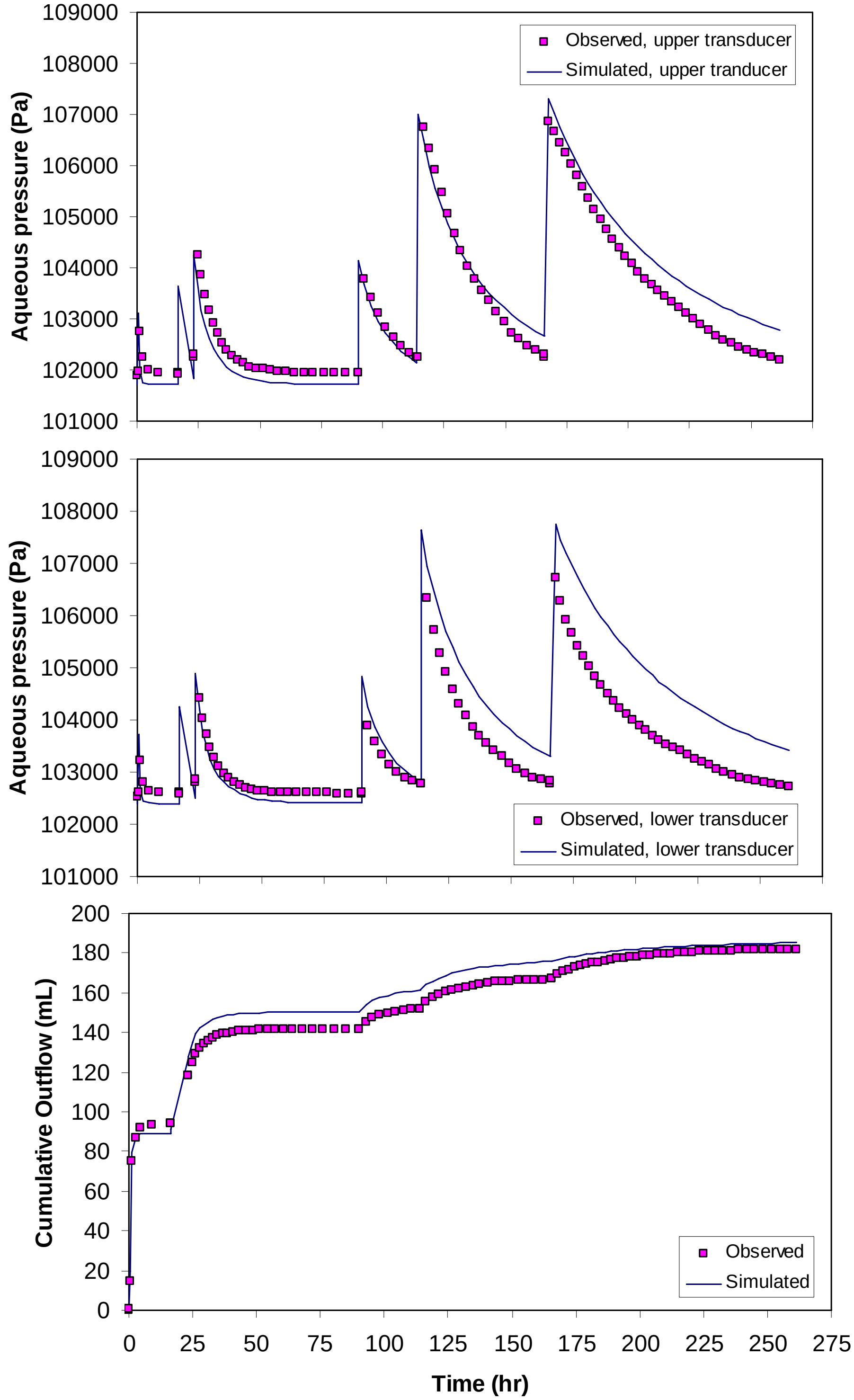

Figure 4.2. Observed and Simulated Aqueous Pressures and Outflow for a Multistep Outflow Experiment Performed on Intact Core Sample C7041, 11.5-12 ft. from the 100-N Area

The prototype datasets described in the previous section will be transmitted to both Bill Webber and JoAnne Rieger early in FY10. They have agreed to review the datasets and to develop schemas for these datasets so that they can be incorporated into HEIS-Geo or an equivalent. Although this process has been initiated, since it requires a collaborative effort by PNNL and CHPRC, completion of these first steps may require more involvement by management on both sides to ensure that all decisions are mutually agreed upon and the work is given high enough priority with tangible goals and deadlines to ensure its timely completion. Assuming that new data schemas can be agreed upon, and are implemented effectively, a schedule for transfer of existing, fully traceable and high-quality data sets will be developed.

One issue that has hampered efforts to consolidate physical and hydraulic property data in the past is the fact that these data are generated for different projects, by different groups that use different methods for measurements and analyses. Just knowing who is doing or has done what is one of the biggest challenges. We recommend that all ongoing projects that involve sediment sampling and characterization at Hanford be notified of this effort to consolidate data and to make it readily accessible for mutual benefit. Then when data are generated, PNNL staff working as points of contact for this task should be notified and the data transferred to them with complete documentation as soon as it is available. The Laboratory will provide quality checks, reformatting, and will perform curve-fitting or inverse modeling of the datasets, as needed. The data and associated parameter sets will then be transferred to CHPRC in an agreed upon, standardized format. The EDM or his delegate will then upload the data to HEIS-Geo. We also recommend that a user list be established so that anyone who expresses an interest in using the data or parameters will be notified periodically when new datasets become available. Longer term plans for these databases and associated analysis tools are discussed by Rockhold (2008).

5.0 Summary and Conclusions

Physical properties and hydraulic parameters and their distributions are required for any type of quantitative assessment of risk and uncertainty associated with predictions of contaminant transport and fate in the subsurface. The central plateau of the Hanford Site in southeastern Washington State contains most of the contamination at the Site and has up to ~100 m of unsaturated and unconsolidated or semi-consolidated sediments overlying the unconfined aquifer. These sediments contain a wide variety of contaminants ranging from organic compounds, such as carbon tetrachloride, to numerous radionuclides including technetium, plutonium, and uranium. Knowledge of the physical and hydraulic properties of the sediments and their distributions is critical for quantitative assessment of the transport of these contaminants in the subsurface, for evaluation of long-term risks and uncertainty associated with model predictions of contaminant transport and fate, and for evaluating, designing, and operating remediation alternatives.

The RDS project, managed by PNNL for the DOE and CHPRC, has compiled physical and hydraulic property data for Hanford Site sediments based on both past and ongoing site characterization efforts. Aside from a one-time effort in the late 1990's to incorporate grain size data from the so-called ROCSAN database into the Hanford Virtual Library, there have been no further attempts on the part of the Hanford site operations or remediation contractors (Fluor-Hanford or CHPRC) to incorporate either physical or hydraulic property data into any broadly accessible databases, such as the Hanford Environmental Information System (HEIS). However, PNNL has been working to organize, catalog, and develop prototype databases with the goal of developing an authoritative, configuration controlled database (Rockhold 2008). Incorporating such data into databases like HEIS that can be easily accessed by operable unit managers, remediation contractors, stakeholders, and others who might be interested in using these data for risk management, remediation, or research purposes should be a high priority.

One of the goals of PNNL's RDS project is to work with the Hanford EDM, now with CHPRC, to develop a protocol and schedule for incorporation of physical property and hydraulic parameter datasets currently maintained by PNNL into HEIS. This requires that the data first be reviewed to ensure quality and consistency. New data schemas must then be developed for HEIS that are approved by the HTAG that oversees HEIS development. After approval, these new data schemas then need to be implemented in HEIS by the EDM before there is an actual repository for the data. This document summarizes some of these ongoing efforts and suggests a long-term strategic plan for continued updating of the physical property and hydraulic parameter datasets and incorporation of these datasets into HEIS.

Prototype datasets have been identified for initial transfer to CHPRC and testing. These datasets will be transferred from PNNL to CHPRC in early FY10.

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