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Development of Vadose Zone Hydraulic Parameter Values

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Several attempts have been made to establish relationships between readily available soil properties, such as grain-size distribution, and less commonly available properties such as saturated hydraulic conductivity (K_{sat}) and the soil moisture retention curve (MRC) (*Evaluation of Pedotransfer Functions for Predicting the Soil Moisture Retention Curve,* Cornelis et al., 2001). Those relationships are referred to as pedotransfer functions (PTF). A PTF has been developed to support estimates of infiltration at the Yucca Mountain site that could have applicability at other arid sites and for other purposes such as modeling the fate and transport of contaminants in the vadose zone. The PTF has direct application to support of fate and transport modeling at the Hanford Site, because it relies on Hanford Site soil and sediment properties.

At least three general approaches have been used to develop PTFs (*Use of the Nonparametric Nearest Neighbor Approach to Estimate Soil Hydraulic Properties* Nemes et al., 2006). Two are parametric approaches that rely on equations with parameters found from fitting those equations to data. Parameters that have been incorporated into PTFs include grain-size distribution, bulk density, porosity, organic matter content, and plasticity index. Generally with these approaches, the more parameters used to develop the PTF, the smaller the uncertainty. Parametric approaches have drawbacks including identifying the correct equation and determining that the probability distributions of errors are similar across the data space. For modeling infiltration at the proposed nuclear repository at Yucca Mountain, Nevada, a nonparametric "sample matching" approach was developed. The available Yucca Mountain data include well-documented grain-size distribution and gravel content (rock-fragment content) for most soil samples, which are readily used as match points to other samples that have developed hydraulic parameter values. This nonparametric approach is beneficial when the form of the relationship between the inputs and outputs is not known in advance, such as with soil hydraulic properties.

Various soil-parameter databases were considered for the basis of the PTF development; most were developed for agricultural applications and contained a large number of soils from locations where more temperate climates prevail, compared to that in the Yucca Mountain region. However, a substantial soil-parameter database has been developed for the U.S. Department of Energy Hanford Site in Washington State, where the soils have developed under arid climatic conditions similar to those of Yucca Mountain, resulting in hydraulic characteristics that could represent those in the Yucca Mountain region. For instance, the average annual precipitation at the Hanford Site is about 17.3 cm/yr, compared to about 12.5 cm/yr for Yucca Mountain (BSC 2004, Section 3.42). The organic carbon content is below 0.5 wt% in Hanford Site sediments, compared to the organic carbon contents that range from about 0.006 to 0.70 wt% in Nye County, Nevada.

The data from the Hanford Site are referred to as the analogous database and are documented in *Variability and Scaling of Hydraulic Properties for 200 Area Soils, Hanford Site* (Khaleel and Freeman 1995). The analogous database includes grain-size distribution, moisture retention, and saturated hydraulic conductivity from the laboratory analysis of 183 soil samples, to develop and provide the following hydraulic-parameter values: residual saturation (θ_r), saturation (θ_s), saturated hydraulic conductivity (K_{sat}), and the moisture-retention curve-fitting parameters, α and n. The analogous database also provides moisture-retention curves. These curves were used to estimate the field capacity (FC), permanent wilting point (PWP), and water-holding capacity (WHC). Field capacity is defined as the soil-moisture content at −0.33 bar (−336.6 cm water) and at −0.10 bar (−102 cm water). Permanent wilting point is defined as the soil moisture content at −60 bar (−61,200 cm water).

The Euclidean distance (ED) is an indicator of how good the match is between any two samples, with the smaller ED values indicating better matches; it removes some subjectivity from the matching process. An exact match has an ED of zero. The ED is applied to the sand, silt, and clay values by determining the difference between sand, silt, and clay fractions of any two soil samples. This application of ED represents the three-dimensional distance between the three parameters. The expression used to calculate ED between sand, silt, and clay for a pair of Yucca Mountain and analogous site samples is:

$$\text{ED (3D)} = [(\text{Sand}_{\text{ymp}} - \text{Sand}_{\text{Hanford}})^2 + (\text{Silt}_{\text{ymp}} - \text{Silt}_{\text{Hanford}})^2 + (\text{Clay}_{\text{ymp}} - \text{Clay}_{\text{Hanford}})^2]^{1/2}.$$

The results based on the newly developed PTF corroborated well with two alternative PTF approaches. One approach considered was ROSETTA (Schaap et al., 2001), which includes a database of 2,134 samples for water retention, 1,306 samples for K_{sat}, and 235 samples for unsaturated hydraulic conductivity obtained from a large number of sources that involve agricultural and non-agricultural soils in temperate climate zones. The other PTF is documented in *Developing Joint Probability Distributions of Soil Water Retention Characteristics* (Carsel and Parrish, 1988) using soil sample data from 42 states.