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Unsaturated Zone Parameter Estimation Using the HYDRUS and Rosetta Software Packages

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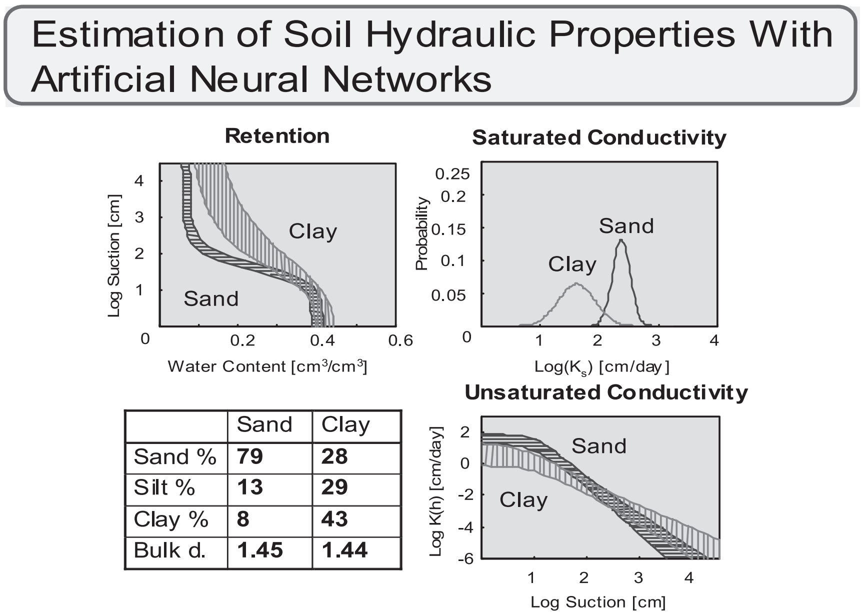
The Salinity Laboratory has long developed and used parameter estimation codes to estimate a variety of soil hydraulic and solute transport parameters from laboratory and/or field experimental data. Much of our earlier work focused on estimating parameters in analytical solute transport models (Skaggs et al., 2002), such as the physical (mobile-immobile) and chemical (two-site) nonequilibrium models embedded in the CFITIM (van Genuchten, 1981) and CXTFIT (Parker and van Genuchten, 1984; Toride et al., 1995) codes. Recently a Windows-based version (STANMOD, Simunek et al., 1999b) of these and related one- and multidimensional analytical transport models became available.

Using parameter optimization techniques for estimating the unsaturated soil hydraulic properties became popular in the mid 1980s (e.g., Kool et al., 1985), initially in conjunction with mostly one- and multi-step outflow experiments. Such optimizations require numerical solutions of the governing Richards equation for variably saturated flow because of the highly nonlinear relationships between the water content, the hydraulic conductivity, and the pressure head (or suction). As more flexible and comprehensive numerical programs such as the HYDRUS codes (Simunek et al., 1998, 1999a; Rassam et al., 2003) became available, these studies were extended to analyses of upward flux or head-controlled infiltration experiments (including tension infiltrometry), evaporation methods, or any other experiment involving some appropriate combination of water flow and solute transport data. In this paper, we briefly review the main features of the HYDRUS codes and their utility for estimating soil hydraulic and solute transport parameters. Also, as an alternative to using HYDRUS for site-specific parameter estimation studies, we briefly summarize the Rosetta code for estimating the unsaturated soil hydraulic parameters and their uncertainty in a more generic manner from soil texture and related surrogate data that are often available. Details of these and other models discussed in this paper can be found at the Web Site of the Salinity Laboratory (www.ussl.ars.usda.gov/models/models.htm).

The Windows-based modular HYDRUS-1D and HYDRUS-2D software packages may be used to address one- and two-dimensional flow and contaminant transport problems, respectively. The HYDRUS codes use the Richards equation for variably-saturated flow and Fickian-based advection-dispersion equations for both heat and solute transport. The flow equation considers water uptake by plant roots, as well as hysteresis in the unsaturated soil hydraulic properties. The solute transport equations include provisions for nonlinear sorption, one-site and two-site non-equilibrium transport, dual-porosity media involving mobile and immobile water, and the transport of solute decay chains. The software packages come with Levenberg-Marquardt type nonlinear parameter optimization modules to allow estimation of a variety of soil hydraulic and solute transport parameters from experimental data. Unknown hydraulic parameters may be estimated from observed water contents, pressure heads, and/or boundary fluxes during transient flow by numerical inversion of the Richards equation. Additional retention or hydraulic conductivity data, as well as a penalty function for constraining the optimized parameters to remain in some feasible region (Bayesian estimation) can be optionally considered. The procedure similarly permits solute transport and/or reaction parameters to be estimated from observed concentrations and related data.

Agricultural applications of HYDRUS include irrigation and drainage design, salinization of irrigated lands, pesticide leaching and volatilization, virus transport in the subsurface, and analysis of riparian systems. Typical non-agricultural problems include the design of radioactive waste disposal sites, contaminant leaching from landfills, design and analysis of capillary barriers, transport and degradation of chlorinated hydrocarbons, and recharge from deep vadose zones. Any of these applications, in principle, may involve parameter estimation. Several strategies can be followed for this purpose. First, one could use water flow information only (e.g., pressure heads and/or fluxes) to estimate the soil hydraulic parameters, followed by estimation of the transport parameters using information from the transport part of the experiment (e.g., solute concentrations). Alternatively, combined water flow and transport information can be used to estimate soil hydraulic and solute transport parameters in a sequential manner. Finally, combined water flow and transport information can be used to simultaneously estimate both the soil hydraulic and solute transport parameters. This last approach is the most beneficial since it uses crossover effects between state variables and parameters, and takes advantage of all available information since concentrations are a function of water flow. Several studies have shown that simultaneous estimation of hydraulic and transport properties yields smaller estimation errors for model parameters than sequential estimation.

Even with the use of parameter estimation software, appropriate experiments for determining the unsaturated soil hydraulic properties can be very time-consuming and costly. One alternative is to use pedotransfer functions (PTFs) to indirectly estimate the hydraulic properties from more easily measured and/or readily available data such as soil texture and bulk density. We developed a Windows-based software package, Rosetta, for this purpose. The PTFs in Rosetta are based on a combined bootstrap-neural network procedure to predict water retention parameters and the saturated and unsaturated hydraulic conductivity, as well as their probability distributions. The PTFs were calibrated on a large number of soil hydraulic data sets derived from three different databases, including the UNSODA unsaturated soil hydraulic database developed at the Salinity Laboratory (Nemes et al., 2001). Rosetta offers a hierarchical set of five PTFs to predict van Genuchten-Mualem type hydraulic parameters depending upon available information, from limited data (soil textural class only) to more extensive data (texture, bulk density, and one or two water retention points). One attractive feature of Rosetta is that it provides uncertainties in its parameter estimates (Figure 1). Uncertainty estimates are generated with the bootstrap method and are given as standard deviations around the estimated hydraulic parameters (Schaap et al., 2001). The uncertainties, which depend upon the invoked PTF model and its input data, are useful in cases where few or no hydraulic data are available. They are particularly useful for risk-based simulations of water flow and solute transport.



	Sand	Clay
Sand %	**79**	**28**
Silt %	**13**	**29**
Clay %	**8**	**43**
Bulk d.	**1.45**	**1.44**

Figure 1. Examples of 90% confidence intervals generated with Rosetta for water retention and the unsaturated hydraulic conductivity for two soils.

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