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Development and Applications of the HYDRUS and STANMOD Software Packages and Related Codes

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Mathematical models have become indispensable tools for studying vadose zone flow and transport processes. We reviewed the history of development, the main processes involved, and selected applications of HYDRUS and related models and software packages developed collaboratively by several groups in the United States, the Czech Republic, Israel, Belgium, and the Netherlands. Our main focus was on modeling tools developed jointly by the U.S. Salinity Laboratory of the USDA, Agricultural Research Service, and the University of California, Riverside. This collaboration during the past three decades has resulted in the development of a large number of numerical [e.g., SWMS_2D, HYDRUS-1D, HYDRUS-2D, HYDRUS (2D/3D), and HP1] as well as analytical (e.g., CXTFIT and STANMOD) computer tools for analyzing water flow and solute transport processes in soils and groundwater. The research also produced additional programs and databases (e.g., RETC, Rosetta, and UNSODA) for quantifying unsaturated soil hydraulic properties. All of the modeling tools, with the exception of HYDRUS-2D and HYDRUS (2D/3D), are in the public domain and can be downloaded freely from several websites.

Abbreviations: GUI, graphical user interface; UCR, University of California, Riverside; USSL, U.S. Salinity Laboratory.

Solving problems involving flow, transport, and biogeochemical processes in the subsurface environment requires appropriate modeling tools consistent with the application. While certain problems may be solved using relatively simple analytical or semianalytical models, other problems may require more sophisticated numerical models, either one- or multidimensional, that simulate water flow, solute transport, and a range of biogeochemical reactions. To have the flexibility in optimally addressing general as well as site-specific environmental problems, one may thus need a toolbox containing a variety of computer programs of varying complexities. A large number of such computer tools have been developed jointly by the U.S. Salinity Laboratory (USSL) and the University of California, Riverside (UCR) during a time span of about 30 yr and released to the public. It is our objective to describe the most pertinent of these computer programs and discuss several applications.

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We describe here the history of development, the main processes involved, and selected applications of HYDRUS and related models and software packages (Table 1). Our main focus is initially on the numerical HYDRUS models, their predecessors, and various modifications and extensions thereof [e.g., SWMS_2D, HYDRUS-1D, HYDRUS-2D, HYDRUS (2D/3D), and HP1] that resulted from the work of several groups of developers in the United States, the Czech Republic, Israel, the Netherlands, and Belgium. We also summarize several other modeling tools, however, that were developed in close collaboration between the USSL and UCR, such as the CXTFIT and STANMOD codes for analytical transport modeling, as well as additional software and databases (e.g., RETC, Rosetta, and UNSODA) for analyzing unsaturated soil hydraulic properties. All of the tools and databases, with the exception of HYDRUS-2D and HYDRUS (2D/3D), are in the public domain. A CD containing the various codes and manuals is freely available from USSL. Most codes can also be downloaded freely from both the HYDRUS website (www.hydrus2d.com or www.pc-progress.cz [verified 3 Mar. 2008]) and the USSL site (www.ars.usda.gov/Services/docs.htm?docid=15992 [verified 3 Mar. 2008]). It is beyond the scope of this work to describe all applications for which the various programs have been used. A comprehensive list of publications showing a large number of applications can be found at www.pc-progress.cz/Pg_Hydrus1D_References.htm (verified 3 Mar. 2008) for HYDRUS-1D and related software and at www.pc-progress.cz/Pg_Hydrus_References.htm (verified 3 Mar. 2008) for HYDRUS-2D and its predecessors.

Table 1. The HYDRUS and related models and software packages.

Model	Version	Operating system	Dimensions†	Brief description (processes)‡	Reference
HYDRUS	3.0	DOS	1	Variably saturated water flow and solute transport in porous media	Kool and van Genuchten (1991)
	5.0	DOS	1	Variably saturated water flow and solute transport in porous media	Vogel et al. (1996)
	6.0	DOS	1	Variably saturated water flow and solute transport in porous media	Šimůnek et al. (1998b)
SOILCO2	1.0	DOS	1	Variably saturated water flow and transport of CO_2 in porous media; MVG	Šimůnek and Suarez (1993c)
UNSATCHEM	2.0	Windows	1	Variably saturated water flow and transport of major ions and CO_2 in porous media; MVG; 16 bit GUI	Šimůnek et al. (1996b)
HYDRUS-1D	2.0	Windows	1	Variably saturated water flow and solute transport in porous media; root water and solute uptake; VG, MVG, BC; hysteresis in soil hydraulic properties; nonlinear solute transport; sequential first-order decay chains; temperature dependence of soil hydraulic and solute transport parameters; two-site sorption model; dual-porosity mobile–immobile water solute transport; inverse problem; 32 bit GUI	Šimůnek et al. (1998b)
	3.0	Windows	1	Version 2.0 + Durner (1994) and Kosugi (1996) soil hydraulic property models; dual-porosity water flow; snow accumulation; compensated root water uptake; virus, colloid, and bacteria transport; transport of major ions and CO_2 (UNSATCHEM); 32 bit GUI	Šimůnek et al. (2005)
SWMS_2D	1.0	DOS	2	Variably saturated water flow and solute transport in porous media; root water and solute uptake; MVG; linear solute transport	Šimůnek et al. (1992)
	2.0	DOS	2	Version 1.0 + iterative solvers for the system of linear equations; predecessor of the 1.0 version of HYDRUS-2D	Šimůnek et al. (1994)
CHAIN_2D	1.0	DOS	2	Version 2.0 of SWMS_2D + nonlinear solute transport; sequential first-order decay chains; gas diffusion; two-site sorption model; temperature dependence of soil hydraulic and solute transport parameters; predecessor of the 2.0 version of HYDRUS-2D	Šimůnek and van Genuchten (1994)
UNSATCHEM-2D	1.0	DOS	2	Variably saturated water flow and transport of major ions and CO_2 in porous media; MVG	Šimůnek and Suarez (1993b)
SWMS_3D	1.0	DOS	3	Variably saturated water flow and solute transport in porous media; root water and solute uptake; MVG; linear solute transport; iterative solvers for the system of linear equations; predecessor of the 1.0 version of HYDRUS (2D/3D)	Šimůnek et al. (1995)
HYDRUS-2D	1.0	Windows	2	SWMS_2D (2.0) + 16 bit GUI	Šimůnek et al. (1996a)
	2.0	Windows	2	CHAIN_2D + 32 bit GUI; dual-porosity mobile–immobile water solute transport; hysteresis in soil hydraulic properties; inverse problem.	Šimůnek et al. (1999a)
HYDRUS (2D/3D)	1.0	Windows	2, 3	HYDRUS-2D (2.0) + SWMS_3D + 32 bit GUI; two- and three-dimensional variably saturated water flow and solute transport in porous media; VG, MVG, Durner (1994), and Kosugi (1996) soil hydraulic property models; hysteresis in soil hydraulic properties; nonlinear solute transport; sequential first-order decay chains; gas diffusion; temperature dependence of soil hydraulic and solute transport parameters; two-site sorption model; dual-porosity mobile–immobile water flow; virus, colloid, and bacteria transport; constructed wetland module	Šimůnek et al. (2006b), Šejna and Šimůnek (2007)
DISK		Windows	2	Software package for analyzing data collected with the tension disk infiltrometer; 32 bit GUI	Šimůnek and van Genuchten (2000)
STANMOD	2.0	Windows	1, 2, 3	Studio of analytical models for analyzing solute transport, including CFitM (van Genuchten, 1980b), CFitIm (van Genuchten, 1981b), Chain (van Genuchten, 1985), CXTFIT (Toride et al., 1995), 3ADE (Leij and Bradford, 1994), N3DADE (Leij and Toride, 1997), and Screen (Jury et al., 1983); 32 bit GUI.	Šimůnek et al. (1999b)
RETC		Windows	NA	Software package for analyzing soil hydraulic properties; VG, BC, Durner (1994), and Kosugi (1996) soil hydraulic property models; 32 bit GUI.	Released online
ROSETTA	1.0	Windows	NA	Hierarchical neural network pedotransfer functions for the van Genuchten–Mualem equations	Schaap et al. (2001)
UNSODA		Windows	NA	Database serving as a repository of measured unsaturated soil hydraulic property data	Leij et al. (1996)
HP1	1.0	Windows	1	One-dimensional water flow; transport of multiple components; mixed equilibrium–kinetic biogeochemical reactions; heat transport in variably saturated media	Jacques and Šimůnek (2005)

† 2 refers to two-dimensional and axisymmetrical three-dimensional; NA, not applicable.

‡ GUI, graphical user interface; BC, Brooks and Corey (1964); MVG, modified van Genuchten soil hydraulic functions (Vogel and Císlerová, 1988).

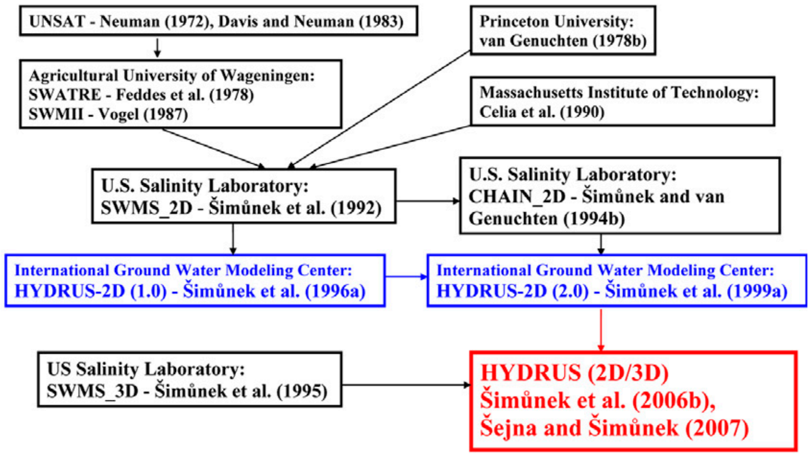

FIG. 1. History of development of HYDRUS and related software packages. Software packages supported by graphical user interfaces are in color (2D, blue; 2D/3D, red).

DOS Numerical Models

UNSAT and SWMII

The two-dimensional HYDRUS models and their predecessors have a long history (Fig. 1). The origin of these models can be traced back to the early work of Dr. Shlomo Neuman and collaborators (Neuman, 1972, 1973, 1975; Neuman et al., 1974), who developed their UNSAT model at the Hydraulic Engineering Laboratory of Technion, Israel Institute of Technology, in Haifa, Israel, long before the introduction of personal computers. The UNSAT model was a finite element model simulating water flow in two-dimensional variably saturated domains as described with the Richards equation (Richards, 1931). The model additionally considered root water uptake as well as a range of pertinent boundary conditions required to ensure wide applicability of the model. The UNSAT model was later modified by Davis and Neuman (1983) at the University of Arizona, Tucson, such that the model could be run on personal computers. This last version of UNSAT formed the basis of the SWMII model developed by Vogel (1987) during his stay with Dr. Reinder Feddes and Dr. Han Stricker at Wageningen University, Wageningen, the Netherlands.

The SWMII model significantly extended the capabilities and ease of use of UNSAT. The code simulated variably saturated water flow in two-dimensional transport domains, implemented the van Genuchten soil hydraulic functions (van Genuchten, 1980a) and modifications thereof (Vogel and Císlerová, 1988), considered root water uptake by taking advantage of some of the features of the SWATRE model (Feddes et al., 1978), and included scaling factors to enable simulations of flow in heterogeneous soils. The code also allowed the flow region to be composed of nonuniform soils having an arbitrary degree of local anisotropy. The SWMII model was a direct predecessor of the SWMS_2D model (Šimůnek et al., 1992) developed later at USSL.

SWMS_2D

The SWMS_2D model (Šimůnek et al., 1992) considerably extended the capabilities of SWMII by including provisions for solute transport. The speed and computational efficiency of the water flow calculations (still a major concern in the early and mid-1990s) were increased by restricting calculations for the second and subsequent iterations during the iterative solution process of the Richards equation only to those parts of the flow domain that registered changes in the pressure head during the first iteration. Solute transport was described using the standard advection–dispersion equation that included linear sorption, first-order degradation in both the liquid and solid phases, and zero-order production in both phases. Several other numerical improvements were at the time also implemented in SWMS_2D. These included solution of the mixed form of the Richards equation as suggested by Celia et al. (1990), thus providing excellent mass balances in the water flow calculations, and higher order corrections to the dispersion term (van Genuchten, 1978c) to improve the numerical solution of the transport equation. While SWMII could simulate water flow in two dimensions in either vertical or horizontal planes, SWMS_2D extended the range of applications also to three-dimensional axisymmetrical flow domains around a vertical axis of symmetry. Examples are flow to a well, infiltration from a surface ring or tension disk infiltrometer, and infiltration from a surface or subsurface dripper.

The original version (1.1) of SWMS_2D used Gaussian elimination to solve the systems of linear algebraic equations resulting from discretization of the governing partial differential equations. The invoked solvers took advantage of the banded nature of the coefficient matrices and, in the case of water flow, of the symmetric properties of the matrix. Since direct solution methods have several disadvantages compared with iterative methods, especially for relatively large problems, we supplemented the direct solvers in Version 1.2 of SWMS_2D (Šimůnek et al., 1994) using iterative solvers adopted from the ORTHOFEM software package of Mendoza et al. (1991). The system of linear algebraic equations for water flow were solved using the preconditioned conjugate gradient method, and for solute transport using the ORTHOMIN (preconditioned conjugate gradient squared) procedure (Mendoza et al., 1991).

Since SWMS_2D was in the public domain and distributed freely by USSL on a CD or downloadable from the USSL website, the code quickly became popular with many users. The HYDRUS website lists a large number of references, from various peer-reviewed journals, in which SWMS_2D was used. The search for this list was performed using Google Scholar. Model applications involved both agricultural and nonagricultural problems. Early agricultural applications included simulations of various irrigation or drainage schemes (e.g., Benjamin et al., 1994; Meshkat et al., 1999) and the transport of various chemicals applied to agricultural soils (e.g., de Vos et al., 2000). Early nonagricultural applications included studies of flow and transport in heterogeneous porous media (e.g., Tseng and Jury, 1994; Roth, 1995; Roth and Hammel, 1996; Hammel and Roth, 1998). These studies showed that due to soil heterogeneity, water and solutes can find flow paths that are much more conductive than would be expected from the average hydraulic conductivity.

CHAIN_2D

The first major upgrade of SWMS_2D was released under the name CHAIN_2D (Šimůnek and van Genuchten, 1994). This model greatly expanded on the capabilities of SWMS_2D by including, among other things, sequential first-order solute decay chains and heat transport. The temperature dependence of the soil hydraulic properties was included by considering the effects of temperature on surface tension, dynamic viscosity, and the density of water. The heat transport equation in CHAIN_2D considered transport due to conduction and advection with flowing water. The solute transport equations considered advective–dispersive transport in the liquid phase, as well as diffusion in the gaseous phase. The transport equations also included provisions for nonlinear nonequilibrium reactions between the solid and liquid phases, linear equilibrium reactions between the liquid and gaseous phases, zero-order production, and two first-order degradation reactions: one that was independent of other solutes, and one that provided the coupling between solutes involved in the sequential first-order decay reactions. Typical examples of sequential first-order decay chains are the transport of radionuclides (van Genuchten, 1985), N species (e.g., Hanson et al., 2006), pesticides (Wagenet and Hutson, 1987), chlorinated aliphatic hydrocarbons (Schaerlaekens et al., 1999; Casey and Šimůnek, 2001), hormones (Casey et al., 2003), and explosives (Dontsova et al., 2006). The additional solute transport processes in CHAIN_2D also allowed simulations of the transport of volatile contaminants, such as methyl bromine or 1,3-dichloropropene (e.g., Wang et al., 1997, 2000).

UNSATCHEM-2D

The SWMS_2D model was further expanded by Šimůnek and Suarez (1993b, 1994) to also simulate the transport of major ions in variably saturated porous media, including major ion equilibrium and kinetic nonequilibrium chemistry. The resulting UNSATCHEM-2D code was intended for prediction of major ion chemistry and water and solute fluxes in soils during transient flow. Since the solution chemistry in the unsaturated zone is significantly influenced by variations in water content, temperature, and CO_2 concentrations in the soil gas phase, all of these variables were included in the model. The CO_2 transport and production model was based on the SOILCO2 model (Šimůnek and Suarez, 1993a,c) described below. The major variables of the chemical system in UNSATCHEM-2D were Ca, Mg, Na, K, SO_4, Cl, NO_3, H_4SiO_4, alkalinity, and CO_2. The model accounted for various equilibrium chemical reactions between these components, such as complexation, cation exchange, and precipitation–dissolution. For the precipitation–dissolution of calcite and dissolution of dolomite, either equilibrium or multicomponent kinetic expressions could be used, which included both forward and backward reactions. Other dissolution–precipitation reactions considered included gypsum, hydromagnesite, nesquehonite, and sepiolite. Since the ionic strength of soil solutions can vary considerably in time and space and often reach high values, both the modified Debye–Hückel and Pitzer expressions were incorporated into the model to calculate single ion activities.

SWMS_3D

The SWMS_3D model (Šimůnek et al., 1995) was a direct extension of the SWMS_2D code (Version 1.2) to three-dimensional flow and transport problems. The model uses the finite element method with tetrahedral linear finite elements to solve the Richards equation for water flow and the advection–dispersion equation with linear sorption for solute transport in three-dimensional transport domains.

Three-dimensional applications often require a large number of finite elements to discretize realistically large transport domains. Even with the fast personal computers currently available, it is virtually impossible to solve, within a reasonable computational time, problems having more than about half a million nodes or more. To decrease the required computational time, Hardelauf et al. (2007) parallelized SWMS_3D to develop PARSWMS, which distributes problems with a large number of elements across multiple processors working in parallel. The PARSWMS code was developed for Linux or UNIX workstations using the installed freewares MPI, PETSc, and PARMETIS. Hardelauf et al. (2007) demonstrated that doubling the number of processors may decrease the computational time by up to nearly 50%.

The majority of applications of the different DOS-based multidimensional numerical models discussed above involved relatively simple geometrical domains since these codes were supported only by simple finite element mesh generators for either structured quadrilateral or hexagonal geometries. Users were responsible for preparing their own inputs characterizing the computational domains and discretizing them into finite elements. Broader applicability and adoption of the codes could be accomplished only by development of graphical tools for easier domain design and their discretization into finite elements. This was accomplished with the second generation of the various modeling tools, starting with Version 1.0 of HYDRUS-2D as described below.

HYDRUS

The one-dimensional HYDRUS models were initially developed mostly independently of their multidimensional counterparts. It was only with the later versions of the Windows-based HYDRUS-1D (Šimůnek et al., 1998c) and HYDRUS-2D (Šimůnek et al., 1999a) software packages that the various processes in these programs were unified. Selected features of earlier one-dimensional codes, such as SUMATRA-1 (van Genuchten, 1978b), WORM (van Genuchten, 1987), and SWMI (Vogel, 1990) had been incorporated into the DOS-based one-dimensional HYDRUS models simulating water flow and solute transport in one-dimensional variably saturated soils (HYDRUS 3.0 of Kool and van Genuchten, 1991; HYDRUS 5.0 of Vogel et al., 1996; HYDRUS 6.0 of Šimůnek et al., 1998b). Most of these codes additionally also considered root water uptake, as well as solute transport subject to linear sorption, first-order degradation in both the liquid and solid phases, and zero-order production in both phases. Interestingly, there was at the time very little common code and overlap between the different versions of the DOS-based HYDRUS codes. For example, the early UNSAT1 and SUMATRA-1 codes of van Genuchten (1978b,c) were based on Hermitian cubic finite element schemes, which proved to be less suitable for highly nonlinear infiltration scenarios than those using standard linear finite elements. Starting in 1998, the Windows-based HYDRUS-1D (Šimůnek et al., 1998c) and HYDRUS-2D (Šimůnek et al., 1999a) software packages unified most or all of the processes and numerical procedures included in the various codes.

SOILCO2

Šimůnek and Suarez (1993a,c) additionally developed a predictive simulation model, SOILCO2, to simulate one-dimensional water flow and multiphase transport of CO_2 based on the Richards and advection–dispersion equations, respectively. The model also included heat transport and a CO_2 production module. Transport of CO_2 was assumed to occur in both the liquid and gas phases. The gas transport equation accounted for production of CO_2 and uptake of CO_2 by plant roots associated with root water uptake. The CO_2 production model considered microbial as well as root respiration, which both depend on water content, temperature, plant growth, salinity, and plant and soil characteristics. Heat flow was included in the model since several CO_2 transport parameters and various partitioning and production coefficients are strongly temperature dependent. An early application of SOILCO2 to field data was presented by Suarez and Šimůnek (1993).

Although all of the above DOS-based programs are still publicly available (most can still be downloaded from the USSL web site), none is currently being developed further since they have been replaced with Windows-based programs or modules as described below.

Windows-Based Numerical Models

Even with well-documented technical or user manuals available, one major problem often preventing the use of DOS-based numerical codes is the extensive work generally required for data preparation, finite element grid design, and graphical presentation of the output results (Šimůnek et al., 1996a). The widespread adoption of numerical models requires techniques that make it easier for users to create, manipulate, and display large data files, and to facilitate interactive data management. Introducing such techniques frees users from cumbersome manual data processing and should enhance the efficiency in which programs are being implemented for a particular example. To avoid or simplify the preparation and management of relatively complex input data files and to graphically display final simulation results, we started in 1995 developing interactive graphical user interfaces (GUIs) for the Microsoft Windows environments that resulted in several software packages described below. While the earlier Windows-based versions were still 16-bit applications, all software packages released starting in 1998 were 32-bit applications.

HYDRUS-1D

The HYDRUS-1D software packages (Šimůnek et al., 1998c, 2005) (Fig. 2) were based on the latest DOS Version 6.0 of HYDRUS (Šimůnek et al., 1998b). Three major upgrades of HYDRUS-1D have been released so far. While the difference between Versions 1.0 and 2.0 was mainly technical (16- vs. 32-bit applications, respectively), Version 3.0 (Šimůnek et al., 2005) represented a major upgrade with several new processes included in the software package. Version 2.0 of HYDRUS-1D (Šimůnek et al., 1998c) may be used to simulate the one-dimensional movement of water, heat, and multiple solutes in variably saturated media. The program uses linear finite elements to numerically solve the Richards equation for saturated–unsaturated water flow and Fickian-based advection–dispersion equations for both heat and solute transport. The flow equation also includes a sink term to account for water uptake by plant roots as a function of both water and salinity stress. The unsaturated soil hydraulic properties can be described using van Genuchten (1980a), Brooks and Corey (1964), and modified van Genuchten (Vogel and Císlerová, 1988) type analytical functions. The heat transport equation considers conduction as well as advection with flowing water. The solute transport equations assume advective–dispersive transport in the liquid phase and diffusion in the gaseous phase. The transport equations further include provisions for nonlinear and nonequilibrium reactions between the solid and liquid phases, linear equilibrium reactions between the liquid and gaseous phases, zero-order production, and two first-order degradation reactions: one that is independent of other solutes, and one that provides the coupling between solutes involved in sequential first-order decay reactions. In addition, physical nonequilibrium solute transport can be accounted for by assuming a two-region, dual-porosity type formulation that partitions the liquid phase into mobile and immobile regions.

The HYDRUS-1D software may be used to analyze water and solute movement in unsaturated, partially saturated, or fully saturated homogeneous layered media. The code incorporates hysteresis by assuming that drying scanning curves are scaled from the main drying curve and wetting scanning curves from the main wetting curve. Root growth is simulated by means of a logistic growth function, while root water uptake can be simulated as a function of both water and salinity stress. The HYDRUS-1D software package additionally implements a Marquardt–Levenberg type parameter estimation technique (Marquardt, 1963; Šimůnek and Hopmans, 2002) for inverse estimation of soil hydraulic (Šimůnek et al., 1998d; Hopmans et al., 2002) and solute transport and reaction (Šimůnek et al., 2002) parameters from measured transient or steady-state flow or transport data. The programs are, for this purpose, written in such a way that almost any application that can be run in a direct mode can equally well be run in an inverse mode and thus for model calibration and parameter estimation. The inverse option has proved to be very popular with many users, leading to a large number of applications ranging from relatively simple laboratory experiments, such as one- and multistep outflow or evaporation

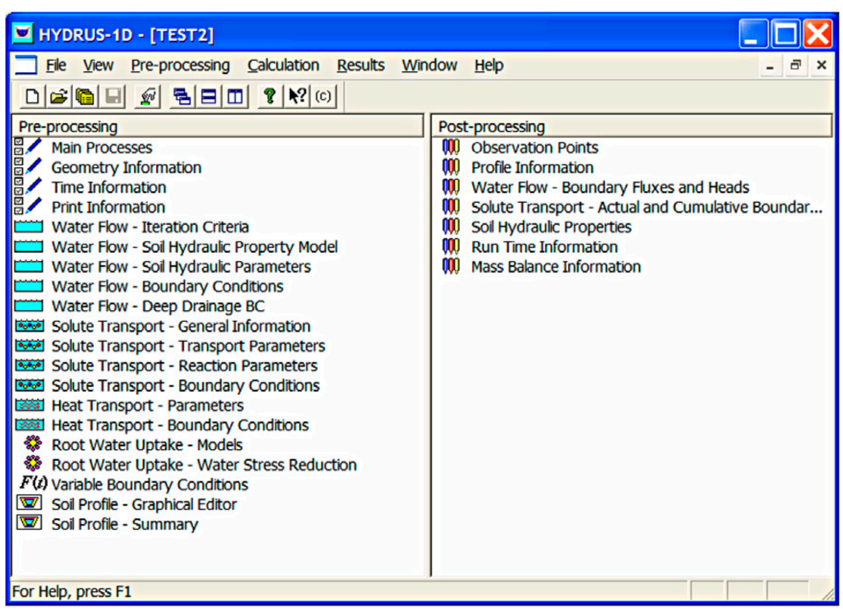

Fig. 2. Main window of the HYDRUS-1D software package. The preprocessing part is on the left and post-processing part on the right. Individual input and output commands are accessible either using menus or directly from the main window.

experiments to more elaborate field problems involving multiple soil horizons and chemicals. We refer to the HYDRUS website for specific examples.

The HYDRUS-1D package uses a Microsoft Windows-based GUI to manage the input data required to run the program, as well as for nodal discretization and editing, parameter allocation, problem execution, and visualization of results. All spatially distributed parameters, such as those for various soil horizons, root water uptake distribution, and the initial conditions for water, heat, and solute movement, are specified in a graphical environment. The program offers graphs of the distributions of the pressure head, water content, water and solute fluxes, root water uptake, and temperature and solute concentrations in the subsurface at preselected times. Also included is a small catalog of unsaturated soil hydraulic properties (Carsel and Parrish, 1988) as well as pedotransfer functions based on neural networks (Schaap et al., 2001).

Version 3.0 of HYDRUS-1D (Šimůnek et al., 2005) includes several new features compared with Version 2.0. Among the new features are additional analytical functions for soil hydraulic properties (Durner, 1994; Kosugi, 1996), compensated root water uptake, and various provisions for simulating nonequilibrium flow and transport (Šimůnek et al., 2003; Šimůnek and van Genuchten, 2008). The flow equation for the latter purpose can consider dual-porosity-type flow, with a fraction of the water content being mobile and a fraction immobile. The transport equations additionally were modified to allow consideration of kinetic attachment–detachment processes of solutes to the solid phase, and hence of solutes having a finite size. This attachment–detachment feature has been used by many recently to simulate the transport of viruses (e.g., Schijven and Šimůnek, 2002), colloids (e.g., Bradford et al., 2002, 2003, 2004), and bacteria (e.g., Gargiulo et al., 2007a,b, 2008). The HYDRUS-1D software further includes modules for simulating CO_2 transport and major ion chemistry modules, adopted from the UNSATCHEM-2D (Šimůnek and Suarez, 1993b) and UNSATCHEM programs (Šimůnek et al., 1996b). Gonçalves et al. (2006) recently demonstrated the use of these new modules by simulating multicomponent major ion solute transport in soil lysimeters irrigated with waters of different qualities. The HYDRUS-1D package was used in this application to described field measurements of the water content, overall salinity, and concentration of individual soluble cations, as well as the Na adsorption ratio and the exchangeable Na percentage.

The water flow part of HYDRUS-1D has been recently used by Seo et al. (2007) in the HYDRUS package for MODFLOW (Harbaugh et al., 2000) to represent the effects of vadose zone processes in this widely used groundwater flow model. Being fully incorporated into the MODFLOW program, the HYDRUS package provides MODFLOW with recharge fluxes at the water table, while MODFLOW provides HYDRUS with the position of the groundwater table that is used as the bottom boundary condition. Twarakavi et al. (2008) compared the HYDRUS package to other contemporary modeling approaches and evaluated its performance for three case studies of increasing complexity.

Finally, we emphasize that HYDRUS-1D is continuously being updated with new processes. Although the new features are not always immediately made available publicly, they are usually shared immediately with colleagues so that they can be properly tested before their general release. For example, Scanlon et al. (2003) and Saito et al. (2006) used a version of HYDRUS-1D that considers coupled water, vapor, and energy movement in soils, as well as mass and energy balances at the soil surface, while Hansson et al. (2004) also considered freeze–thaw processes. Šimůnek et al. (2001), Haws et al. (2005), Köhne et al. (2004, 2006), Pot et al. (2005), and Kodešová et al. (2008), among many others, used a version of HYDRUS-1D that considers the dual-permeability flow and transport model of Gerke and van Genuchten (1993). Pang and Šimůnek (2006) evaluated bacteria-facilitated Cd transport in gravel columns using the HYDRUS-1D code with capabilities to simulate colloid-facilitated solute transport (Šimůnek et al., 2006a). Finally, Šimůnek and Nimmo (2005) used a version that allowed simulations of water flow in accelerated centrifugal fields.

HYDRUS-2D

Most or all processes in HYDRUS-1D were included also in HYDRUS-2D, including water uptake by plant roots as a function of both water and salinity stress, a range of soil hydraulic functions, solute decay chains, hysteresis, provisions for nonlinear and nonequilibrium reactions, physical nonequilibrium (dual-porosity) type solute transport, and parameter estimation capabilities. While Version 1.0 of HYDRUS-2D (Šimůnek et al., 1996a) was based on the SWMS_2D model (Šimůnek et al., 1994), Version 2.0 (Šimůnek et al., 1999a) was derived from CHAIN_2D (Šimůnek and van Genuchten, 1994). A unique feature of HYDRUS-2D is that it can handle flow regions delineated by irregular boundaries as well as three-dimensional regions exhibiting radial symmetry about the vertical axis. The code includes the MeshGen2D mesh generator (Lain and Šejna, 1992; Šejna et al., 1994), which was specifically designed for variably saturated subsurface flow and transport problems. The mesh generator may be used for defining very general domain geometries and for discretizing the transport domain into an unstructured finite element mesh.

Similarly as discussed above for HYDRUS-1D, HYDRUS-2D, before having been recently fully replaced with HYDRUS (2D/3D) as described below, was continuously being updated with new features and processes. New dynamic boundary conditions suitable for various microirrigation schemes implemented into HYDRUS-2D were used, for example, by Gärdenäs et al. (2005), Lazarovitch et al. (2005), and Hanson et al. (2006). Hansson et al. (2005) simulated water flow patterns in flexible pavements with a version of HYDRUS-2D that considered, in addition to subsurface flow, also the surface runoff described using the kinematic equation.

HYDRUS (2D/3D)

The HYDRUS (2D/3D) software package (Šimůnek et al., 2006c; Šejna and Šimůnek, 2007) (Fig. 3) is an extension and replacement of HYDRUS-2D (Version 2.0) and SWMS_3D. This software package is a complete rewrite of HYDRUS-2D and its extensions for two- and three-dimensional geometries. In addition to features and processes available in HYDRUS-2D and SWMS_3D, the new computational modules of HYDRUS (2D/3D) consider (i) water flow and solute transport in a dual-porosity system, thus allowing for preferential flow in fractures or macropores while storing water in the matrix (Šimůnek et

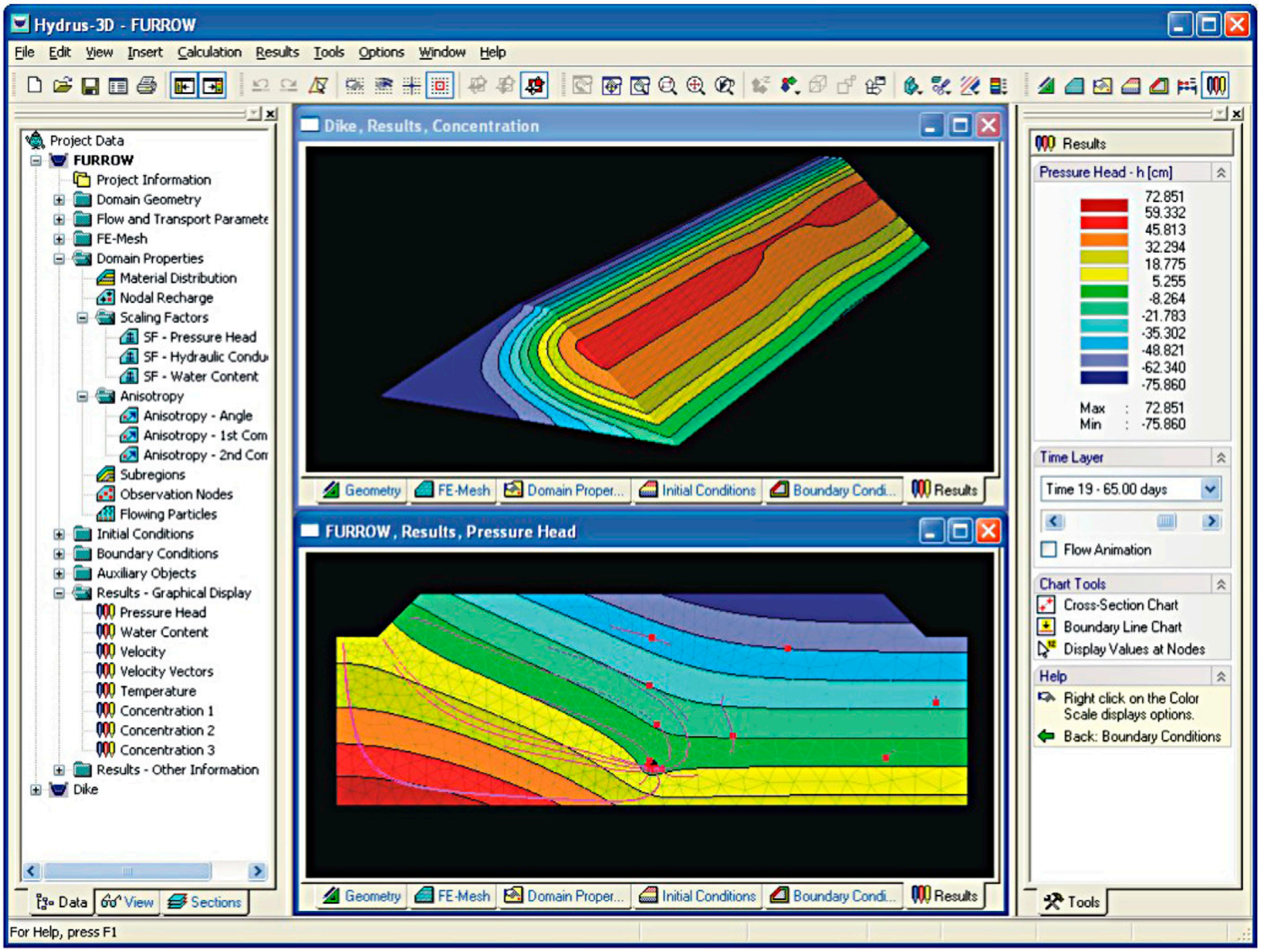

FIG. 3. Main window of the HYDRUS (2D/3D) software package. Input and output data are accessible using the data tree of the navigation bar on the left. The computational domain with its finite element discretization, various domain properties, initial and boundary conditions, and results are displayed in one or multiple view windows in the middle. Various tools for manipulating data in the view window are available on the edit bar on the right. The tabs in the view window allow fast access to different type of data.

al., 2003), (ii) root water uptake with compensation, (iii) the spatial root distribution functions of Vrugt et al. (2001), (iv) the soil hydraulic property models of Kosugi (1996) and Durner (1994), (v) the transport of viruses, colloids, and bacteria using an attachment–detachment model, filtration theory, and blocking functions (e.g., Bradford et al., 2004), (vi) a constructed wetland module (only in two dimensions) (Langergraber and Šimůnek, 2005, 2006), (vii) the hysteresis model of Lenhard et al. (1991) to eliminate pumping by keeping track of historical reversal points, (viii) new print management options, (ix) dynamic, system-dependent boundary conditions, (x) flowing particles in two-dimensional applications, and (xi) calculations of actual and cumulative fluxes across internal mesh lines.

New features of the GUI of HYDRUS (2D/3D) include, among other things, (i) a completely new GUI based on high-end three-dimensional graphics libraries, (ii) the Multiple Document Interface architecture with multiple projects and multiple views, (iii) a new organization of geometric objects, (iv) a navigation window with an object explorer, (v) many new functions improving the user friendliness, such as drag-and-drop and context-sensitive pop-up menus, (vi) improved interactive tools for graphical input, (vii) options to save cross-sections and mesh lines for charts within a given project, (viii) a new display options dialog where all colors, line styles, fonts, and other parameters of graphical objects can be customized, (ix) extended print options, (x) extended information in the Project Manager (including project previews), and (xi) an option to export input data for the parallelized PARSWMS code (Hardelauf et al., 2007).

An interesting application of HYDRUS (2D/3D) is presented by Sansoulet et al. (2008), who simulated transient spatial distributions of water fluxes in a three-dimensional transport domain under a banana (*Musa* sp.) plant.

DISC

The DISC software package (Šimůnek and van Genuchten, 2000) is a dramatic simplification of HYDRUS-2D for analyzing tension disk infiltrometer data by parameter estimation. The DISC code numerically solves the Richards equation for saturated–unsaturated water flow in a three-dimensional region exhibiting radial symmetry about the vertical axis. The software includes the Marquardt–Levenberg (Marquardt, 1963) parameter optimization algorithm for inverse estimation of soil hydraulic properties from measured transient cumulative infiltration and related data obtained during a typical tension disk permeameter experiment (Šimůnek and van Genuchten, 1996, 1997). Šimůnek and van Genuchten (1997) concluded that the best practical scenario for estimating soil hydraulic parameters from a tension disk infiltration experiment is to use the cumulative infiltration curve measured at several consecutive tensions applied to the soil surface, in conjunction with knowledge of the initial and final water content. These results suggest that one should be able to use information typically being collected with a tension disk infiltrometer to estimate not only the unsaturated hydraulic conductivity function but, without further experiments, also the soil water retention curve (Šimůnek et al., 1998a). The applicability of the suggested inverse technology using field data was recently demonstrated by Ramos et al. (2006).

UNSATCHEM

The UNSATCHEM software package (Šimůnek et al., 1996b) resulted from combining various features from SOILCO2 (water flow, heat transport, and CO_2 transport), UNSATCHEM-2D (major ion chemistry), and Version 1.0 of HYDRUS-1D (especially the GUI). We refer to the original codes for detailed descriptions of the many processes that were combined into UNSATCHEM. The UNSATCHEM package allows simulations of one-dimensional water flow, heat transport, multiphase transport of CO_2, transport of major ions, and major ion equilibrium and kinetic nonequilibrium chemistry in variably saturated porous media. The model as such can consider the effects of varying water content, temperature, CO_2–producing microbiological activity, and CO_2 transport in the soil environment on geochemical transport. The UNSATCHEM code was used to evaluate alternative strategies for sodic soil reclamation by Šimůnek and Suarez (1997), while an application assessing As oxyanion transport in gold mine heap leach facilities was demonstrated by Decker et al. (2006), the latter using a modified version that included additional species such as As and pyrite. Major ion chemistry and CO_2 transport modules of UNSATCHEM were fully incorporated into Version 3.0 of HYDRUS-1D.

HP1

The most complex modeling tool in terms of available chemical and biological reactions was recently developed by coupling HYDRUS-1D with the PHREEQC geochemical code (Parkhurst and Appelo, 1999). This coupling resulted in a new comprehensive simulation tool, HP1 (acronym for HYDRUS1D–PHREEQC, Version 1) (Jacques and Šimůnek, 2005; Jacques et al., 2006). The combined code contains modules simulating (i) transient water flow in variably saturated media, (ii) the transport of multiple components, (iii) mixed equilibrium–kinetic biogeochemical reactions, and (iv) heat transport. The HP1 program is a significant expansion of the individual HYDRUS-1D and PHREEQC programs by combining and preserving most of their original features and capabilities into a single numerical model. The code still uses the Richards equation for variably saturated flow and advection–dispersion type equations for heat and solute transport; however, the program can now simulate also a broad range of low-temperature biogeochemical reactions in water, the vadose zone, and groundwater systems, including interactions with minerals, gases, exchangers, and sorption surfaces, based on thermodynamic equilibrium, kinetics, or mixed equilibrium–kinetic reactions.

Jacques et al. (2003, 2008a,b), Jacques and Šimůnek (2005), and Šimůnek et al. (2006b) demonstrated the versatility of HP1 on several examples such as (i) the transport of heavy metals (Zn^{2+}, Pb^{2+}, and Cd^{2+}) subject to multiple cation exchange reactions, (ii) transport with mineral dissolution of amorphous SiO_2 and gibbsite [$Al(OH)_3$], (iii) heavy metal transport in a medium with a pH-dependent cation exchange complex, (iv) infiltration of a hyperalkaline solution in a clay sample (this example considered kinetic precipitation–dissolution of kaolinite, illite, quartz, calcite, dolomite, gypsum, hydrotalcite, and sepiolite), (v) long-term transient flow and transport of major cations (Na^+, K^+, Ca^{2+}, and Mg^{2+}) and heavy metals (Cd^{2+}, Zn^{2+}, and Pb^{2+}) in a soil profile, (vi) Cd leaching in acid sandy soils, (vii) radionuclide transport (U and its aqueous complexes), and (viii) the fate and subsurface transport of explosives (trinitrotoluene [TNT] and its daughter products 4-amino-2,6-dinitrotoluene [4ADNT], 2-amino-4,6-dinitrotoluene [2ADNT], and 2,4,6-triaminotoluene [TAT]).

Analytical Solute Transport Models

Parallel to the development of numerical models, joint collaborative work at USSL and UCR also produced a large number of analytical models for solute transport. These solutions pertained to one-dimensional equilibrium transport (e.g., van Genuchten, 1981a,b; van Genuchten and Alves, 1982), one-dimensional nonequilibrium transport (van Genuchten and Wierenga, 1976; van Genuchten and Wagenet, 1989; Toride et al., 1993), two- and three-dimensional equilibrium transport (Leij et al., 1991), and two- or three-dimensional nonequilibrium transport (Leij et al., 1993). Much of this work has been incorporated into a series of computer programs for both forward and inverse analyses of solute transport in soils and groundwater. The first computer codes for inverse estimation of solute transport parameters were the CFITM (van Genuchten, 1980b) and CFITIM codes (van Genuchten, 1981b), which considered the analysis of laboratory soil column breakthrough curves in terms of equilibrium and nonequilibrium transport models, respectively. These models were updated by Parker and van Genuchten (1984) to yield the widely used CXTFIT code. This program allowed analysis of column breakthrough data, as well as distributions vs. depth. The CFITM, CFITIM, and CXTFIT models were the first computerized parameter estimation codes for estimating selected equilibrium and nonequilibrium transport parameters from observed laboratory and field data. They provided a much-needed alternative to the then widely accepted but much more approximate trial and error or graphical methods for analyzing laboratory or field transport data (van Genuchten and Wierenga, 1986).

The CXTFIT code of Parker and van Genuchten (1984) was later updated by Toride et al. (1995) to allow analysis of a much broader range of laboratory and field data. The program permitted more flexible initial and boundary conditions, included more general zero- and first-order production or decay scenarios, and considered both local-scale equilibrium and nonequilibrium processes in the stochastic stream-tube models. The CXTFIT code also included a variety of stochastic stream-tube models that consider the effects of areal variations in the pore-water velocity on field-scale transport. The CXTFIT models were later extended by Leij and Bradford (1994) to three-dimensional equilibrium transport to produce the 3DADE software package, and by Leij and Toride (1997) to three-dimensional nonequilibrium transport to yield the N3DADE code. All of the above transport codes, except N3DADE, were developed for both the forward and inverse analyses.

The various analytical transport models above were all DOS-based codes. A major development next was their inclusion in the public-domain Windows-based STANMOD (STudio of ANalytical MODels) computer software package (Šimůnek et al., 1999b) (Fig. 4). In addition to CFITM, CFITIM, CXTFIT, 3DADE, and N3DADE, STANMOD also included the CHAIN code of van Genuchten (1985) for analyzing the advective–dispersive transport of up to four solutes involved in sequential first-order decay reactions (e.g., for radionuclide decay chains or the simultaneous movement of various interacting N or organic chemicals). Another one-dimensional analytical model included in STANMOD is the screening model of Jury et al. (1983) for describing the transport, degradation, and volatilization of soil-applied volatile organic chemicals. The STANMOD package hence is a very flexible tool for approximate analysis of one- two-, or multidimensional solute transport problems in soils and groundwater.

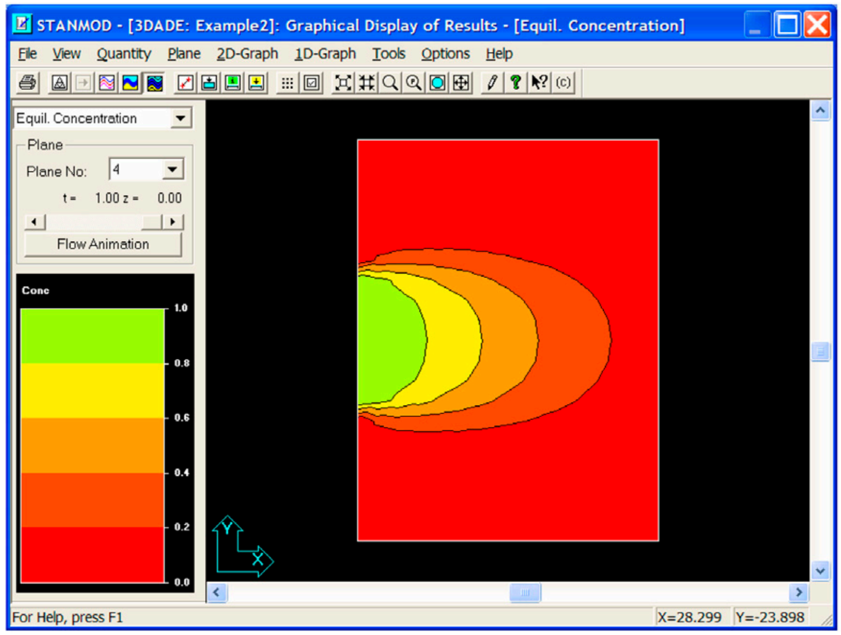

FIG. 4. Graphical display of results obtained with the STANMOD software package.

Unsaturated Soil Hydraulic Property Software

A third area of collaborative software development at USSL and UCR has been in the area of hydraulic property estimation, leading to the RETC code for analyzing soil hydraulic property data, the Rosetta software for estimating the hydraulic properties using pedotransfer functions, and the UNSODA soil hydraulic property database. These three software packages are briefly summarized below.

RETC

Much of the hydraulic property research at USSL started with the publication of van Genuchten's (1980a) study in which statistical pore-size distribution models for the unsaturated soil hydraulic conductivity (Mualem, 1976) were combined with a relatively flexible equation for the soil water retention curve to yield closed-form constitutive relationships that could be readily incorporated in numerical simulators like HYDRUS. The van Genuchten equations have become quite popular in the subsurface hydrologic literature (Kundzewicz and Koutsoyiannis, 2007) by providing an attractive alternative to the then popularly used equations of Brooks and Corey (1964). The hydraulic functions were first programmed in the SOHYP model (van Genuchten, 1978a), but later extended in the RETC code (van Genuchten et al., 1991) using fewer restrictions on the van Genuchten m and n parameters. The programs may be used to predict the unsaturated hydraulic conductivity from observed soil water retention data assuming that one observed conductivity value (not necessarily at saturation) is available. The RETC program also permits fitting of analytical functions simultaneously to observed water retention and hydraulic conductivity data. In 1999, we supplemented the RETC program with a GUI (Fig. 5) similar to STANMOD, and expanded the program to also include the lognormal distribution model of Kosugi (1996) and the dual-porosity formulation proposed initially by Durner (1994). In addition to the inverse options available in RETC, we also added a direct option for calculating the soil hydraulic functions from specified parameters.

Rosetta

Numerical models such as the HYDRUS codes simulating variably saturated flow all require information about the unsaturated soil hydraulic properties. Considering that direct measurements of the soil hydraulic properties is relatively tedious, difficult, and time consuming, many have attempted to predict

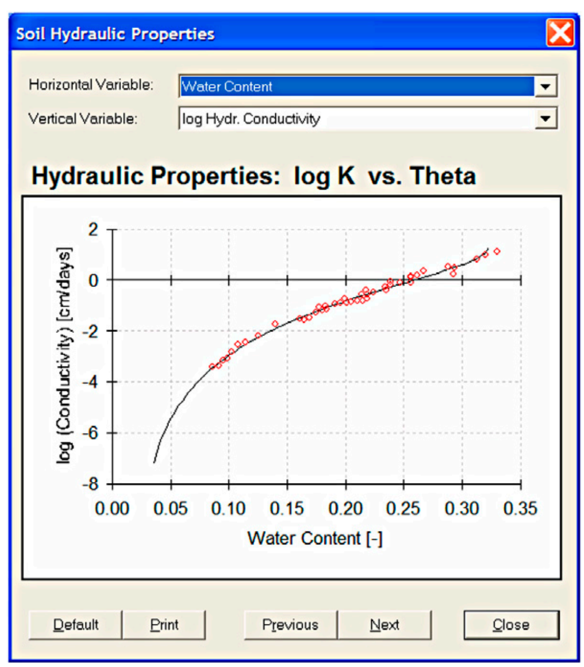

FIG. 5. Display by RETC of hydraulic conductivity data fitted with the van Genuchten-Mualem model (van Genuchten, 1980a).

soil hydraulic properties from more easily measured surrogate soil properties, such as soil texture and other more readily available information. Relationships between the soil hydraulic and other (textural) properties are commonly called pedotransfer functions (PTFs). Pedotransfer functions have been developed using various mathematical and statistical approaches, such as regression or neural network analyses (Schaap et al., 1998, 2001). Pedotransfer functions can be used to predict either the soil hydraulic properties directly, such as the water content at specified pressure heads or the saturated hydraulic conductivity, or parameters in the analytical models used for the soil hydraulic properties.

Schaap et al. (1998) calibrated hierarchical neural network PTFs for the van Genuchten–Mualem equations on a large database of soil hydraulic and related properties, and implemented the resulting PTFs into the Rosetta software package (Schaap et al., 2001). Figure 6 shows a dialog window from the HYDRUS-1D software package that implements the Rosetta Lite module (a simplification of Rosetta) of Schaap et al. (2001) to predict van Genuchten (1980a) soil hydraulic parameters using five different levels of input data. The simplest model (Model 1) uses the average of fitted hydraulic parameters within a textural class in the USDA textural triangle. These averages provide an alternative to the class-average values obtained by Carsel and Parrish (1988). The four other models in Rosetta use progressively more detailed input data, starting with the sand, silt, and clay fractions (Model 2), then adding a measured bulk density value (Model 3), and additionally requiring water contents at 33 (Model 4) and 1500 (Model 5) kPa suctions (i.e., at 330 and 15,000 cm), which are traditionally considered to be the field capacity and permanent wilting point, respectively. All estimated hydraulic parameters in Rosetta itself are accompanied by uncertainty estimates that permit an assessment of the reliability of Rosetta's predictions. These uncertainty estimates were generated by combining the neural networks with the bootstrap method (for more information, see Schaap and Leij, 2000; Schaap et al., 1998, 2001).

UNSODA

The UNSODA (UNsaturated SOil Hydraulic DAtabase) database was developed to serve as a repository of measured unsaturated soil hydraulic property data (water retention, hydraulic conductivity, and soil water diffusivity), and related soils information (particle-size distribution, bulk density, organic matter content, etc.) potentially useful for theoretical analysis of the hydraulic properties. The initial DOS-based version of the database was released in 1996 (Leij et al., 1996), but later updated (Nemes et al., 2001) in Microsoft Access 97 format to provide more flexibility in data entry and retrieval and possible interfacing with other programs. The database can be used to: (i) store and edit data; (ii) search for data sets based on user-defined query specifications; (iii) write the contents of selected data sets to an output device; and (iv) describe the unsaturated hydraulic data with closed-form analytical expressions. The UNSODA database may be used as a source of surrogate hydraulic data or for the development and evaluation of indirect methods for estimating the unsaturated hydraulic properties. The latest version contains information on close to 800 soil samples from around the world. The UNSODA database allows analysis of the unsaturated soil hydraulic data using the parametric models of Brooks and Corey (1964) and van Genuchten (1980a), although users can easily add additional hydraulic models. Several studies have relied on data from the UNSODA database to analyze alternative constitutive relationships (e.g., Leij et al., 1997; Kravchenko and Zhang, 1998; Kosugi, 1996; Schaap and van Genuchten, 2006), for predicting the hydraulic properties from particle-size data (e.g., Arya et al., 1999a,b), and for deriving PTFs (Schaap et al., 1998; Schaap and Leij, 2000).

User Feedback and Software Support

The various programs discussed here, especially the HYDRUS and STANMOD codes and their predecessors, have been used over the years in a large number of applications. We refer to the HYDRUS website (www.hydrus2d.com) for an extensive list of examples. As an example, we list here several references for a single application: drip irrigation and associated processes. References include Meshkat et al. (1999), Assouline (2002), Schmitz et al. (2002), Cote et al. (2003), Skaggs et al. (2004), Beggs et al. (2004), Li et al. (2005), Lazarovitch et al. (2005, 2007), Gärdenäs et al. (2005), and Hanson et al. (2006, 2008). Many other example applications have been compiled (see Rassam et al., 2003, 2004; Selker, 2004). Feedback from users like these has been extremely helpful in identifying strengths and weaknesses of the codes, defining additional processes or features that should be included, and for identifying coding errors. Much of the feedback and user support during the last 10 yr has been through the Frequently Asked Questions (FAQs) and troubleshooting pages of the HYDRUS web site.

The HYDRUS web site also hosts several discussion forums where users, after registering, can submit questions about the different software packages and how to use them for their particular applications. Users there can also discuss various topics related to modeling or respond to questions posted by other users. The large number of users of these discussion forums has made the forums nearly self-supporting in terms of software support and feedback. This is important because of the shear number of software questions that otherwise had to be answered by the software developers only. We note that the HYDRUS website also provides tutorials for several software packages, including brief downloadable

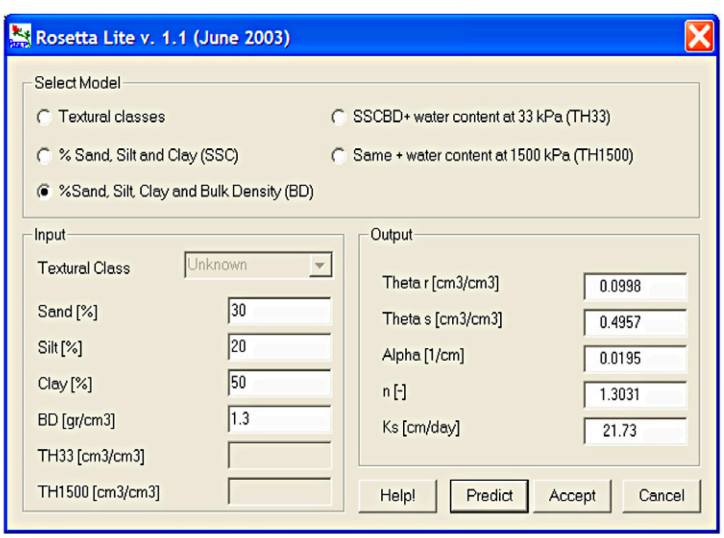

FIG. 6. The Rosetta Lite dialog window from the HYDRUS-1D software package.

videos in which these tutorials are performed step by step, thus allowing software users to teach themselves interactively about the basic components of the software, including the process of data entry and display of calculated results. We also dramatically extended the documentation for several software packages. For example, the installation of the latest HYDRUS (2D/3D) is accompanied by 240 pages of information in the technical manual, a 200-page user manual, and more than 1000 pages of online context-sensitive help. Each Windows-based software package furthermore comes with a suite of test problems, most of which are described in detail in the corresponding technical manuals. Major sources of information for new users are always previously published studies in which the programs have been used. Of course, a major satisfaction for software developers like us is to see the programs being actively used in various applications, and to see results of the applications published in the literature. We therefore are continuously updating the list of such publications at www.pc-progress.cz/Pg_Hydrus1D_References.htm for HYDRUS-1D and related software packages, and at www.pc-progress.cz/Pg_Hydrus_References.htm for HYDRUS-2D (or 2D/3D) and its predecessors.

Conclusions

Collaboration between the USSL and the UCR during the past 30 yr has resulted in the development of a large number of popularly used computer tools for studying vadose zone flow and transport processes. These tools include numerical models for one- or multidimensional variably saturated flow and transport (e.g., HYDRUS-1D and HYDRUS-2D), analytical models for solute transport in soils and groundwater (e.g., CXTFIT and STANMOD), and tools or databases for analyzing or predicting the unsaturated soil hydraulic properties (e.g., RETC and UNSODA). The wide use of these models is in large part due to their ease of use because of the availability of interactive GUIs. The modeling tools cover a large number of processes, from relatively simple one-dimensional solute transport problems to multidimensional flow and transport applications at the field scale, including relatively complex problems involving a range of biogeochemical reactions. An example of the latter is the HP1 program that couples the HYDRUS-1D software package with the PHREEQC geochemical code.

We believe that the software tools have served, and are serving, an important role in vadose zone research. This is reflected by their frequent use in a variety of applications (many of them leading to peer-reviewed publications) and the favorable reviews the programs have received recently. For example, the HYDRUS-2D software package was reviewed by Diodato (2000) and Tyler (2004). The STANMOD software package was reviewed by Divine (2003), the HYDRUS-1D software package by Scanlon (2004), and the latest HYDRUS (2D/3D) program by McCray (2007). The need for codes such as HYDRUS and STANMOD is further reflected by the frequency of downloading from the HYDRUS website. For example, HYDRUS-1D was downloaded more than 200 times in March 2007 by users from 30 different countries, and more than 1000 times in 2006. The HYDRUS website receives, on average, some 700 individual visitors each day.

Acknowledgments

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