# Integrated modeling of flow and transport processes in saltaffected soils

M.Th. van Genuchten<sup>1</sup> and J. Šimůnek<sup>2</sup>

<sup>1</sup>George E. Brown, Jr. Salinity Laboratory, USDA, ARS, Riverside, CA, USA, rvang@ussl.ars.usda.gov

## 1 INTRODUCTION

Irrigation has contributed significantly to increased crop production worldwide. Unfortunately, irrigation has contributed also to increased salinization of agricultural lands, and has caused the destruction of agriculture in many areas. As much as 25% of the world's irrigation areas may be salt affected, while 40% may be saline, sodic or waterlogged (e.g., Ghassemi et al., 1995). Salinity is inevitably associated with the adopted irrigation and drainage practices. Effective management of salt-affected soils hence requires detailed knowledge of the many coupled processes involved. Computer models have become increasingly important tools to assist in the management, analysis, and solution of site-specific irrigation, salinization and/or crop production problems.

Traditionally, much of the research in salinity and irrigation/drainage has progressed along disciplinary lines (e.g., soil physics, agricultural engineering, soil and geochemistry, microbiology, plant physiology) in which the various physical, chemical and microbiological processes were too often studied and implemented in relative isolation. The introduction of increasingly powerful computers, advanced numerical methods and improved understanding of subsurface flow and transport processes, now provide tremendous opportunities for integrating the various processes involved. One such integrated approach is provided by the HYDRUS models developed at the Salinity Laboratory in collaboration with the University of California, Riverside. In this paper we summarize ongoing research related to the HYDRUS-1D and HYDRUS-2D computer software packages (Šimůnek et al., 1998, 1999) for simulating subsurface one- and multi-dimensional water flow and solute transport. Brief overviews are given of the various features incorporated in the software packages, recent applications, and future plans.

## 2 OVERVIEW OF HYDRUS SOFTWARE FEATURES

The HYDRUS codes are Windows-based (MS Windows 95, 98, 2000, XP, and/or NT environments) software packages for simulating water, heat and/or solute movement in one-and two-dimensional soil and groundwater systems. Table 1 gives an overview of the different processes currently incorporated in HYDRUS. Variably-saturated water flow is simulated using the standard Richard equation, which may be applied to unsaturated systems, or to systems that are partially or completely saturated. Root-water uptake as a function of water and salinity stress is simulated using stress response functions that can have the familiar threshold slope features, or consist of more realistic sigmoidal functions (van Genuchten, 1987). Solute transport is simulated using standard advection-dispersion equations, augmented as

<sup>&</sup>lt;sup>2</sup>Department of Environmental Sciences, University of California, Riverside, CA, USA

needed with nonlinear sorption isotherms and/or chemical (two-site) or physical (mobile-immobile) nonequilibrium processes. Heat transport is also considered.

Table 1. Features included in current versions of the HYDRUS software packages

Feature	Comments
Variably-saturated water flow	Richards equation (1-D, 2-D, axisymmetric flow)
Root water uptake	Water and salinity stress effects on water uptake
Solute transport	Advection-dispersion transport equations
Multiple solutes	Consecutive decay chains
Nonlinear sorption	Freundlich-Langmuir isotherms, or simplifications thereof
Nonequilibrium sorption	One-site and two-site nonequilibrium sorption
Preferential flow	Mobile-immobile water; other processes
Heat transport	Convective and conductive heat movement
Unsaturated soil hydraulic properties	Several constitutive models; hysteresis
Pedotransfer functions	Textural class averages and Rosetta-based estimates
Parameter estimation	Marquardt-Levenberg optimization
Graphical User Interfaces (GUIs)	Windows-based interactive pre- and post-processors

An attractive feature of the HYDRUS codes that has greatly facilitated their utility for a broad range of applications is the inclusion of parameter estimation (inverse) procedures. The objective function that is minimized for this purpose in the HYDRUS models consists of three terms: (1) deviations between measured and calculated variables (e.g., observed pressure heads, water contents, concentrations and/or fluxes), (2) differences between independently measured and predicted soil hydraulic or other data (e.g., specific soil water retention and hydraulic conductivity data), and (3) deviations between prior knowledge of, for example, the soil hydraulic parameters.

The HYDRUS models are further supported by Microsoft Windows based Graphical User Interfaces (GUIs) for data-preprocessing, generation of structured or unstructured finite element numerical grid systems, problem execution, and visualization of the simulation results. Figure 1 gives an example of the finite element grid and numerical results (in this case pressure heads) for alternate furrow irrigation in a tile-drained field. Additional details of the HYDRUS codes are given in the technical manuals (Šimůnek et al., 1998; 1999), as well as in a recent textbook (Rassam et al., 2003). Some of the above features are discussed also on the HYDRUS website (<a href="http://www.hydrus2d.com">http://www.hydrus2d.com</a>) from which HYDRUS-1D and its manual can be downloaded freely.

## **3 RECENT EXAMPLES**

The HYDRUS codes have been applied to a broad range of subsurface flow and transport problems. Recent applications include: (1) analysis of a variety of surface and subsurface irrigation problems (e.g., Skaggs et al., 2004), (2) tile drainage design and performance, (3) salinity management, (4) the fate and subsurface transport of toxic trace elements, (5) analysis of riparian systems, (6) virus, colloid, and bacteria transport (e.g., Bradford et al., 2004), (7) transport of pesticides (including fumigants) and their degradation products, (8) nitrogen dynamics and leaching, (9) studies of alternative root water uptake models, (10), tree crop agroforestry, (11) predicting soil moisture and temperature profiles around buried land mines, (12) evaluating slug-tests for large-diameter, hand-dug wells, (13) capillary barrier design, (14) the transport of TCE and its degradation products, (15), analyses of heat pulse probes for

measuring soil water fluxes, (16) analyses of the decay of historical monuments, (17) the transport of endocrine disruptors, hormones, and pharmaceuticals, (18) evaluation of landfill designs, (19) studies of water and vapor movement in deep vadose zones, (20) studies of preferential flow and transport, and (21) fluid flow and chemical migration within the capillary fringe. References to several of these applications are given elsewhere (Simunek and van Genuchten, 2003; van Genuchten and Šimůnek, 2004).

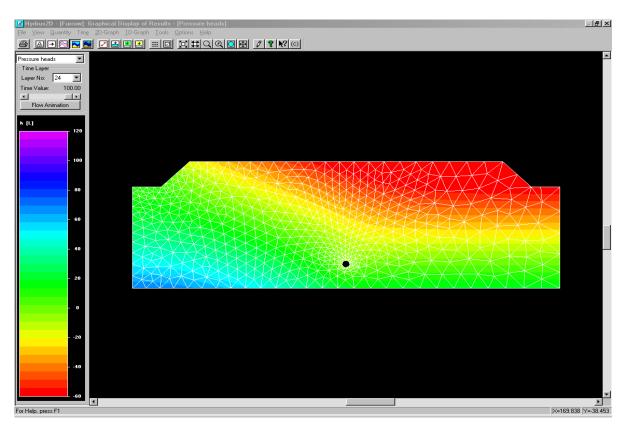


Figure 1. Example of the finite element mesh and pressure head profile for a tile-drainage example.

# 4 ONGOING RESEARCH AND FUTURE PLANS

A large number of new features have recently been included in the HYDRUS software packages, and will be available in forthcoming new versions. These features include (1) preferential flow and transport as modeled with a range of dual-porosity, dual-permeability, and kinematic wave models (Šimůnek et al., 2004), (2) multicomponent solute transport (Jacques et al., 2003; Jacques and Šimůnek, 2005), (3) the coupled movement of water and energy, including vapor transport, snow hydrology, and/or freezing/thawing cycle (e.g., Hansson et al., 2004), (4) an energy balance at the soil surface (using the Penman-Monteith method for calculating potential ET), (5) overland flow to improve the design of surface irrigation systems, (6) colloid and colloid-facilitated transport, and (7) constructed wetlands (Langergraber and Šimůnek, 2005). Overviews of recent work on multicomponent geochemical transport, colloid and colloid-facilitated transport, coupled overland and subsurface flow, and preferential flow are given in a recent paper by van Genuchten and Šimůnek (2004).

# 5 CONCLUSIONS

In this paper we briefly summarized various features of the HYDRUS-1D and HYDRUS-2D software packages, as well as recent applications and our future plans. Because of their generality, we believe that the two models are extremely useful tools for predicting a variety of subsurface flow and contaminant transport problems, as well as for analyzing a broad range of site-specific irrigation, drainage and salinity management problems.

## 6 REFERENCES

- Bradford, S.A., Bettahar, M., Šimůnek, J. & van Genuchten, M.Th. 2004. Straining and attachment of colloids in physically heterogeneous porous media, *Vadose Zone J.*, 3: 384-394.
- Ghassemi, F., Jakeman, A.J. & Nik, H.A. 1995. Salinisation of Land and Water Resources: Human Causes, Extent, Management and Case Studies. Univ. of New South Wales Press, Sydney, Australia, 520 p.
- Hansson, K., Simunek, J., Mizoguchi, M., Lundin, L.-C. & van Genuchten, M.Th. 2004. Water flow and heat transport in frozen soil: Numerical solution and freeze/thaw applications. *Vadose Zone J.* 3: 93-704.
- Jacques, D., Šimůnek, J. Mallants, D. & van Genuchten, M.Th. 2003. The HYDRUS-PHREEQC multicomponent transport model for variably-saturated porous media: Code verification and application, MODFLOW and More 2003: Understanding through Modeling, Conference Proceedings, ed. E. Poeter, Ch. Zheng, M. Hill, and J. Doherty, International Ground Water Modeling Center, Colorado School of Mines, 23-27.
- Jacques, D. & Šimůnek, J. 2005. Multicomponent variable saturated transport model, Description, manual, verification and examples, Waste and Disposal, SCK•CEN, BLG-998, Mol, Belgium.
- Langergraber, G. & Šimůnek, J. 2005 Modeling variably-saturated water flow and multi-component reactive transport in constructed wetlands. *Vadose Zone Journal*, (submitted).
- Rassam, D., Šimůnek, J. & van Genuchten, M.Th. 2003. *Modelling Variably-Saturated Flow with HYDRUS-* 2D. ND Consult, Brisbane, Australia, 275 p,
- Šimůnek, J. & van Genuchten, M.Th 2002. The HYDRUS software packages for simulating water, heat and solute movement in the subsurface: Features, recent applications and future plans. In: Proc. Second Federal Interagency Hydrologic Modeling Conference, *Hydrologic Modeling for the 21st Century*, Las Vegas, NV, July 28 August 1, 2002, CD Rom, Session 8C, 12p, U.S. Geological Survey, Subcommittee on Hydrology, Denver, CO.
- Šimůnek, J., Šejna, M. & van Genuchten, M. Th. 1998. The HYDRUS-1D software package for simulating water flow and solute transport in two-dimensional variably saturated media, Version 2.0. *IGWMC-TPS-70*, Int. Ground Water Modeling Center, Colorado School of Mines, Golden, Colorado, 202p.
- Šimůnek, J., Šejna, M. & van Genuchten, M. Th. 1999. The HYDRUS-2D software package for simulating twodimensional movement of water, heat, and multiple solutes in variably saturated media, Version 2.0, *IGWMC-TPS-53*, Int. Ground Water Modeling Center, Colorado School of Mines, Golden, Colorado, 251 p.
- Šimůnek, J., Jarvis, N.J., van Genuchten, M.Th. & Gärdenäs, A. 2003. Review and comparison of models for describing non-equilibrium and preferential flow and transport in the vadose zone. *J. Hydrol.* 272 (1-4): 14-35
- Skaggs, T.H., Trout, T.J., Šimůnek, J. & Shouse, P.J. 2004. Comparison of HYDRUS-2D simulations of drip irrigation with experimental observations. *J. Irrig. & Drain. Eng.*, ASCE, 130(4):304-310.
- van Genuchten, M. Th. 1987. A numerical model for water and solute movement in and below the root zone. Unpublished Research Report, U.S. Salinity Laboratory, USDA, ARS, Riverside, California.
- van Genuchten, M.Th. & Šimůnek, J. 2004. Integrated modeling of vadose-zone flow and transport processes. In: R.A. Feddes, G.H. de Rooij & J.C. van Dam (eds.), *Unsaturated-Zone Modeling; Progress, Challenges and Applications*; Wageningen UR Frontis Series, Vol. 6, Chapter 2, pp. 37- 69, Kluwer Academic Publishers, Dordrecht, The Netherlands.