New Features of the HYDRUS Computer Software Packages

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Abstract

The capabilities of the HYDRUS-1D and HYDRUS (2D/3D) software packages have been substantially expanded since two earlier HYDRUS workshops held in Prague, Czech Republic (March 2008) and Tokyo, Japan (June 2008). Multiple processes were added to both HYDRUS packages, including compensated root water and solute uptake models and triggered irrigation. Computational modules of both packages have been made about 2-3 times faster by using capabilities of advanced processors and compilers, such as using the loop vectorization. Major developments were introduced in version 2 of HYDRUS (2D/3D). This version can now handle for the first time complex, general, three-dimensional geometries, while domain properties, initial conditions, and boundary conditions can be specified on geometrical objects, rather than on the finite element mesh. Completely new modules accounting for processes not available in the standard HYDRUS version were introduced. These new modules include the HP2, C-Ride, DualPerm, UnsatChem, Wetland, and Fumigant modules. These new modules simulate flow and transport processes in two-dimensional transport domains and are fully supported by the HYDRUS graphical user interface. Several processes in these specialized modules of HYDRUS (2D/3D) have been made also part of HYDRUS-1D.

1. Introduction

The HYDRUS-1D and HYDRUS (2D/3D) programs (Šimůnek et al., 2008) are finite element models for simulating the one-, two- and three-dimensional movement of water, heat, and multiple solutes in variably saturated media. The standard versions of HYDRUS programs numerically solve the Richards equation for saturated-unsaturated water flow and convection-dispersion type equations for heat and solute transport. The flow equation incorporates a sink term to account for water uptake by plant roots. The heat transport equation considers movement by both conduction and convection with flowing water. The governing convection-dispersion solute transport equations are written in a very general form by including provisions for nonlinear nonequilibrium reactions between the solid and liquid phases, and linear equilibrium reaction between the liquid and gaseous phases. Hence, both adsorbed and volatile solutes, such as pesticides, can be considered. The solute transport equations also incorporate the effects of zero-order production, first-order degradation independent of other solutes, and first-order decay/production reactions that provide the required coupling between the solutes involved in the sequential first-order chain. The transport models also account for convection and dispersion in the liquid phase, as well as diffusion in the gas phase, thus permitting the model to simultaneously simulate solute transport in both the liquid and gaseous phases. HYDRUS considers up to fifteen solutes, which can either be coupled in a unidirectional chain or move independently of each other. Physical nonequilibrium solute transport can be accounted for by assuming a two-region, dual porosity type formulation, which partitions the liquid phase into mobile and immobile regions. Attachment/detachment theory, including the filtration theory, is included to simulate transport of viruses, colloids, and/or bacteria.

Table 1. Selected new options in HYDRUS-1D (since 2008).

Version	New Options
4.04	• Option to specify the nonequilibrium phase concentration initially at equilibrium with the equilibrium phase concentration • Option to specify initial conditions in total (instead of liquid) concentrations • Option to print fluxes instead of temperatures for observation nodes
4.05	• HP1 – support of dual-porosity models • Linking of optimized parameters of different soil layers • Constant mobile water content in multiple layers (in the Mobile-Immobile Water Model) when optimizing immobile water content
4.06	• The Per Moldrup's tortuosity models (Moldrup et al., 1997, 2000) were implemented as an alternative to the Millington and Quirk (1960) model
4.07	• Surface energy balance (i.e., the balance of latent, heat, and sensible fluxes) for bare soils • Daily variations of meteorological variables can be generated by the model using simple meteorological models • Preliminary (at present rather simple) support of the HYDRUS package for MODFLOW
4.08	• Compensated root water and solute (passive and active) uptake based on Šimůnek and Hopmans (2009) • Executable programs made about three times faster due to the loop vectorization
4.12	• New additional output (e.g., solute fluxes for observation nodes and profiles of hydraulic conductivities (thermal and isothermal) and fluxes (liquid, vapor, and total))
4.13	• Version 2.1.002 of HP1, new GUI supporting HP1 • Conversions of the mass units for the threshold-slope salinity stress model from electric conductivity to osmotic head
4.15	• Input of sublimation constant and initial snow layer • New conversions of constants (EC, osmotic potential) for the salinity stress response function
4.16	• Option to set field capacity as an initial condition (Twarakavi et al., 2009) • Display of wetting hydraulic functions for hysteretic soils • Triggered irrigation • Interception can be considered with the standard HYDRUS input (without the need for meteorological input)

We continue to expand the capabilities of the HYDRUS-1D and HYDRUS (2D/3D) software packages and many new processes and options have been added since the two HYDRUS workshops held in 2008 in Prague, Czech Republic (in March) and Tokyo, Japan (in June). Multiple processes have been added to both HYDRUS packages since 2008, including the compensated root water and solute uptake model and/or triggered irrigation, and many others. Tables 1 and 2 list selected new processes and options that have been implemented in recent versions of HYDRUS-1D and HYDRUS (2D/3D), respectively. Note that we continue to expand the capabilities of the HYDRUS modeling environment (Table 2) by developing specialized modules for more complex applications that cannot be solved using its standard versions. In this manuscript we list many of these changes and describe the new modules in more detail.

2. Specialized Modules

Completely new modules accounting for processes not available in the standard HYDRUS version were introduced. These new modules include the **HP2**, **C-Ride**, **DualPerm**, **UnsatChem**, **Wetland**, and **Fumigant** modules. All these modules simulate flow and transport processes in two-dimensional transport domains and are fully supported by the HYDRUS graphical user interface. Many processes included in these specialized modules of HYDRUS (2D/3D) are currently also available as part of HYDRUS-1D.

2.1. The HP1/HP2 Modules

The one-dimensional program **HP1**, which couples the **PHREEQC** geochemical code (Parkhurst and Appelo 1999) with **HYDRUS-1D**, was first released in 2005 (Jacques and Šimůnek 2005), and successfully used in many applications. This comprehensive simulation tool (HP1 is an acronym for **H**YDRUS-**P**HREEQC-**1**D) can simulate (1) transient water flow, (2) the transport of multiple components, (3) mixed equilibrium/kinetic biogeochemical reactions, and (4) heat transport in one-dimensional variably-saturated porous media (soils). **HP2** (Šimůnek et al., 2012d) is then a two-dimensional alternative of the HP1 module. Both HP1 and HP2 can simulate a broad range of low-temperature biogeochemical reactions in water, the vadose zone and/or ground water systems, including interactions with minerals, gases, exchangers and sorption surfaces based on thermodynamic equilibrium, kinetic, or mixed equilibrium-kinetic reactions. More details about both modules are presented in several papers of these proceedings (e.g., Jacques et al., 2013; Šimůnek et al., 2013).

2.2. The C-Ride Modules

The **C- Ride** module (Šimůnek et al., 2012c) simulates the transport of particle-like substances (e.g., colloids, viruses, bacteria, and nanoparticles) and colloid-facilitated solute transport (Šimůnek et al., 2006), the latter often observed for many strongly sorbing contaminants such as heavy metals, radionuclides, pharmaceuticals, pesticides, and explosives. These contaminants are predominantly associated with the solid phase, which is commonly assumed to be stationary. However, such contaminants may also sorb/attach to mobile and deposited colloidal particles (e.g., microbes, humic substances, suspended clay particles, and metal oxides), which then can act as pollutant carriers and thus provide a rapid transport pathway for the pollutants. This module fully accounts for the dynamics of colloid (attachment/straining) and solute (kinetic/equilibrium sorption to soil and mobile/deposited colloids) transfer between the different phases. The schematic of the colloid-facilitated solute transport model is shown in Figure 1.

Table 2. Selected new options in HYDRUS (2D/3D) (since 2008).

Version	New Options
1.09	• New more efficient algorithm for particle tracking
1.10	• Import of domain properties, initial and boundary conditions from another project with (slightly) different geometry or FE mesh (both 2D and 3D)
1.11	• The Per Moldrup's tortuosity models (Moldrup et al., 1997, 2000) were implemented as an alternative to the Millington and Quirk (1960) model
2.01	**Computational module:** • Initial conditions can be specified in the total solute mass (previously only liquid phase concentrations were allowed) • Initial equilibration of nonequilibrium solute phases with equilibrium solute phase • Gradient boundary conditions • A subsurface drip boundary condition (with a drip characteristic function reducing irrigation flux based on the back pressure) (Lazarovitch et al., 2005) • A surface drip boundary condition with dynamic wetting radius (Gärdenäs et al., 2005) • A seepage face boundary condition with a specified pressure head • Triggered Irrigation, i.e., irrigation can be triggered by the program when the pressure head at a particular observation node drops below a specified value • Time-variable internal pressure head or flux nodal sinks/sources (previously only constant internal sinks/sources) • Fluxes across meshlines in the computational module for multiple solutes (previously only for one solute) • HYDRUS calculates and reports surface runoff, evaporation and infiltration fluxes for the atmospheric boundary • Water content dependence of solute reactions parameters using the Walker's (1974) formula was implemented • An option to consider root solute uptake, including both passive and active uptake (Šimůnek and Hopmans, 2009) • An option to use a set of Boundary Condition records multiple times • Options related to the **Fumigant** transport (e.g., removal of tarp, temperature dependent tarp properties, additional injection of fumigant) • The **UNSATCHEM** module simulating transport of and reactions between major ions • The new **CWM1** constructed wetland module **GUI:** • Supports for complex general three-dimensional geometries (Professional Level) • Domain properties, initial conditions, and boundary conditions can be specified on "Geometric Objects" (defining the transport domain) rather than on the finite element mesh • Import of various quantities (e.g., domain properties, initial and boundary conditions) from another HYDRUS projects even with (slightly) different geometry or FE mesh • Geometric objects can be imported using DXF and TIN (triangular irregular network) files • Display of results using Isosurfaces • Support of **ParSWMS** (a parallelized version of SWMS_3D) (Hardelauf et al., 2006)
2.02	• The **DualPerm** module simulating flow and transport in dual-permeability porous media • The **C-Ride** module simulating colloid transport and colloid-facilitated solute transport • The **HP2** module (coupled HYDRUS and PHREEQC) for simulating biogeochemical reactions

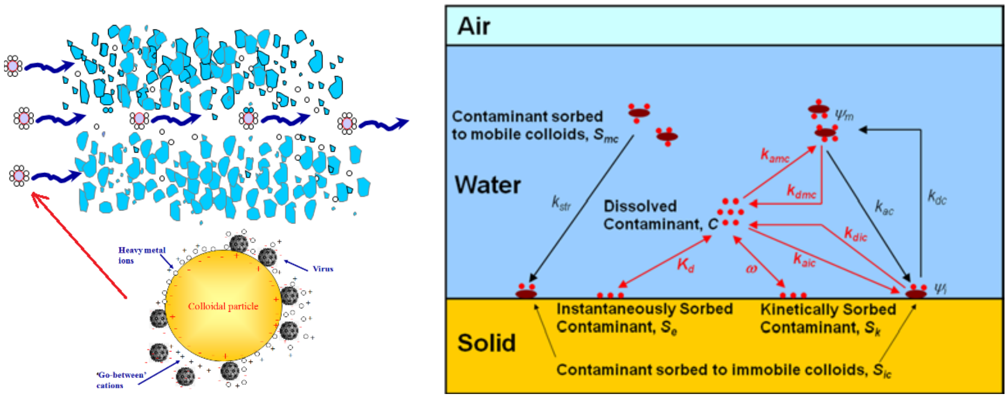

Figure 1. Schematic of the colloid-facilitated solute transport model.

2.3. The DualPerm Module

The **DualPerm** module (Šimůnek et al., 2012b) simulates preferential and/or nonequilibrium water flow and solute transport in dual-permeability media using the approach suggested by Gerke and van Genuchten (1993). The module assumes that the porous medium consists of two interacting regions: one associated with the inter-aggregate, macropore, or fracture system, and one comprising micropores (or intra-aggregate pores) inside soil aggregates or the rock matrix. Water flow can occur in both regions, albeit at different rates. Modeling details are provided by Šimůnek and van Genuchten (2008). An example of the pressure head profiles for a tension disc (with a disc radius of 10 cm) infiltration experiment in the transport domain, 50 cm wide and 150 cm deep, in the matrix and fracture domains for different ratios of the anisotropy coefficients (K_x^A/K_z^A=1, 10, and 0.1) is shown in Figure 2.

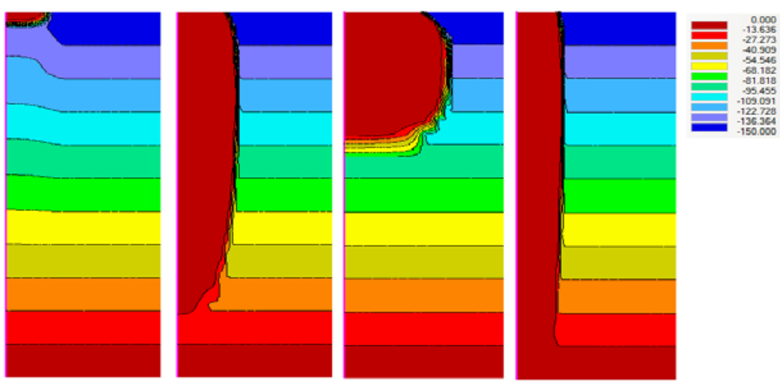

Figure 2. Pressure head profiles for the matrix (left), isotropic fracture, and fracture with K_x^A/K_z^A=10, and fracture with K_x^A/K_z^A=0.1 (right).

2.4. The UnsatChem Module

The geochemical **UnsatChem** module (Šimůnek et al., 2012a) has been implemented into both the one- and two-dimensional computational modules of Hydrus. This module simulates the transport of major ions (i.e., Ca, Mg, Na, K, SO4, CO3, and Cl) and their equilibrium and kinetic geochemical interactions, such as complexation, cation exchange and precipitation-dissolution (e.g., calcite, gypsum, and/or dolomite). Possible applications include studies of the salinization/ reclamation of agricultural soils, sustainability of various irrigation systems, and the disposal of brine waters from mining operations. Since the computational driver for this module was developed some two decades ago (Šimůnek and Suarez, 1994), the UnsatChem module (especially its one-dimensional version) has found a wide use in many applications.

2.5. The Wetland Module

The **Wetland** module simulates aerobic, anoxic, and anaerobic transformation and degradation processes for organic matter, nitrogen, phosphorus, and sulphur during treatment of polluted wastewater in subsurface constructed wetlands (Langergraber and Šimůnek, 2012). Constructed wetlands are engineered water treatment systems that optimize the treatment processes found in natural environments. Constructed wetlands have become popular since they can be quite efficient in treating different types of polluted water and provide sustainable, environmentally friendly solutions. A large number of physical, chemical and biological processes are simultaneously active and may mutually influence each other. The Wetland module uses two biokinetic model formulations [CW2D of Langergraber and Šimůnek (2005) and CWM1 of Langergraber et al. (2009)] to account for complex conditions that may occur in various types of wetlands. An example of the application of the Wetland module to simulate the spatial distribution of heterotrophic organisms in a subsurface constructed wetland is shown in Figure 3.

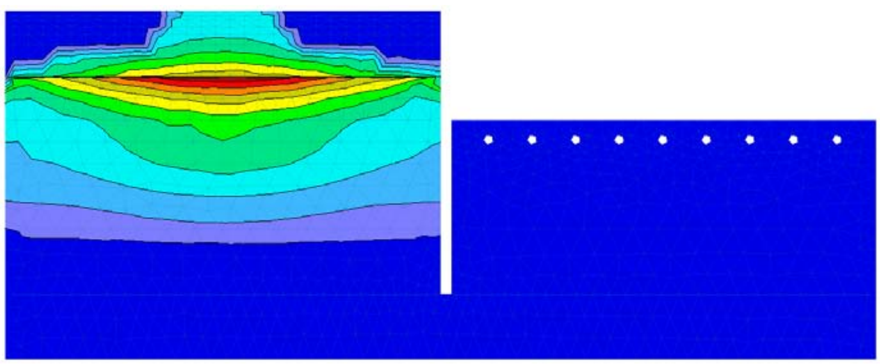

Figure 3. Steady-state distribution of heterotrophic organisms in a subsurface constructed wetland.

2.6. The Fumigants Module

The **Fumigants** module implements multiple additional options that are required to simulate processes related to fumigants applications and transport. This module allows users to specify an additional injection of fumigants into the transport domain at a specified location at a specified time and to consider the presence or absence of a surface tarp, a temperature dependence of tarp properties, and its removal at specified time. The Fumigants module has been recently used to investigate the effect of different application scenarios, such as tarped broadcast, tarped bedded shank injection and a tarped drip line-source application and various factors (e.g., initial water content, tarp permeability) on fumigant volatilization (Fig. 4) (Spurlock et al., 2013).

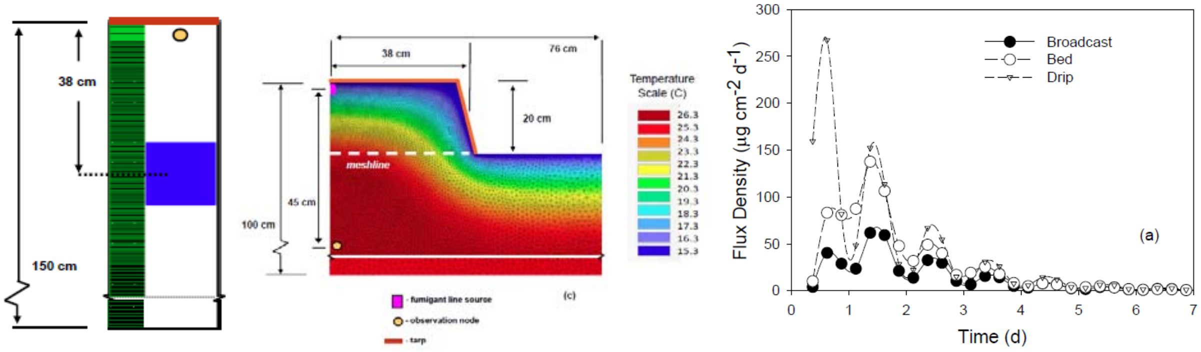

Figure 4. Tarped broadcast (left) and tarped bed drip scenarios (center). Volatilization fluxes for different scenarios (adopted from Spurlock et al., 2013).

3. Graphical User Interface (GUI) of HYDRUS (2D/3D)

3.1. Geometries in the Professional Level of HYDRUS (2D/3D)

The latest 3D-Professional Level of HYDRUS supports complex general three-dimensional geometries that can be formed from three-dimensional objects (**Solids**) of general shapes. Three-dimensional objects are formed by boundary **Surfaces**, which can be either **Planar** surfaces or **Curved** surfaces (**Quadrangle**, **Rotary**, **Pipe**, or **B-Spline**). Figure 5 provides examples of various curved surfaces, while Figure 6 shows how these individual objects can be combined to form complex three-dimensional geometries.

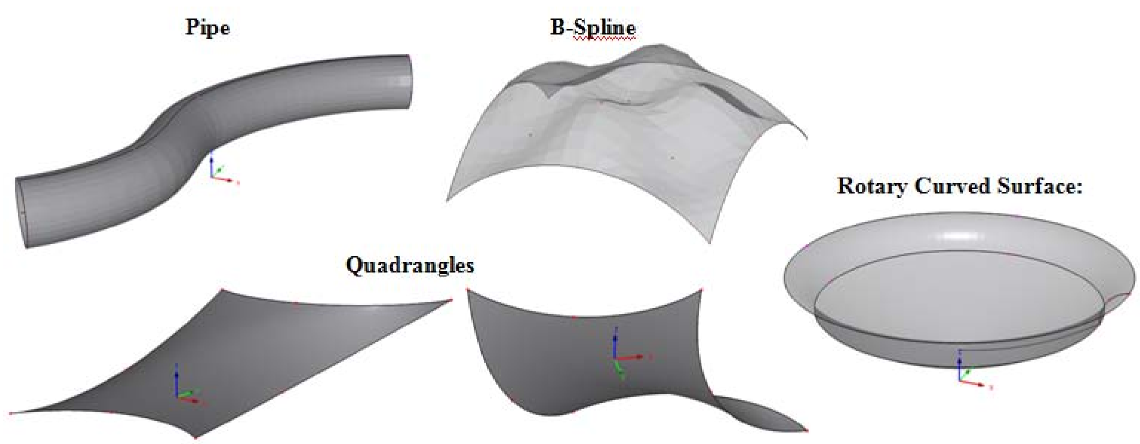

Figure 5. Examples of curved surfaces (Rotary, Pipe, B-Spline, and Quadrangle Surfaces).

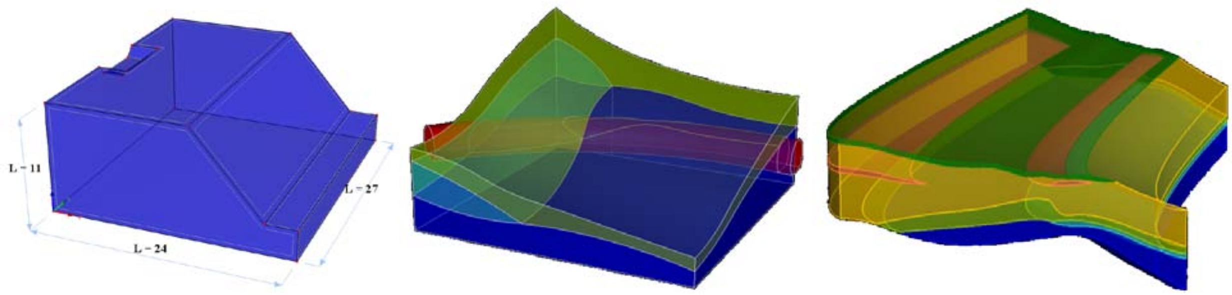

Figure 6. Transport domains formed using planar (left) or curved (center, right) surfaces.

3.2. Domain Properties, Initial Conditions, and Boundary Conditions Specified on Geometric Objects

Various spatially variable properties (e.g., material distribution, initial conditions, boundary conditions, domain properties, etc) can be specified in Version 2.0 of HYDRUS, either directly on the Finite Element Mesh (FEM) (as done in Version 1.0), or on Geometric Objects (e.g., boundary curves, rectangles, circles, surfaces, solids) (Fig. 7).

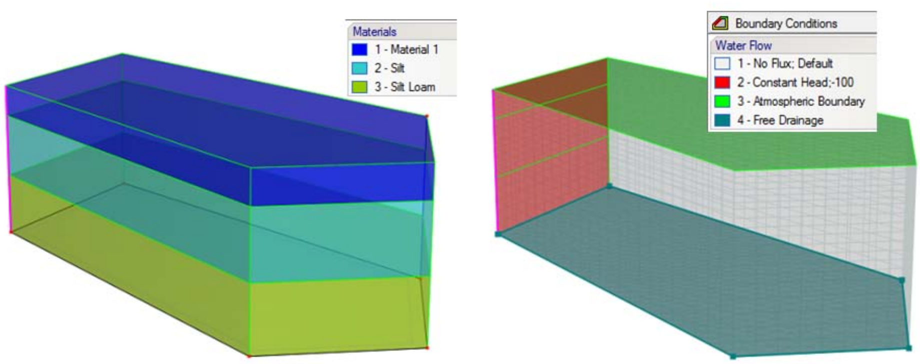

Figure 7. The transport domain with materials (left) and boundary conditions (right) specified on Geometric Objects.

3.3. Display of Standard and Alternative Variables

Many different spatially-variable properties can be displayed in the center “View” window of HYDRUS GUI, depending on what processes are being simulated. These variables are divided between standard variables, such as pressure heads, water contents, and/or liquid concentrations, and alternative variables, such as different types of water contents (mobile, immobile, and total) or concentrations (liquid, solid, gas, or total). While the standard variables can be selected from the “Data” tab of the Navigator bar, the alternative variables can be selected from the View tab of the Navigator bar (Fig. 8).

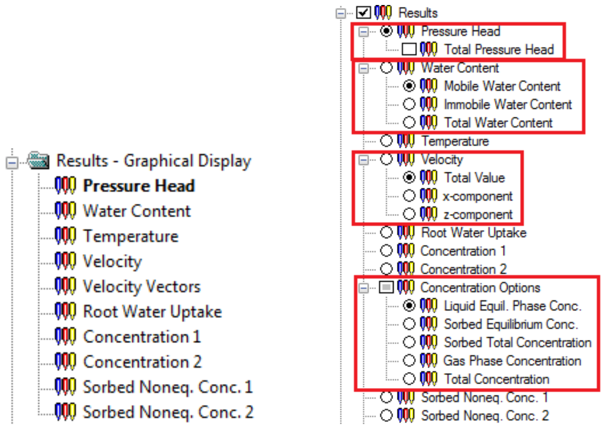

Figure 8. Standard and alternative variables that can be displayed in the View window.

4. Conclusions

The HYDRUS models 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 (HYDRUS website lists over one thousand references, in which HYDRUS has been used). The need for codes such as HYDRUS is further reflected by the frequency of downloading the program from the HYDRUS web site. For example, HYDRUS-1D was downloaded more than 10,000 times in 2012 by users from some 50 different countries. The HYDRUS web site receives on average some 700 individual visitors each day.

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