REVIEWS

Numerical Modeling of Contaminant Transport Using HYDRUS and its Specialized Modules

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Abstract | A broad range of numerical models have been developed during the past several decades to describe the fate and transport of agricultural, industrial, and other contaminants in soils and groundwater. Such models are now increasingly implemented in both research and engineering projects addressing subsurface pollution problems. Of particular concern is especially non-point source pollution stemming from plant and animal production. In this paper we first briefly review different types of mathematical models that are being used to describe the transport of agricultural chemicals in both the vadose zone and groundwater. We next review various versions of the HYDRUS computer software packages, including several specialized modules that were recently developed for simulating the movement of water, heat, and solutes in the subsurface.

Early versions of the HYDRUS models considered the transport of only one chemical species and assumed that the behavior of this solute was independent of other species present in the soil solution. Physical non-equilibrium transport could be accounted for in later versions of HYDRUS by assuming a two-region or dual-porosity type formulations that partition the liquid phase into mobile and immobile regions. Chemical nonequilibrium transport could be accounted for by assuming kinetic interactions between solutes in the liquid and solid phases. Physical and chemical nonequilibrium formulations were extended later also to particle transport by including provisions for filtration theory, and time- and/or depth-dependent blocking functions.

Subsequent versions of the HYDRUS codes also considered the transport of multiple solutes, which either could be coupled by means of a uni-directional first-order degradation chain, or move independently of each other. While this approach proved effective for evaluating the subsurface transport of many chemicals (e.g., nitrogen species, pesticides, radionuclides), many environmental problems require analyses of the transport of multiple chemical species that could interact mutually, create complexed species, precipitate, dissolve, and/or compete with each other for sorption sites. Several specialized modules have now been developed to simulate transport processes not accounted for in the earlier standard versions of HYDRUS. These include a wetlands module, the HP1/2/3 multicomponent transport modules, the facilitated transport C-Ride module, a module

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for fumigants, and the major ion Unsatchem module. All of these modules simulate flow and transport processes in two-dimensional transport domains and are supported by the HYDRUS (2D/3D) graphical user interface. Many processes of these specialized modules are also available as part of the public domain HYDRUS-1D software. Brief overviews of these more recent modules are included in this manuscript.

1 Introduction

Modern agriculture produces and uses an unprecedented number of chemicals in plant and animal production. A broad range of pesticides, fertilizers, and fumigants are now routinely applied to agricultural lands, thus causing agricultural operations to be one of the most important sources of especially non-point source pollution.[1] Additionally, salts and toxic trace elements are often unintended consequences of irrigation in arid and semi-arid regions. While many agricultural chemicals are beneficial in surface soils, their leaching into the deeper vadose zone and groundwater can pose environmental problems. Thus, management practices are needed to keep agricultural contaminants in the root zone and prevent their transport into nearby surface water and groundwater. Animal production now increasingly uses also a range of pharmaceuticals and hormones, many of which, along with pathogenic microorganisms, are being released into the environment through animal waste. Animal wastes and wash water are frequently applied to agricultural lands. Potential concerns about pharmaceuticals and hormones appearing in the environment include increased incidences of cancer, development of antibiotic resistant bacteria, abnormal physiological processes and reproductive impairment, and increased toxicity of chemical mixtures. While agriculture causes mostly non-point source pollution, similar problems arise with point-source pollution from industrial and municipal waste disposal sites, nuclear waste repositories, leaking underground storage tanks, chemicals spills, mine tailings, and many other sources.[1–3]

Once released into the environment, point- or non-point source contaminants generally are subjected to a large number of simultaneous physical, chemical, and biological processes, including advective-dispersive transport, sorption-desorption, volatilization, precipitation-dissolution, complexation, and biodegradation. Most of the predictive models currently being used consider the transport of only one chemical species and assume that the behavior of this solute is independent of that of other species in the soil solution. In reality, the soil solution is always a mixture of many ions which mutually may interact in various ways as well as may compete with each other for available sorption sites.[4,5] Many environmental problems require analyses of the coupled transport and reaction of multiple chemical species. Agricultural examples include optimization of fertilizer management practices, and management and reclamation of saline and sodic soils.[6] Non-agricultural examples include acid mine drainage, radionuclide transport, the environmental fate of metal-organic mixed wastes, analyses of redox zones in organic-contaminated aquifers, disposal of brine/saline waters produced during mining of coalbed or shale gas, and reactive permeable barriers for aquifer remediation.[2,7,8] In the following sections we will consider several of such complex problems that lead to multicomponent transport.

A large number of models of varying levels of complexity and dimensionality are now available to describe the basic physical and chemical processes affecting water flow and pollutant transport in the subsurface. Modeling approaches range from relatively simple analytical and semi-analytical solutions, to much more complex numerical codes that permit consideration of a large number of simultaneous nonlinear processes. While analytical and semi-analytical solutions undoubtedly remain popular for relatively simple applications,[9,10] the development of more accurate and numerically stable solution techniques and the ever-increasing power of personal computers are now facilitating the much wider use of numerical models. The use of numerical models is also significantly enhanced by their availability in both the public and commercial domains, and by the development of sophisticated graphics-based interfaces that dramatically simplify their use.

The HYDRUS software packages[11] are now widely used to evaluate the fate and transport of various chemicals in especially the vadose zone

between the soil surface and the groundwater table. However, the codes are also applicable to flow and transport in saturated or variably-saturated systems. The popularity of the HYDRUS models is due in part to the implementation of a large number of processes in the codes, their flexibility in allowing application to a broad range of agricultural, industrial and environmental problems, the possibility to consider inverse (parameter estimation) problems, and their ease of use. In this manuscript we will briefly review the development of the various HYDRUS versions, including the most recent versions of HYDRUS-1D and HYDRUS (2D/3D) for one- and multidimensional transport problems, respectively, and its specialized modules. We also briefly discuss selected applications.

2 The HYDRUS Computer Software Packages

The HYDRUS-1D and HYDRUS (2D/3D) codes are finite element models for simulating the one-, two- and three-dimensional movement of water, heat, and multiple solutes in variably saturated media. Tables 1 and 2 provide a historical perspective of the development of the HYDRUS-1D and HYDRUS (2D/3D) programs, respectively, their various versions, and when different processes and options were first developed or added. Both tables also list the specialized HYDRUS modules, such as Wetland, HP1/2, and UnsatChem, and when they were included into the software packages. To limit the number of references to previous HYDRUS versions, we refer to Šimůnek et al.,[11] which provides a more detailed summary of past development of the HYDRUS codes and their many earlier versions.

The standard versions of the HYDRUS programs[11] numerically solve the Richards equation for saturated-unsaturated water flow and advection-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 conduction as well as advection with flowing water. The governing advection-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 reactions between the liquid and gaseous phases. Hence, both adsorbed and volatile solutes, such as certain pesticides, can be considered. The 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 solutes involved in a sequential first-order chain. The transport models further account for advection and dispersion in the liquid phase, as well as diffusion in the gas phase, thus permitting the models to simulate solute transport simultaneously in both the liquid and gaseous phases. The codes consider up to 15 solutes, which can either be coupled in a unidirectional chain or are allowed to move independently of each other.

The HYDRUS codes can consider a range of physical and chemical nonequilibrium transport situations. 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. Chemical nonequilibrium solute transport can be accounted for by dividing the available sorption sites into two fractions and by assuming instantaneous sorption on one fraction of sorption sites and time-dependent sorption on the remaining sites. Physical and/or chemical nonequilibrium models have been extended recently to particle transport by including provisions for filtration theory, and time- and/or depth-dependent blocking functions.

3 Solute Transport

3.1 Transport of single ions

Early versions of both HYDRUS codes could simulate only the transport of a single ion, which was assumed to be either nonreactive or could be linearly sorbed onto the solid phase, and which could be subject to zero- and first-order degradation/production reactions. The one-dimensional version of the transport equation for variably-saturated flow conditions in that case is given by

$$\frac{\partial(\theta c + \rho_b s)}{\partial t} = \frac{\partial}{\partial z}\left(\theta D \frac{\partial c}{\partial z}\right)$$

$$-\frac{\partial(qc)}{\partial z} - \theta c \mu_w - \rho_b s \mu_s + \rho_b \gamma_s + \theta \gamma_w - r \quad (1)$$

where t is time [T], z is the spatial coordinate [L], θ is the volumetric water content [L^3L^{-3}], q is the volumetric flux density [LT^{-1}], c [ML^{-3}] and s [MM^{-1}] are concentrations in the liquid and solid phases, respectively, ρ_b is the bulk density [ML^{-3}], D is the hydrodynamic dispersion coefficient [L^2T^{-1}], μ_w and μ_s are first-order degradation coefficients for the liquid and solid phases [T^{-1}], respectively, γ_w [$ML^{-3}T^{-1}$] and γ_s [T^{-1}] are zero-order production coefficients for the liquid and solid phases, respectively, and r is a sink term for root solute uptake [$ML^{-3}T^{-1}$].

Table 1: History of development of the standard HYDRUS-1D code and its specialized modules.

Version (year)	Processes and options
1.0 (1998)	• Variably-saturated water flow, and heat and solute transport in one-dimensional porous media • Root water and solute uptake • van Genuchten, modified van Genuchten, and Brooks and Corey models for the soil hydraulic properties (see HYDRUS manual for references), hysteresis in the hydraulic properties • Nonlinear solute transport, sequential first-order decay chains, volatile solutes • Temperature dependence of soil hydraulic and solute transport parameters • Chemical nonequilibrium—two-site sorption model • Physical nonequilibrium—dual-porosity solute transport with mobile-immobile water • 16 bit GUI
2.0 (1998)	• Inverse problems using the Marquardt-Levenberg optimization algorithm • 32 bit GUI
3.0 (2005)	• Durner and Kosugi models for the soil hydraulic properties • Dual-porosity water flow • Snow fall/melting • Compensated root water uptake • Virus, colloid, and bacteria transport (using attachment/detachment concepts and filtration theory)[12] • **UnsatChem module**—transport and reactions of major ions and transport of carbon dioxide
4.0 (2008)	• Vapor flow • Coupled water, vapor, and energy transport • Hysteresis model of Lenhard et al.[13] and Lenhard and Parker[14] to eliminate pumping effects by keeping track of historical reversal points • Dual-porosity water flow and solute transport, with solute transport subject to two-site sorption in the mobile zone • Daily variations in evaporation, transpiration, and precipitation rates • **DualPerm module**—dual-permeability type water flow and solute transport[15] • **Meteo module**—potential evapotranspiration calculated with the Penman-Monteith combination equation or the Hargreaves equation • **HP1 code**—obtained by coupling HYDRUS with the PHREEQC biogechemical code[16]
4.04 (2008)	• Option to specify initial conditions in terms of total (instead of liquid only) concentrations • Option to specify nonequilibrium phase concentration to be initially at equilibrium with the equilibrium phase concentration
4.05 (2008)	• 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 (2008)	• Implementation of the tortuosity models of Moldrup et al.[17,18] as an alternative to the Millington and Quirk[19] model
4.07 (2008)	• Surface energy balance (i.e., the balance of latent, heat, and sensible fluxes) for bare soils • Daily variations in meteorological variables generated with the model using simple meteorological models • Preliminary (at present relatively simple) support of the HYDRUS package for MODFLOW
4.08 (2009)	• Compensated root water and solute uptake (passive and active) based on Šimůnek and Hopmans[20] • Executable programs made about three times faster due to the loop vectorization
4.12 (2009)	• New additional output (e.g., solute fluxes at observation nodes and profiles of hydraulic conductivities (thermal and isothermal) and fluxes (liquid, vapor, and total))
4.13 (2009)	• Version 2.1.002 of HP1, new GUI supporting HP1 (gas transport, time-variable soil physical properties) • Conversions of mass units for the threshold-slope salinity stress model from electric conductivity to osmotic head
4.15 (2012)	• Input of sublimation constant and initial snow layer • New conversions of constants (EC, osmotic head) for the salinity stress response function
4.16 (2013)	• Option to set field capacity as an initial condition[21] • Triggered irrigation • Interception can be considered with the standard HYDRUS input (no need for meteorological input)

Table 2: History of development of the standard HYDRUS-2D and HYDRUS (2D/3D) programs and their specialized modules.

Version (year)	Processes and options
HYDRUS-2D	
1.0 (1996)	• Variably-saturated water flow and (linear and equilibrium) solute transport in two-dimensional porous media • Root water and solute uptake • van Genuchten and modified van Genuchten models for the soil hydraulic properties • Linear equilibrium solute transport • 16 bit GUI (including the **MeshGen-2D** unstructured mesh generator)
2.0 (1999)	• Heat transport • Brooks and Corey, Durner, and Kosugi models for the soil hydraulic properties; hysteresis in soil hydraulic properties • Nonlinear solute transport, sequential first-order decay chains, volatile solutes • Temperature dependence of soil hydraulic and solute transport parameters • Chemical nonequilibrium—two-site sorption model • Inverse problem using the Marquardt-Levenberg optimization algorithm • 32 bit GUI
HYDRUS (2D/3D)	
1.0 (2007)	• Variably-saturated flow, and heat and solute transport in two- and three-dimensional media • Durner and Kosugi models for the soil hydraulic properties • Hysteresis model of Lenhard et al.[13] and Lenhard and Parker[14] to eliminate pumping effects by keeping track of historical reversal points • Physical nonequilibrium—dual-porosity solute transport with mobile-immobile water • New dynamic system-dependent boundary conditions • Compensated root water uptake, spatial root distribution functions of Vrugt et al.[22] • Virus, colloid, and bacteria transport (using attachment/detachment concepts and filtration theory)[12] • Flowing particles in 2D • **Wetland module**—based on the biokinetic model CW2D (in 2D)[23]
2.0 (2011)	• Option to specify initial conditions in total (instead of liquid) concentrations • Option to specify the nonequilibrium phase concentration initially at equilibrium with the equilibrium phase concentration • Gradient boundary conditions • A subsurface drip boundary condition (with a drip characteristic function reducing irrigation flux based on the back pressure)[24] • A surface drip boundary condition with dynamic wetting radius[25] • A seepage face boundary condition with a specified pressure head • Triggered irrigation[26] • Water content dependence of solute reactions parameters using the Walker's[27] formula was implemented. • Compensated root water and solute uptake (passive and active) based on Šimůnek and Hopmans[29] • Implementation of the tortuosity models of Moldrup et al.[17,18] as an alternative to the Millington and Quirk[19] model • An option to use a set of boundary condition records multiple times • **Fumigant module**—options related to the fumigant transport (e.g., removal of tarp, temperature dependent tarp properties, additional injection of fumigant) • **Wetland module**—includes the second biokinetic model CWM1 (in 2D)[28] • **UnsatChem module**—transport and reactions of major ions and transport of carbon dioxide (in 2D) • Support for **ParSWMS**, a parallelized version of SWMS-3D, an early version of the three-dimensional computational module of HYDRUS (2D/3D)[29]
2.02 (2012)	• **DualPerm module**—dual-permeability type water flow and solute transport (in 2D)[15] • **HP2 module**—obtained by coupling HYDRUS-2D with the PHREEQC biogeochemical code • **C-Ride module**—colloid transport and colloid-facilitated solute transport (in 2D)[30]

3.1.1 Equilibrium solute transport: The most common way to relate the liquid and solid phase concentrations is to assume instantaneous sorption and to use adsorption isotherms. The simplest form of the adsorption isotherm is a linear equation, $s = K_d c$, where K_d is the distribution coefficient [$L^3 M^{-1}$]. Substitution of this equation into (1) leads to a constant value for the retardation factor R (i.e., $R = 1 + \rho_b K_d / \theta$). While the use of a linear isotherm greatly simplifies the mathematical description of solute transport, sorption and exchange are generally nonlinear and most often depend also on the presence of competing species in the soil solution. Many models have been used in the past to describe nonlinear sorption. The most common nonlinear models are the Freundlich and Langmuir isotherms, which in HYDRUS are combined into the general form.

$$s = \frac{K_f c^{\beta}}{1 + \eta c^{\beta}} \qquad (2)$$

where K_f [$M^{-\beta} L^{3\beta}$], β [$-$] and η [$M^{-\beta} L^{3\beta}$] are general isotherm coefficients. Eq. (2) reduces to the traditional Freundlich isotherm when $\eta = 0$, and to the Langmuir isotherm when $\beta = 1$. The solute retardation factor for nonlinear adsorption is not constant, as is the case for linear adsorption, but changes as a function of concentration. Šimůnek and van Genuchten[1] list in their Table 1 a range of linear and other sorption models frequently used in contaminant transport studies.

3.1.2 Chemical non-equilibrium solute transport: An alternative to describing sorption as an instantaneous process using algebraic equations such as eq. (2), is to assume a kinetic sorption process in which case the time dependency of the reaction is described using ordinary differential equations. The most popular and simplest formulation of a chemically controlled kinetic reaction arises when first-order linear kinetics is assumed:

$$\frac{\partial s}{\partial t} = \alpha_k (K_d c - s) \qquad (3)$$

where α_k is a first-order kinetic rate coefficient [T^{-1}]. Several other nonequilibrium adsorption expressions were also used in the past (see Table 1 in ref. 31). Models based on this and other kinetic expressions are often referred to as one-site sorption models.

While eq. (3) can be used to also describe the transport of particles, the transport of viruses, colloids, bacteria, and nanoparticles is more commonly modeled using a modified form of the advection-dispersion equation in which the kinetic sorption equation is replaced with an equation describing the kinetics of particle attachment and detachment as follows:

$$\rho \frac{\partial s}{\partial t} = \theta k_a \psi c - k_d \rho s \qquad (4)$$

where c is the (colloid, virus, bacteria) concentration in the aqueous phase [$N_c L^{-3}$], s is the solid phase (colloid, virus, bacteria) concentration [$N_c M^{-1}$], in which N_c is the number of (colloid) particles, k_a is the first-order deposition (attachment) coefficient [T^{-1}], k_d is the first-order entrainment (detachment) coefficient [T^{-1}], and ψ is a dimensionless colloid retention function [$-$] to account for time-dependent blocking and/or depth-dependent retention processes.

Many variants, combinations, and generalizations of (2), (3), and (4) can be formulated. One option is to further expand the one-site first-order kinetic model into a two-site sorption model that divides available sorption sites into two fractions.[32,33] In this approach, sorption on one fraction (type-1 sites) is assumed to be instantaneous and described using isotherms such as (2), while sorption on the remaining (type-2) sites is considered to be time-dependent and described using an ordinary differential equation such as (3). The two-site sorption model has been used in a great number of studies and will not be discussed here further.

Alternatively, one could assume also that sorption occurs kinetically on two different sets of sites, with the rates of sorption being different on both kinetic sites. The two kinetic processes can then be used to represent different chemical and/or physical processes, such as the removal of particles from the liquid phase. While the first kinetic process could be used for chemical attachment, the second kinetic process could represent physical straining.[34–36] The two kinetic sorption model is widely used to simulate the transport of various particle-like substances, such as viruses,[37–39] colloids,[12,34,40] bacteria,[35,36,41] and nanoparticles.[42,43]

3.1.3 Physical non-equilibrium solute transport: While chemical nonequilibrium models of the type discussed above assume that chemical factors are the cause of nonequilibrium transport, physical nonequilibrium models

assume that nonequilibrium flow or transport is caused by physical factors.[15,44] Physical nonequilibrium models usually divide the pore system into two regions: one region in which water is either stagnant (being immobile) or moves only very slowly, and a second region in which water can move more quickly (being mobile). For example, larger soil particles or soil aggregates, but also the matrix of rocks, may have their own micro-porosity containing relatively immobile water, while water will flow mostly only between the larger particles or soil aggregates, or within rock fractures. Alternative descriptions arise if water flow is assumed to be completely restricted to, or merely dominant, in the macropores (or inter-aggregate pores and fractures), while water in the matrix (the intra-aggregate pores or rock matrix) is assumed to move only very slowly or not at all. Physical nonequilibrium models have been reviewed recently by Jarvis,[45] Šimůnek and van Genuchten,[31] and Köhne et al.[46,47] The two reviews by Köhne et al.[46,47] in particular provide a large number of citations in which various physical nonequilibrium solute transport models (including HYDRUS) have been used.

We note that the HYDRUS codes include also provisions to simultaneously consider chemical and physical nonequilibrium transport processes. This option is especially attractive when simulating the transport of sorbing solutes in preferential flow pathways, or when particles are transported (roll) over solid surfaces at a different rate than in the bulk aqueous phase.[40,48]

3.2 Transport of multiple ions subject to sequential first-order decay reactions

Versions 1 of the windows-based HYDRUS codes (Tables 1 and 2) included an option to simulate the transport of multiple solutes subject to sequential first-order decay reactions. Figure 1 shows schematically how these decay reactions are implemented. In the figure, c, s, and g represent concentrations in the liquid, solid, and gaseous phases, respectively, the subscripts s, w, and g refer to solid, liquid and gaseous phases, respectively, straight arrows represent the different zero-order (γ) and first-order (μ, μ') rate reactions, while circular arrows indicate equilibrium distribution coefficients between the liquid and gaseous phases (k_g) and liquid and solid phases (k_d).

The decay chain option in HYDRUS, in which solute A degrades to produce solute B, solute B produces solute C, and so on, has proved to be very attractive for modeling the fate and transport of different types of solutes. Typical examples of sequential first-order decay chains involve radionuclides, mineral nitrogen species, certain pesticides, chlorinated aliphatic hydrocarbons, hormones, antibiotics, and explosives. Mallants et al.[49] used this structure to simulate the transport of the radionuclides ^{226}Ra, ^{222}Rn, and ^{210}Pb, with Ra and Pb sorbing to the solid phase and Rn being volatile and diffusing also in the gas phase. Another example with radionuclides is given by Pontedeiro et al.[50] who evaluated the subsurface transport of ^{238}U, ^{234}U, ^{230}Th, ^{226}Ra, and ^{210}Pb after being released from a conventional mining installation processing ore containing naturally occurring radioactive materials.

HYDRUS was used similarly in several studies[51–53] to simulate the transport of nitrogen species involved in a nitrification/denitrification chain. The reaction pathway in this case involves the hydrolysis of urea ((NH_2)$_2$CO) by heterotrophic bacteria to form ammonium (NH_4^+), which is sequentially nitrified by autotrophic bacteria to nitrite (NO_2^-) and nitrate (NO_3^-), with nitrate in
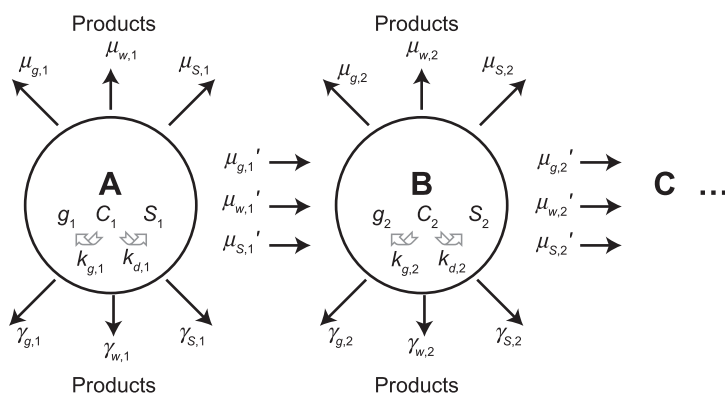
Figure 1: Schematic of the general structure of first-order decay reactions for three solutes (A, B and C) as implemented in the HYDRUS codes.

turn being denitrified to form di-nitrogen (N_2 and N_2O). In this reaction pathway, ammonium is a sorbing and volatile species that can be present in the liquid phase as well as in the solid and gaseous phases.

Additional HYDRUS-1D examples for sequential decay chains are given by Wehrhan et al.[54] and Unold et al.[55] who investigated the fate and transport of the antibiotic sulfadiazine (SDZ) and its main transformation products in pig manure. Casey and Šimůnek[56] and Schaerlaekens et al.[57] considered first-order degradation for the transport of trichloroethylene (TCE). Microbiological degradation of perchloroethylene (PCE) under anaerobic conditions follows a series of chain reactions in which, sequentially, trichloroethylene (TCE), cis-dichloroethylene (c-DCE), vinylchloride (VC), and ethene are generated.

The transport of hormones was investigated using HYDRUS-1D by Casey et al.,[58–60] Das et al.,[61] and Fan et al.[62] Casey et al.[58,60] and Das et al.[61] studied the transport of estrogenic hormones, i.e., 17β-estradiol and its primary metabolite estrone, in natural soil. Casey et al. (2004)[59] and Das et al.[61] evaluated the transport of androgenic hormones (i.e., testosterone and its primary metabolite androstenedione). Papiernik et al.[63] further used HYDRUS-1D to evaluate the transport of the herbicide isoxaflutole and its diketonitrile and benzoic acid metabolites. Bradford et al.[64] similarly used a variant of the sequential first-order decay model to simulate the transport and retention behavior of monodispersed and aggregated species of pathogenic *E. coli* O157:H7. We further note the work by Dontsova et al.[65,66] who analyzed the fate and transport of explosives. Additional examples in which HYDRUS was used to simulate the transport of first-order degradation chains can be found in the literature.

3.3 *Transport of mutually dependent multiple ions*

While the above models for solutes subject to sequential first-order degradation reactions has proved to be very attractive in dealing with different chemicals, they cannot be used to describe many transport scenarios in which several solute species are present simultaneously in the soil solution. This is because the soil solution is always a mixture of many ions which may mutually interact, create complexed species, precipitate, dissolve, and/or could compete with each other for sorption sites.[4,67] For such conditions, one needs to use multicomponent reactive transport models that consider the various mutual interactions between the different solutes and integrate those

interactions and reactions with transport modules for water and solutes.

Following Šimůnek and Valocchi,[4] geochemical transport models can be broadly divided into two major groups: models with specific chemistry and general models. Models with specific chemistry are usually constrained to very specific applications since they are restricted to certain prescribed chemical systems. On the other hand, models with generalized chemistry provide users with much more flexibility in designing particular chemical systems, thus permitting a much broader range of applications. Users can then either select species and reactions from large geochemical databases, or are able to define their own species with particular chemical properties and reactions.

Models simulating the transport of major ions, such as LEACHM[68] and UNSATCHEM,[6,69] and various reclamation models[4] are typical examples of models with specific chemistry. These models typically consider the transport of major ions and their mutual reactions such as complexation, cation exchange, and precipitation/dissolution. The UNSATCHEM add-on module to HYDRUS (2D/3D), discussed below, is an example of such a model.

Models are now also increasingly available for simulating carbon and nitrogen cycles. Examples are CENTURY,[70] LEACHN,[68] RZWQM,[71] and COUP.[72] Environmental models of this type typically distribute organic matter, carbon, and organic and mineral nitrogen over multiple computational pools, while allowing organic matter to be decomposed by multiple microbial biomass populations. They can account for most of the major reaction pathways, such as inter-pool transfer of carbon and nitrogen, nitrification (ammonium to nitrate-N), denitrification (leading to the production of N_2 and N_2O), volatilization losses of ammonia (NH_3), and microbial biomass growth and death. The Wetland add-on module to HYDRUS (2D/3D), discussed below, is an example of such a model.

Most codes with general geochemistry are limited to solute transport and biogeochemical reactions, while water flow paths must be calculated outside of the reactive transport code. Typical examples are PHREEQC,[73] CRUNCH,[74] and PHAST.[75] Only a few models allow the velocity field to be calculated internally (e.g., MIN3P).[76] Several codes for transient variably-saturated flow have also been coupled to general biogeochemistry models. These include 3DHYDROGEOCHEM,[77] TOUGHREACT,[78] and the HYDRUS (2D/3D) add-on module HP1/2/3[16,79] discussed below.

Several interesting applications of both the specific and general chemistry models have recently appeared in a special issue of Vadose Zone Journal entitled "Reactive Transport Modeling".[67] The models with specific chemistry were used in studies by Langergraber and Šimůnek,[28] Reading et al.,[80] and Suarez et al.[81] Langergraber and Šimůnek[28] illustrated the use of reactive transport modeling with the Wetland module within the HYDRUS software as a tool for evaluating complex physical and chemical processes within wetland systems constructed for the treatment of various contaminants. Reading et al.[80] used the UNSATCHEM code to evaluate the use of gypsum to ameliorate a nonsaline sodic clay soil in North Queensland, Australia, while Suarez et al.[81] used UNSATCHEM to evaluate reactions controlling the fate and transport of boron in soils, which are critical for optimal management of B-containing waste waters in arid systems.

General reactive transport models have been used in recent studies.[82–84] Bea et al.[82] used the MIN3P-D multicomponent reactive transport code to describe processes occurring within a mine tailing impoundment and their impact on CO_2 sequestration. Chang et al.[83] used PHREEQC in combination with laboratory column experiments to evaluate the efficacy of Fe(II)-containing solutions as an in-situ means for reducing toxic hexavalent chromium (Cr(VI)) to trivalent chromium (Cr(III)), which subsequently coprecipitates with Fe(III). Lichtner and Hammond (2012)[84] used PFLOTRAN to evaluate geochemical processes controlling the aqueous phase distribution and solid phase speciation of a hexavalent uranium [U(VI)] plume below the Hanford 300 Area bordering the Columbia River in Hanford, WA.

4 Specialized HYDRUS Modules

In this section we summarize several newly implemented HYDRUS modules, some of which represent examples of reactive transport with specific chemistry (notably the Wetland and UnsatChem modules), while others consider general reactive transport (the HP1 and HP2 models). Also briefly discussed are several modules not intended for the transport of multiple solutes but providing additional modeling capabilities, such as to account for preferential flow (the DualPerm module), colloid-facilitated solute transport (the C-Ride module), or fumigant transport (the Fumigant module). Except for the older HP1, all modules simulate flow and transport processes in two-dimensional transport domains and are fully supported by the HYDRUS (2D/3D) graphical user interface.

Many of the processes are also available as part of HYDRUS-1D.

4.1 *The HP1/HP2 modules*

The one-dimensional program HP1, which couples the PHREEQC geochemical code[73] with HYDRUS-1D, was first released in 2005,[16] and used successfully in many applications. HP1, which is an acronym for HYDRUS-PHREEQC-1D, is a relatively comprehensive simulation module that can be used to 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. HP2[79] is the two-dimensional equivalent of HP1. The HP1 and HP2 modules both 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.

The versatility of HP1 was demonstrated by Jacques and Šimůnek[16] and Jacques et al.[5,7] on several examples, including (a) the transport of heavy metals (Zn^{2+}, Pb^{2+}, and Cd^{2+}) subject to multiple cation exchange reactions, (b) transport with mineral dissolution of amorphous SiO_2 and gibbsite ($Al(OH)_3$), (c) heavy metal transport in a medium having a pH-dependent cation exchange complex, (d) 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), (e) 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, (f) cadmium leaching in acid sandy soils, (g) radionuclide transport, and (h) long term uranium migration in agricultural field soils following mineral P-fertilization.

More recent applications of HP1 include Bessinger and Marks,[85] who used HP1 to evaluate laboratory and field experiments involving the treatment of mercury-contaminated soils with activated carbon, and Jacques et al.[86,87] who used HP1 to model chemical degradation of concrete during leaching with rain and different types of water. Jacques et al.[87] also considered the effects of chemically degrading concrete on its hydraulic properties such as porosity, tortuosity, and the hydraulic conductivity. Jacques et al.[88] additionally combined HP1 with the general optimization UCODE program[89] to inversely optimize hydraulic, solute transport, and cation exchange

parameters pertaining to column experiments subject to transient water flow and solute transport with cation exchange.

The versatility of HP2 was demonstrated recently by Šimůnek et al.[79] on several examples: (a) a sodic soil reclamation problem using furrow irrigation, which demonstrated the cation exchange features of HP2, and (b) the release and migration of uranium from a simplified uranium mill tailings pile towards a river. These examples included the processes of water flow, solute transport, precipitation/dissolution of the solid phase, cation exchange, complexation, and many other reactions. As an example of possible modeling output, Figures 2 and 3 show uranium concentration profiles at two different times, and final pH, calcite, and gypsum profiles, respectively, for the uranium tailings example adapted from Yeh and Tripathi.[90] Detailed information about this project, as well as instructions on how to implement the project using HP2, can be found in Šimůnek et al.[79]

4.2 *The C-Ride module*

The C-Ride module[91] considers the transport of particle-like substances (e.g., colloids, microorganisms, and nanoparticles) as well as colloid-facilitated transport,[30] the latter often observed for many strongly sorbing contaminants such as heavy metals, radionuclides, pharmaceuticals, pesticides, and explosives. These contaminants are associated predominantly with the solid phase, which is commonly assumed to be stationary. However, the 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.

The C-Ride module fully accounts for the dynamics of colloid transfer (attachment/straining) and solute transfer (kinetic/equilibrium sorption onto soil and mobile/deposited colloids) between the different phases. A schematic of the colloid transport and colloid-facilitated transport module is shown
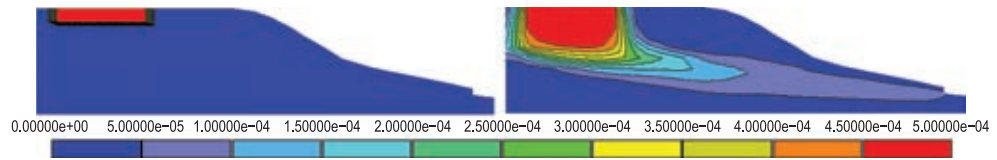
Figure 2: Uranium concentration profiles at times 0 (left), and 500 (right) d for the Uranium Tailing Pile Leaching example.
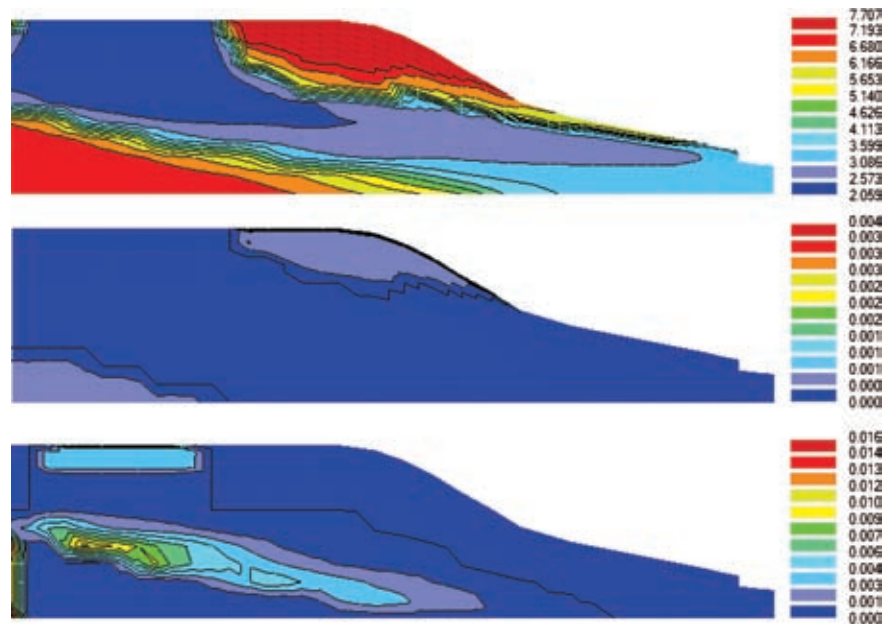

Figure 3: Plots of pH (top), calcite (mol/L) (middle), and gypsum (mol/L) (bottom) after 1000 d for the Uranium Tailing Pile Leaching example.

in Figure 4. The module assumes that the porous medium consists of three phases (i.e., solid, air and water). Following van der Weerd and Leijnse,[92] the C-Ride module assumes that (a) only one type of colloid exists in the system, and that the colloids can be described by their mean behavior, (b) colloids are stable and that their mutual interactions in the liquid phase may be neglected, (c) immobile colloids do not affect the flow and transport properties of the porous medium because of possible clogging of small pores, and (d) the transport of colloids is not affected by sorption of contaminants on colloids. Colloids are assumed to exist in three states (Fig. 4, top): mobile (suspended in water), C_c [$N_c L^{-3}$], attached to the solid phase, S_c^{att} [$N_c M^{-1}$], and strained by the solid phase, S_c^{str} [$N_c M^{-1}$]. Colloid phase changes are described in terms of nonlinear first-order processes of attachment, k_{ac} [T^{-1}], detachment, k_{dc} [T^{-1}], and straining, k_{str} [T^{-1}].

C-Ride further assumes that contaminants can be dissolved in the liquid phase, C [ML^{-3}], as well as can be sorbed instantaneously (S_e [MM^{-1}]) and kinetically (S_k [MM^{-1}]) to the solid phase, and to colloids in all of their states (S_{mc}, S_{ic} [MN_c^{-1}]). Six different states of contaminants (Fig. 4, bottom) are thus distinguished: dissolved, instantaneously or kinetically sorbed to the solid phase, and sorbed to mobile or immobile colloids (the latter either strained or attached to the solid phase). The coefficients k_{amc}, k_{aic}, k_{dmc}, k_{dic} [T^{-1}] in Figure 4 represent various first-order attachment/detachment rates to/from mobile and immobile colloids. The coefficients K_d and ω represent instantaneous and kinetic solute sorption to the solid phase, respectively, while the factors ψ account for nonlinearity of the various processes.[30,91]

Figure 5 shows a conceptual model for cadmium (and virus) transport facilitated by
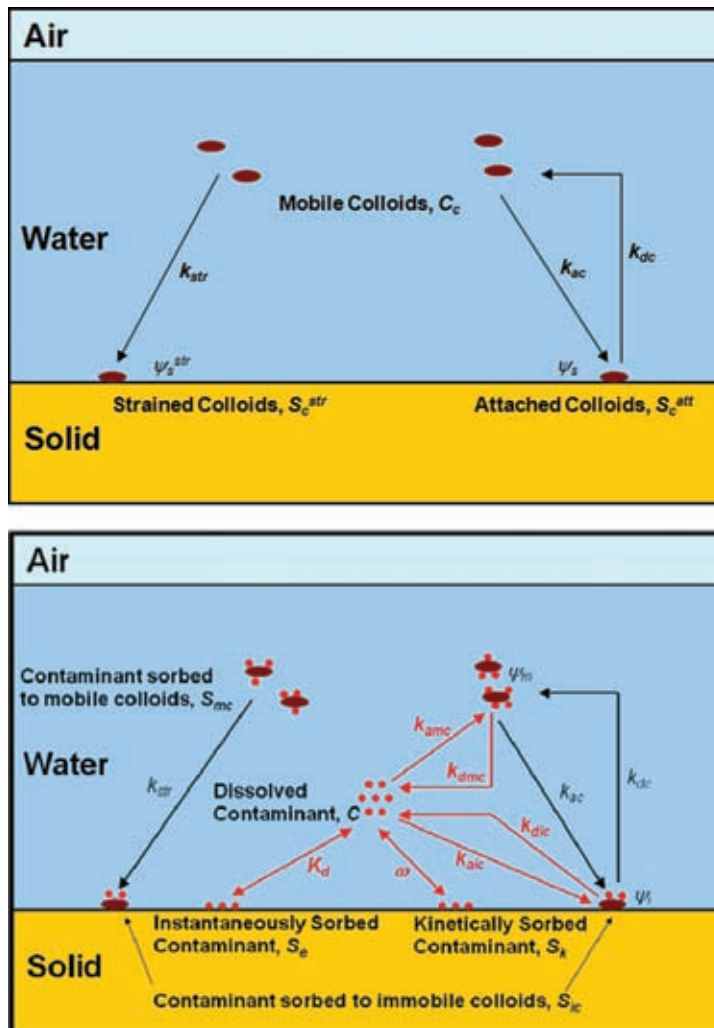
Figure 4: Schematic of the C-Ride module for colloid transport (top) and colloid-facilitated solute transport (bottom).
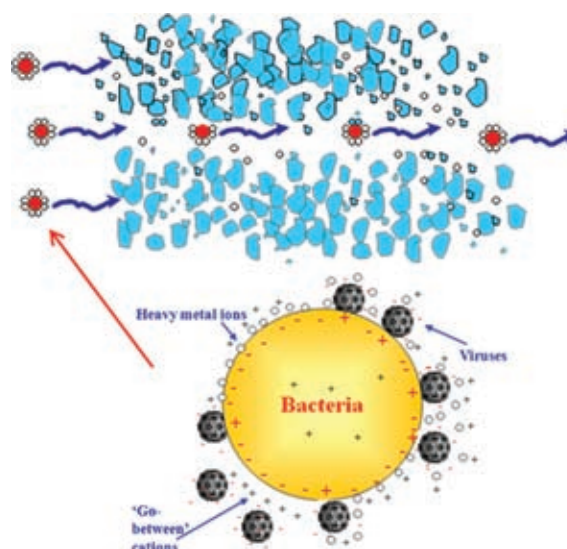
Figure 5: Schematic of a conceptual model for bacteria-facilitated transport of heavy metal ions and viruses.

B. subtilis spores or *E. coli* in saturated coarse alluvial gravels.[96] This application of the C-Ride module successfully simulated Cd transport involving advection, dispersion, kinetic adsorption-desorption of Cd to/from the aquifer and to/from mobile/immobile bacteria, and kinetic attachment/detachment of the bacteria to/from the aquifer.

4.3 The DualPerm module

The DualPerm module[94] simulates preferential and/or nonequilibrium water flow and solute transport in dual-permeability media using the approach suggested by Gerke and van Genuchten.[15] 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.[31] The dual-permeability formulation has seen many applications, especially in 1D.[95–97] Several of these examples are discussed by Köhne et al.[46,47]

An example of pressure head profiles calculated for a tension disc infiltration experiment is shown in Figure 6. The transport domain for the matrix and fracture was taken to be 50 cm wide and 150 cm deep, while the disc radium was assumed to be 10 cm. Different ratios of the anisotropy of the hydraulic conductivity were employed in the simulations ($K_x^A/K_z^A = 1$, 10, and 0.1 from left to right in the figure). Various parameters used for

these calculations using the DualPerm module are given by Šimůnek et al.[94]

4.4 The UnsatChem module

The UnsatChem geochemical module[98] has been implemented into both the one- and two-dimensional computational versions of HYDRUS. This module simulates the transport of major ions (i.e., Ca^{2+}, Mg^{2+}, Na^+, K^{2+}, SO_4^{2-}, CO_3^{2-}, and Cl^-) and their equilibrium and kinetic geochemical interactions, such as complexation, cation exchange and precipitation-dissolution (e.g., of 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 already some 20 years ago,[69] the UnsatChem module (especially its one-dimensional version) has been used in many applications.[99–105]

Gonçalves et al.[106] and Ramos et al.[107] recently demonstrated the applicability of Unsatchem to simulating multicomponent major ion transport in soil lysimeters irrigated with waters of different quality. The UnsatChem module of HYDRUS-1D was used in their work to describe field measurements of the water content, overall salinity, the concentration of individual soluble cations, as well as the Sodium Adsorption Ratio (SAR), Electric Conductivity (EC), and the Exchangeable Sodium Percentage (ESP). Figure 7 summarizes results for this application.
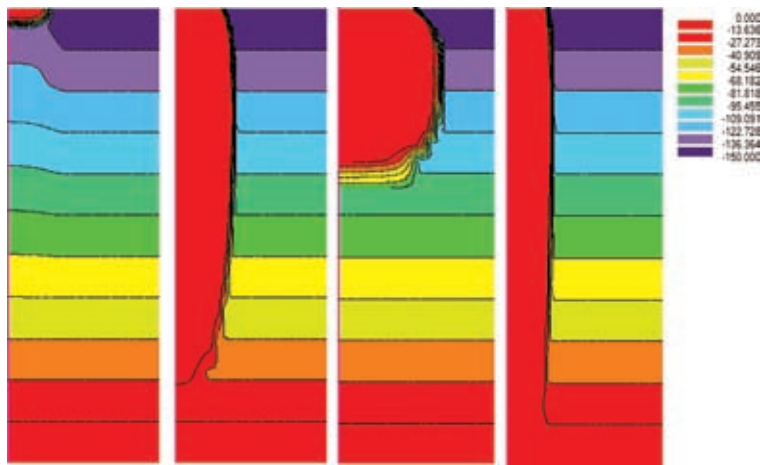
Figure 6: Pressure head profiles for the matrix (left), an isotropic fracture, a fracture with $K_x^A/K_z^A = 10$, and a fracture with $K_x^A/K_z^A = 0.1$ (right).
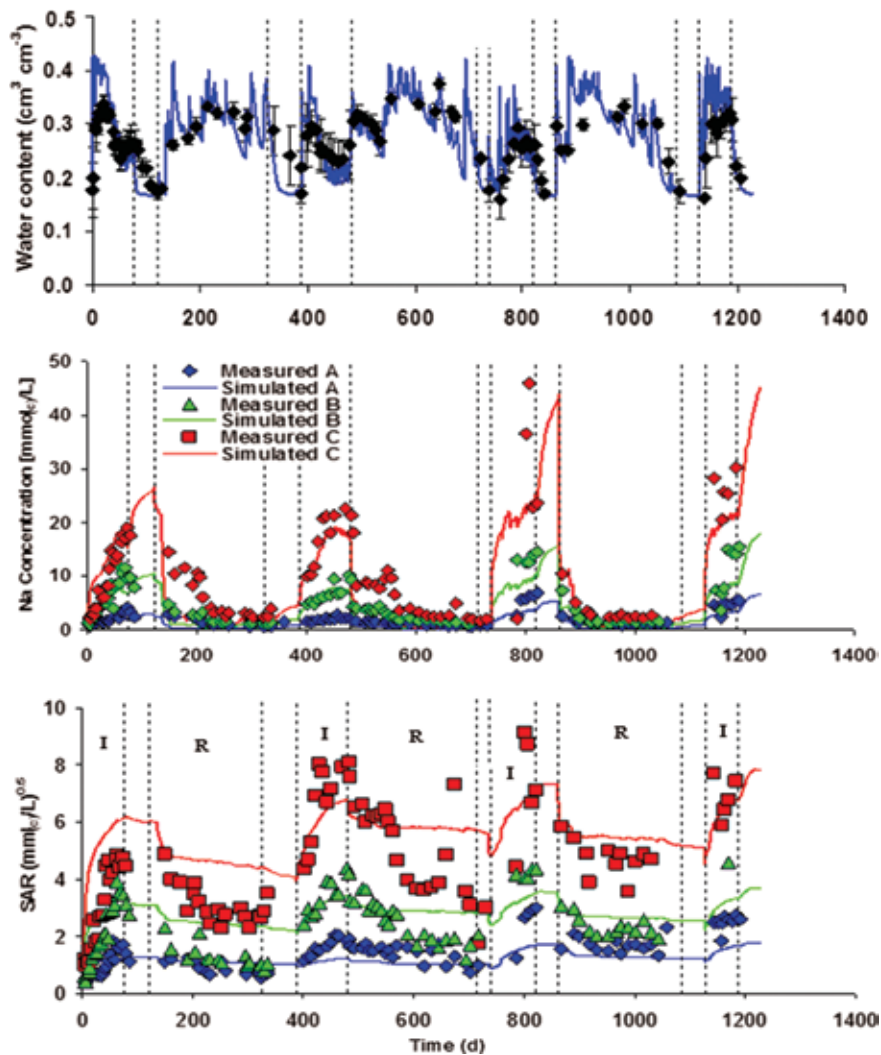
Figure 7: Measured and simulated volumetric water contents (top), soluble sodium concentrations (middle), and sodium adsorption ratios (SAR) for lysimeters irrigated with waters of different quality (A, B, and C). I and R correspond to the irrigation and rainfall periods, respectively. Adapted from Gonçalves et al.[106]
Source: This material is reproduced with permission of John Wiley & Sons, Inc.
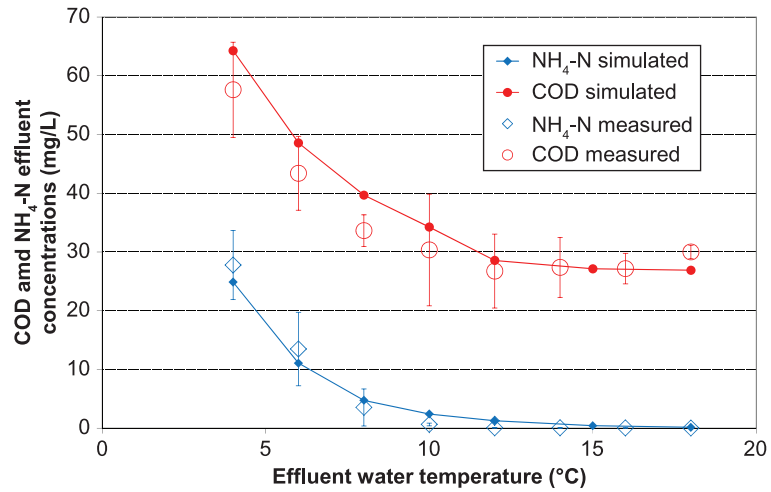
Figure 8: Measured and simulated COD and NH$_4$-N effluent concentrations of a vertical flow constructed wetland. Adapted from Langergraber.[110]
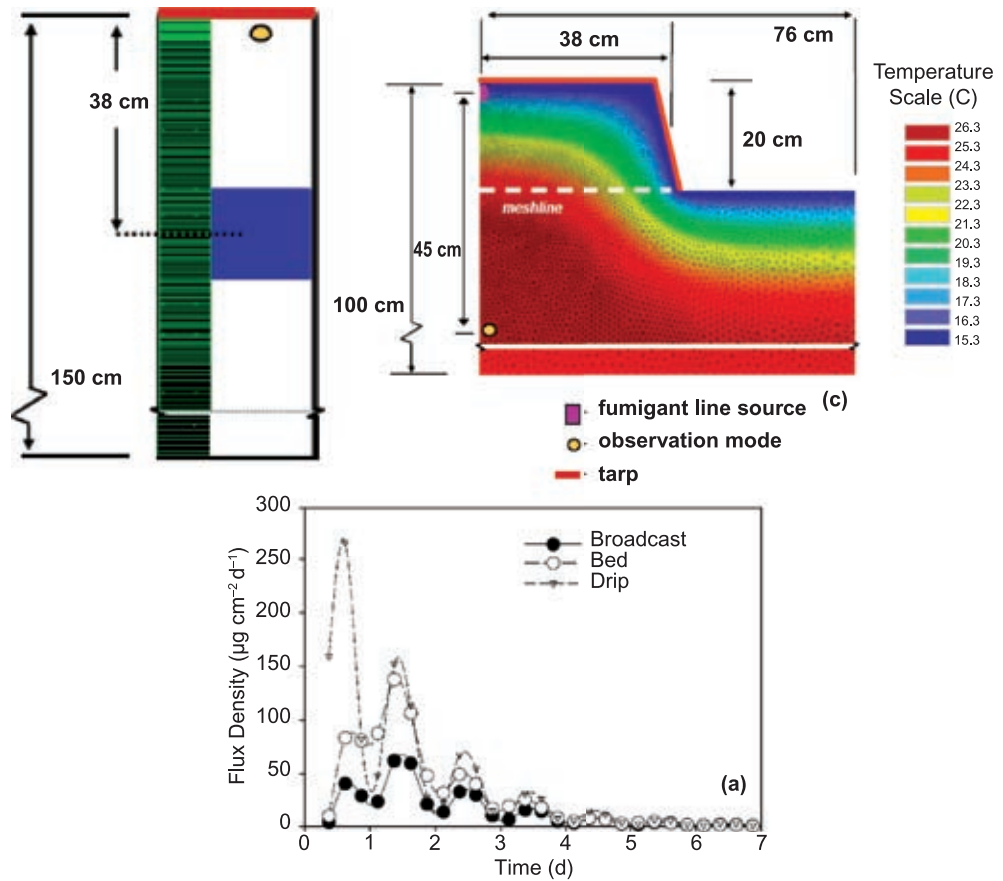
Figure 9: Tarped broadcast (top left), tarped bed drip (top right) and volatilization fluxes (bottom) for different fumigants application scenarios (adopted from Spurlock et al.).[119]

4.5 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.[28] Constructed wetlands are engineered water treatment systems that optimize treatment processes found in natural environments. Constructed wetlands have become popular since they can be

relatively 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 and stimulate each other.

The Wetland module uses two biokinetic model formulations (CW2D of Langergraber and Šimůnek[23] and CWM1 of Langergraber et al.)[108] to account for complex conditions that may occur in various types of wetlands. Both biokinetic model formulations have been developed for constructed wetlands treating municipal wastewater. A good match with measured effluent concentration data could be achieved, especially for vertical flow constructed wetlands with intermittent loadings.[109–111] As an example, Figure 8 shows a comparison of simulated and measured effluent concentrations of a vertical flow constructed wetland treating municipal wastewater. In addition to applications involving municipal wastewater, the Wetland model has been also used for constructed wetlands treating combined sewer overflow,[112–115] treating effluent of a wastewater treatment plant for irrigation purposes,[116] and treating run-off from agricultural sites including predictions of the effects of streamside management zones.[117,118]

4.6 The Fumigants module

The Fumigants module implements multiple additional options required to simulate processes related to fumigant applications and transport. This module allows users to specify an additional injection of fumigants into the transport domain at a specified location and time, consider the presence or absence of a surface tarp, allow the tarp properties to depend on temperature, and permit tarp removal at a specified time. The Fumigants module was recently used to investigate the effect of different application scenarios, such as tarped broadcasting, tarped bedded shank injection, tarped drip line-source application, and other options (e.g., having different initial water contents and tarp permeability) on fumigant volatilization.[119] Figure 9 illustrated an application.

5 Conclusions

In this paper we provided an overview of the HYDRUS codes and various specialized modules that were recently added to the computer software packages. We believe the that HYDRUS models have provided, and will continue to provide, an important service to the soil environmental and hydrological communities, especially but not limited to vadose zone processes. This is reflected by their frequent use in a wide range of applications

in both basic and applied research and engineering. For example, the HYDRUS website (http://www.pc-progress.com/en/Default.aspx) lists over one thousand publication in which the HYDRUS codes have been used. The codes 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. Examples of the latter are the HP1/HP2 modules that couple the HYDRUS software packages with the PHREEQC geochemical code, and the Wetland module that includes two biokinetic model formulations (CW2D and CWM1). The need for codes such as HYDRUS is reflected further by the frequency of downloading 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 about 700 individual visitors each day.

The wide use of the HYDRUS models is in large part due also to their ease of use because of the implementation of relatively sophisticated interactive graphical user interfaces, which are continuously being updated in attempts to make the codes as attractive as possible for non-expert users. Feedback from users is continuously being used also to improve the codes, to identify particular strengths and weaknesses of the models, and to define additional processes or features that should be included in the models. We believe that the codes and associated manuals hence are serving an important role in the transfer of vadose zone research and development technologies to both the scientific community and practitioners.

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