Modeling of irrigation and related processes with HYDRUS

Naftali Lazarovitch\textsuperscript{a,\*}, Isaya Kisekka\textsuperscript{b}, Tobias E. Oker\textsuperscript{c}, Giuseppe Brunetti\textsuperscript{d}, Thomas Wöhling\textsuperscript{e,f}, Li Xianyue\textsuperscript{g}, Li Yong\textsuperscript{h}, Todd H. Skaggs\textsuperscript{i}, Alex Furman\textsuperscript{j}, Salini Sasidharan\textsuperscript{k}, Iael Raji-Hoffman\textsuperscript{b}, and Jiří Šimůnek\textsuperscript{l,\*}

\textsuperscript{a}French Associates Institute for Agriculture and Biotechnology of Drylands, Jacob Blaustein Institutes for Desert Research, Ben-Gurion University of the Negev, Be’er Sheva, Israel
\textsuperscript{b}Department of Land Air and Water Resources, University of California Davis, Davis, CA, United States
\textsuperscript{c}College of Agricultural and Environmental Sciences, University of Georgia, Tifton Campus, GA, United States
\textsuperscript{d}Department of Civil Engineering, University of Calabria, Rende, Italy
\textsuperscript{e}Technische Universität Dresden, Chair of Hydrology, Dresden, Germany
\textsuperscript{f}Lincoln Agritech Ltd, Environmental Research, Hamilton, New Zealand
\textsuperscript{g}Inner Mongolia Agricultural University, Hohhot, China
\textsuperscript{h}Hohai University, Nanjing, China
\textsuperscript{i}U.S. Salinity Laboratory, USDA-ARS, Riverside, CA, United States
\textsuperscript{j}Technion, Israel Institute of Technology, Israel
\textsuperscript{k}Department of Biological & Ecological Engineering, Oregon State University, Corvallis, OR, United States
\textsuperscript{l}Department of Environmental Sciences, University of California, Riverside, CA, United States

*Corresponding authors: e-mail address: lazarovi@bgu.ac.il; jiri.simunek@ucr.edu

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Abstract

Future agriculture calls for increased input (e.g., water, nutrients, pesticides) use efficiency while maintaining or improving productivity, minimizing environmental impacts, and increasing profitability. Complete understanding of complex irrigation systems requires laborious, time-consuming, and expensive field investigations, which invariably involve only a limited number of treatments. On the other hand, fully calibrated process-based models, such as HYDRUS, can quickly evaluate different irrigation management strategies without the need for labor-intensive fieldwork and have become valuable research tools for predicting complex and interactive water flow and solute transport processes in and below the root zone. HYDRUS codes have been used worldwide in several hundreds of studies evaluating various types of irrigation (e.g., sprinkler, furrow, basin, and surface and subsurface drip), their scheduling (e.g., the timing of irrigation and its amount), and solute-related factors (e.g., fertigation, chemigation, salinization, and sodification).

The objective of this manuscript is to review the current modeling capabilities of HYDRUS to evaluate various irrigation methods and related processes. The manuscript starts with a section describing governing flow and transport equations solved numerically by the HYDRUS codes, the corresponding initial and boundary conditions, and related factors such as soil hydraulic properties and root water and nutrient uptake. Modeling of different irrigation techniques is described in subsequent sections, followed by sections dealing with solute-related topics such as fertigation, chemigation, and salinization/sodification. Topics, including the effects of spatial variability, optimization of irrigation systems, and special irrigation methods, are covered in the later sections. The manuscript emphasizes the advantages and opportunities of HYDRUS in describing various processes in the root zone of irrigated plants that support sustainable irrigated agriculture. All the project files of the discussed examples and their descriptions are available for download at https://www.pc-progress.com/en/Default.aspx?hyd5-AdvancesInAgronomy.

1. Introduction

1.1 General introduction

Sustainably meeting the comprehensive dietary needs of each individual on this globe is a concern that is growing alongside the world population. The major steps needed to meet this goal include decreasing food waste, changing our diets by consuming more plant and less animal protein, and intensifying production on existing cultivated areas while reducing the environmental impact of production. Irrigated agriculture is the primary user of freshwater, accounting for nearly 85% of the total global water consumption (Jury and Vaux Jr., 2007) and providing about 40% of total
food production (Sepulcre-Cantó et al., 2007). Irrigation water demand is expected to increase in the future due to foreseen alterations in rainfall caused by climate change and increased food and biofuel demands. Water scarcity is increasing worldwide, necessitating the development of more efficient irrigation practices.

Complete understanding of irrigation systems and corresponding complex physical, chemical, and biological interactions in the soil–plant–atmosphere system requires laborious, time-consuming, and expensive field investigations. Such investigations invariably involve only a limited number of treatments that only provide information about the studied systems and conditions (e.g., for a particular climate, plants, soils, and irrigation methods). This information then needs to be extrapolated to other relevant conditions. Numerical models have become indispensable tools for evaluating, summarizing, and extrapolating information about vadose zone flow and transport processes in the root zones of irrigated systems. Despite their complexity, the use of numerical models is increasing thanks to a better understanding of water flow and transport processes, the development and improvement of mathematical methods for solving governing equations, and accelerated development of computers capable of computing different processes simultaneously for short time and small space increments (van Genuchten and Šimůnek, 2004). There is now a growing use of models for the visualization of irrigation (Assouline, 2002; Gärdénäs et al., 2005) and fertilization–related processes (Cote et al., 2003; Gärdénäs et al., 2005; Hanson et al., 2006). Fully calibrated process-based models can quickly evaluate different irrigation management strategies for different climate and soil conditions and various crops without the need for labor-intensive fieldwork, and they have become valuable research tools for predicting complex and interactive water flow and solute transport processes in and below the root zone.

1.2 HYDRUS introduction

The HYDRUS software packages (Šimůnek et al., 2008, 2012, 2016b, 2018, 2022a,b) represent typical examples of such process–based mathematical models. These software packages numerically solve the Richards equation for variably saturated water flow and advection–dispersion equations for heat and solute transport (and many other processes and factors) in one–, two–, and three–dimensional variably saturated soil domains. A sink term in the flow and transport equations accounts for plant roots’ uptake of water and nutrients. Heat transport occurs due to conduction and
convection with flowing water. Advective-dispersive transport in the liquid phase, as well as diffusion in the gaseous phase, is considered in the solute transport equations, which also include provisions for nonlinear nonequilibrium reactions between the solid and liquid phases, linear equilibrium reactions between the liquid and gaseous phases, and various zero-order and first-order degradation reactions. In addition, 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 filtration theory, is additionally included to enable simulations of the transport of viruses, colloids, and/or bacteria.

The HYDRUS software packages and its various predecessors, e.g., SWMS-2D, CHAIN-2D, HYDRUS-1D, HYDRUS-2D, and HYDRUS (2D/3D), have a long history that goes back to the early 1990s and have been used in several thousands of studies involving various agricultural, industrial, and environmental applications as documented in detail by Šimůnek et al. (2008, 2012, 2016b). These applications have resulted in several hundreds of manuscripts evaluating various types of irrigation (e.g., sprinkler, furrow, basin, and surface and subsurface drip), their management (e.g., the timing of irrigation and its amount), and associated solute-related factors (e.g., fertigation chemigation, salinization, and sodification) (Šimůnek et al., 2016b).

The last comprehensive review of the HYDRUS software packages was published in the Vadose Zone Journal in 2016 (Šimůnek et al., 2016b) when two independent packages for one-dimensional (i.e., HYDRUS-1D, version 4) and two- and three-dimensional (i.e., HYDRUS (2D/3D), version 3) applications still existed. These two software packages have recently been merged, resulting in a single HYDRUS (Version 5) software package, consisting of an interactive graphics-based user interface (Šejna et al., 2022) and multiple computational programs for simulating water, heat, and solute movement in one-, two-, and three-dimensional variably saturated porous media (Šimůnek et al., 2022a,b). Version 5 of HYDRUS (compared to its earlier versions), in addition to providing various new graphical capabilities, such as depth-time graphs for various variables of one-dimensional simulations, also includes several new modules that greatly expand the numerical capabilities of the software package, some of which are highly relevant for agricultural and irrigation applications.

While various new modules implemented into HYDRUS 5 have been individually described in their corresponding manuscripts (see references given below), they have not comprehensively been listed in one text.
The **Furrow module** to simulate the coupled surface-subsurface water flow and solute transport in blocked and open-ended furrows has recently been developed by Brunetti et al. (2018b). This hybrid Finite Element-Finite Volume pseudo-3D model combines the two-dimensional Richards-based Finite-Element solver, HYDRUS-2D, for subsurface flow with a one-dimensional Finite-Volume discretization of the zero-inertia and advection equations for overland flow. The model has been successfully validated in synthetic and experimental scenarios by Brunetti et al. (2018b). This add-on module has been fully incorporated into the GUI of the HYDRUS 5.

The **PFAS module** (Silva et al., 2020) can simulate the fate and transport of polyfluoroalkyl substances (PFAS) under dynamic vadose zone conditions. PFAS are a class of thousands of related chemicals used for their water-repellent and fire-retardant qualities. They are sometimes called “forever chemicals” because they persist in the environment and accumulate in people and animals. They have been linked to health problems, including testicular and kidney cancers, high cholesterol, and thyroid disease. The contamination of agricultural soils by these long-lasting toxins can be traced to sludge from treatment plants spread over the years as fertilizer on farm-lands to add nutrients. These chemicals behave differently than traditional organic contaminants. Rather than being present in the gas phase (a process considered in the standard HYDRUS model), these chemicals sorb to the air-water interface. The PFAS module thus replaces the storage term for the air phase with the storage term for the sorption to the air-water interface. It additionally considers the concentration effects on surface tension and viscosity.

Another new module is the **Dynamic Plant Uptake (DPU) module** (Brunetti et al., 2019a), which simulates the translocation and transformation of neutral compounds in the soil-plant domain. Traditionally, HYDRUS deals only with processes in the subsurface and general plant uptake, leaving what happens with water and chemicals once they enter plants unaccounted for. However, plants (fruits or leaves) represent the most common pathway for environmental contaminants to enter the human and animal food chain. Plants can uptake chemicals from contaminated environments (e.g., by irrigation water) and bioaccumulate and metabolize them in by-products, which can be dangerous for human health. The DPU module couples HYDRUS with a multicompartment Dynamic Plant Uptake model of Trapp (2007), which accounts for multiple differentiated metabolism pathways in plant tissues, and allows one to simulate the entire pathway.
from irrigation to soil, from soil to roots, and from roots to stems, fruits, and leaves, while considering relevant biochemical reactions in all these compartments.

Additional new modules in Version 5, less relevant to irrigation applications, are COSMIC (Brunetti et al., 2019b), Particle Tracking (Zhou et al., 2021), Fumigant (Spurlock et al., 2013b), and C-Ride (Šimůnek et al., 2006). The **COSMIC module** (Brunetti et al., 2019b) calculates above-ground neutron fluxes using the physically based COsmic-ray Soil Moisture Interaction Code (COSMIC) of Shuttleworth et al. (2013). The **Particle Tracking module** (Zhou et al., 2021) tracks hypothetical particles in the subsurface, and its results can be used to calculate soil water travel times and water age for different locations in the soil profile. The **Fumigant module** considers additional options and factors related to the transport of fumigants, i.e., chemicals used to sterilize soils before planting crops (e.g., tarp removal, temperature-dependent tarp properties, an additional injection of fumigants) (Spurlock et al., 2013b). Finally, the **C-Ride module** (Šimůnek et al., 2006) can simulate variably saturated water flow, colloid transport, and colloid-facilitated solute transport in porous media.

### 1.3 Manuscript Objectives

As discussed above, HYDRUS models have been used in several hundreds of manuscripts evaluating various types of irrigation, their management, and associated solute-related factors. Some of these older applications, mainly furrow and drip irrigation, were reviewed by Šimůnek et al. (2016b). The objective of this manuscript is to further expand on this older review and to examine HYDRUS’s current modeling abilities to evaluate various irrigation methods and related processes. The manuscript begins with a section describing governing flow and transport equations solved numerically by the HYDRUS codes, the corresponding initial and boundary conditions, and related factors such as soil hydraulic properties and root water and nutrient uptake. Modeling of different irrigation techniques is described in subsequent sections, followed by sections dealing with solute-related topics, including fertigation, chemigation, and salinization/sodification. Topics such as the effects of spatial variability, optimization of irrigation systems, and special irrigation methods are covered in the later sections.
The manuscript emphasizes the advantages and opportunities of HYDRUS in describing various processes in irrigated plant root zones that support sustainable irrigated agriculture.

The manuscript provides many examples of HYDRUS simulating various types of irrigation and related processes. The use of various (standard and special) boundary conditions available in the software to simulate different irrigation types is demonstrated throughout the manuscript. Different ways of displaying the obtained results are also presented. Finally, the manuscript proposes possible directions for software development so that it continues to be relevant in optimizing irrigation scheduling in the twenty-first century.

2. Mathematical and physical background

2.1 Governing flow and transport equations

Water flow and solute transport in soils are described in the HYDRUS models using the modified Richards (1) and convection-dispersion (2) equations, respectively (Šimůnek et al., 2022a,b):

\[ \frac{\partial \theta(h)}{\partial t} = \frac{\partial}{\partial x_i} \left[ K(h) \left( K_{ij}^A \frac{\partial h}{\partial x_i} + K_{ijz}^A \right) \right] - S(h) \]  
\[ \frac{\partial (\rho bs + \theta c + ag)}{\partial t} = \frac{\partial}{\partial x_i} \left( \theta D_{ij}^{\omega} \frac{\partial c}{\partial x_j} \right) + \frac{\partial}{\partial x_i} \left( aD_{ij}^{q} \frac{\partial q}{\partial x_j} \right) - \frac{\partial (q_{i,c})}{\partial x_i} - \phi \]  

The Richards Eq. (1) combines the mass balance equation with the Darcy-Buckingham equation, and it contains the following variables: \( \theta \) is the volumetric water content \([L^3 L^{-3}]\), \( h \) is the pressure head or matric potential \([L]\), \( t \) is time \([T]\), \( x_i \) is the spatial coordinate \([L]\), \( K \) is the unsaturated hydraulic conductivity \([LT^{-1}]\), \( K_{ij}^A \) are components of a dimensionless anisotropy tensor \( K^A \), and \( S \) is the sink/source term \([L^3 L^{-3} T^{-1}]\), usually accounting for root water uptake (transpiration). Alternative formulations to Eq. (1) that partition the liquid phase into mobile and immobile (or less mobile) regions (i.e., dual-porosity or dual-permeability models) are also available in the HYDRUS code to account for nonequilibrium or preferential flow (e.g., Šimůnek et al., 2003, 2008; Šimůnek and van Genuchten, 2008; Šimůnek et al., 2016b). This partial differential equation is strongly nonlinear, and as a result, only a relatively few simplified analytical solutions can be derived. Most practical applications require a numerical solution,
which can be obtained using various numerical methods such as finite differences or finite elements.

The equation governing the transport of dissolved solutes in the vadose zone (2) is obtained by combining the solute mass balance equation with equations defining the total mass of the chemical (on the left side) and the solute flux densities and solute reactions (on the right side). In its most general interpretation, the solute transport Eq. (2) allows chemicals to reside in all three phases of the soil (i.e., gaseous, liquid, and solid) and a broad range of transport mechanisms (including advective transport, diffusion, and hydrodynamic dispersion in both the liquid and gaseous phases), and it facilitates different types of chemical reactions that lead to losses or gains in the total chemical concentration. Advective-dispersive transport in the liquid phase, as well as diffusion in the gaseous phase, is considered in the solute transport equations, which also include provisions for linear and nonlinear (i.e., Freundlich, Langmuir, or Freundlich–Langmuir adsorption isotherms), and equilibrium and nonequilibrium (i.e., one- or two-site sorption models) reactions between the solid and liquid phases, linear equilibrium reactions between the liquid and gaseous phases (i.e., Henry’s law), and various zero-order and first-order degradation reactions.

In Eq. (2), \( \rho_b \) is the bulk density [ML\(^{-3}\)], \( a \) is the volumetric air content [L\(^3\)L\(^{-3}\)], \( s \) [MM\(^{-1}\)], \( c \) [ML\(^{-3}\)], and \( g \) [ML\(^{-3}\)] are concentrations in the solid, liquid, and gaseous phases, respectively, \( D_{ij}^{\text{lw}} \) and \( D_{ij}^{\text{lg}} \) are components of the effective dispersion tensors in the liquid and gaseous phases [L\(^2\)T\(^{-1}\)], respectively, \( q_i \) is the volumetric flux density [LT\(^{-1}\)], and \( \phi \) is the rate of change of mass per unit volume by reactions or other sources (negative) or sinks (positive) such as plant solute uptake [ML\(^{-3}\)T\(^{-1}\)]. The PFAS module replaces in Eq. (2) the air phase storage term (the third term on the left side) with the storage term for the sorption to the air-water interface, \( A_i \Gamma \), where \( A_i \) is the air-water interfacial area ([L\(^2\)L\(^{-3}\)] or [L\(^{-1}\)]), and \( \Gamma \) is the interfacial adsorbed concentration (i.e., mass per unit area of the interface) [ML\(^{-2}\)].

Again, alternative formulations to Eq. (2) that partition the liquid phase into mobile and immobile (or less mobile) regions (i.e., dual-porosity or dual-permeability models) are also available in the standard HYDRUS code to account for physical nonequilibrium or preferential solute transport (e.g., Šimůnek et al., 2003; Šimůnek and van Genuchten, 2016). Alternative formulations are also used in the add-on modules, such as UnsatChem and C-Ride.

The HYDRUS models numerically solve the governing flow and transport equations, meaning that the transport domain and simulation time are
divided into small pieces called finite elements or finite differences. Triangles and quadrilaterals are typical spatial finite elements in two dimensions, and tetrahedral, triangular prisms, and hexahedrals in three dimensions (Šimůnek et al., 2022a,b).

### 2.2 Initial and boundary conditions

The flow and transport equations can be solved, providing that applicable initial and boundary conditions are specified. Initial conditions characterizing the system’s initial state can be specified either in terms of water contents or pressure heads for the flow equation and in terms of (liquid-phase or total) concentrations for the transport equation. When nonequilibrium (either physical or chemical nonequilibrium) solute transport models are used, the initial condition also needs to be specified for the nonequilibrium phase (i.e., concentrations in the mobile phase or at the kinetic sorption sites).

One of the main advantages of the HYDRUS codes is their flexibility in defining boundary conditions (BC), allowing simulations of various realistic irrigation scenarios. While the codes can accommodate standard system-independent boundary conditions, when conditions on boundaries are known beforehand, such as the Dirichlet (prescribed boundary pressure heads) and Neumann (prescribed boundary fluxes) boundary conditions, they can also accommodate a large number of system-dependent boundary conditions, when conditions on boundaries are not known apriori but are the results of interactions between external (e.g., meteorological) conditions and conditions in (feedback from) the subsurface system.

The soil–air interface, exposed to atmospheric conditions, is an example of a system-dependent boundary. While the potential flux across this interface is controlled exclusively by external conditions (e.g., precipitation, irrigation, evaporation), the actual flux also depends on the (transient) water content conditions in the soil. Soil surface boundary conditions may change from prescribed flux to prescribed head type conditions (and vice-versa). This occurs, for example, when the precipitation/irrigation rate exceeds the infiltration capacity of the soil, resulting in either surface runoff or accumulation of excess water on top of the soil surface, depending upon the soil conditions. Similarly, the potential evaporation rate calculated from meteorological conditions (the evaporative demand of the atmosphere) may exceed the capability of the soil to deliver enough water toward the soil surface. In this case, the potential evaporation rate can be significantly reduced to an actual evaporation rate controlled by the soil.
Other system-dependent boundary conditions, less commonly used with irrigation applications, include the seepage face BC, deep drainage BC, or flow to tile drains. Additionally, several boundary conditions implemented in HYDRUS have been specially developed for irrigation applications. These include, for example, subsurface drip characteristic function, surface drip with dynamic wetting, triggered irrigation, and a reservoir BC.

2.2.1 Subsurface drip characteristic function
The infiltration rate of water from a subsurface cavity (dripper) is affected by many factors, including the pressure in the cavity, its size and geometry, and the hydraulic properties of the surrounding soil (Lazarovitch et al., 2005). When a specified discharge of a subsurface source (e.g., a subsurface emitter) is larger than the soil infiltration capacity, the pressure head in the source outlet increases and becomes positive. The built-up pressure may significantly reduce the source discharge rate. HYDRUS implements a special system-dependent boundary condition for flow from a subsurface source that uses the drip characteristic function:

\[ Q = Q_0 \left( h_{in} - h_s \right)^c \]  

(3)

where \( h_s \) is the pressure head at the source-soil interface [L], often called the back pressure, \( Q_0 \) [L\(^3\)T\(^{-1}\)] ([L\(^2\)T\(^{-1}\)] in 2D) is the nominal discharge (Optimal Flux in the HYDRUS GUI) of the source for the reference inlet pressure \( h_{in} \) [L] (usually being 10 m) and the back pressure equal to zero, \( Q \) [L\(^3\)T\(^{-1}\)] ([L\(^2\)T\(^{-1}\)] in 2D) is the source discharge for the actual back pressure \( h_s \) [L], and \( c \) [-] is an empirical constant (Exponent in the HYDRUS GUI) that reflects the flow characteristics of the emitter. Normally, \( c = 0.5 \) corresponds to a turbulent flow emitter, and \( c = 1 \) to a laminar one. This equation states that when \( h_s \) increases, the pressure difference between the soil and the source inlet decreases, and the discharge rate correspondingly decreases (Lazarovitch et al., 2005).

2.2.2 Surface drip with dynamic wetting
The wetted area’s radius for drip irrigation gradually increases as irrigation time increases. The radius of this area for transient conditions can be calculated in HYDRUS as described by Gärdenäs et al. (2005). The irrigation flux \( Q \) is initially applied to a single boundary node representing the dripper with the Neumann (flux) boundary condition. When the pressure head required to accommodate the specified irrigation flux \( Q \) is larger than zero, the
boundary condition in this particular node is changed to the Dirichlet (head) boundary condition with a zero pressure head value, and the actual infiltration flux \( Q_a \) through this node is calculated. The excess flux \((Q - Q_a)\) is then applied to the neighboring node, again with the specified Neumann boundary condition. This procedure is iteratively repeated until the entire irrigation flux \( Q \) is accounted for, thus providing the radius of the wetted area. Since the infiltration flux into the dry soil is larger at the start of irrigation, the wetted area continuously increases as irrigation proceeds.

### 2.2.3 Triggered irrigation

Irrigation can be either defined externally (by specifying the irrigation rate and the initial and final irrigation times in the HYDRUS input) or triggered internally by the model, depending on the conditions in the soil (e.g., Dabach et al., 2013). Irrigation may be triggered in HYDRUS when a user-specified pressure head is reached in a selected observation node defined somewhere in the transport domain (likely in the root zone). The irrigation then starts after a user-specified lag period at a user-specified irrigation rate or pressure head at a user-specified boundary, and it lasts for a user-specified irrigation time duration. In 1D applications, triggered irrigation with a specified irrigation rate is applied at the soil surface, thus likely representing sprinkler irrigation. In 2D applications, irrigation can be triggered at the time-variable head, time-variable flux, or atmospheric boundaries, likely representing surface or subsurface drip irrigation or sprinkler irrigation.

### 2.2.4 Reservoir boundary condition

The reservoir boundary condition (Šimůnek et al., 2018) allows users to consider a reservoir that is external to the HYDRUS transport domain, while water can be added (injected) to or removed (pumped) from this reservoir. Flow into or out of the reservoir through its interface with the subsurface transport domain depends on the conditions in the transport domain (e.g., the position of the groundwater table) and external fluxes (pumping or injection):  

\[
\frac{dV_w}{dt} = Q_{in} - Q_p + (P - E)S \frac{dV_{w\epsilon}}{dt} = Q_{in}\epsilon_{in} - Q_p\epsilon_p + P\sigma \epsilon_r
\]

where \( V_w \) is the volume of water in the reservoir \([L^3]\), \( Q_{in} \) is the water flow rate into (or out of) the reservoir from the soil profile across the reservoir wall \([L^3T^{-1}]\), \( Q_p \) is the pumping/injection rate \([L^3T^{-1}]\), \( P \) and \( E \) are
precipitation and evaporation rates \([\text{LT}^{-1}]\), respectively, and \(S\) is the surface area of the reservoir \([\text{L}^2]\). In the latter equation, \(c\) is the solute concentration in the reservoir \([\text{ML}^{-3}]\), \(c_{in}\) is the solute concentration associated with the mass transfer between the soil profile and water reservoir \([\text{ML}^{-3}]\) \(c_{in}\) is equal to \(c\) when water infiltrates into the soil profile and equal to the solute concentration in the soil profile when water exfiltrates into the reservoir), \(c_p\) is the solute concentration associated with pumping or injection (equal to \(c\) for pumping or to the concentration of water being injected into the reservoir) \([\text{ML}^{-3}]\), and \(c_p\) is the solute concentration associated with precipitation.

Since mass balances of water and solute in the external reservoir are constantly being updated (based on all incoming and outgoing fluxes), the boundary conditions across the transport domain are dynamically adjusted depending on the water level in the reservoir. Reservoir boundary conditions potentially have many applications, such as dynamically estimating the water level in wells (e.g., Sasidharan et al., 2018, 2019), furrows during irrigation (e.g., Bristow et al., 2020; Šimůnek et al., 2016a), or wetlands.

2.3 Soil hydraulic properties

The numerical solution of the Richards Eq. (1) requires knowledge of the unsaturated soil hydraulic properties, i.e., the retention curve \(\theta(h)\) and the hydraulic conductivity function \(K(h)\), which are, in general, highly nonlinear functions of the pressure head. HYDRUS permits using five different analytical models for the hydraulic properties (Brooks and Corey, 1964; Durner, 1994; van Genuchten, 1980; Vogel and Číslarová, 1988; Kosugi, 1996).

The soil hydraulic parameters must be either specified by users, selected from a soil catalog listing them for 12 main textural classes, or estimated using pedotransfer functions. The van Genuchten and Brooks and Corey parameters in the soil catalog were taken from Carsel and Parrish (1988) and Rawls et al. (1982), respectively. HYDRUS users can also use pedotransfer functions (PTFs) based on neural networks (Schaap et al., 2001) to predict van Genuchten’s (1980) parameters based on textural information.

2.4 Solute transport and reaction parameters

The advection-dispersion Eq. (2), numerically solved by the HYDRUS software, is written in a relatively general form so that it can represent many
different solutes, such as tracers, nitrogen species, pesticides, heavy metals, radionuclides, and many other chemicals. Different solutes are characterized by different transport and reaction parameters, and particular values then represent a specific chemical in a given soil environment. When solute transport is selected in the HYDRUS software, all transport and reaction parameters are initially set for a tracer, such as a chloride or a bromide (i.e., no sorption and no reactions). It is up to HYDRUS users to enter the proper parameters (e.g., sorption parameters, degradation parameters, Henry’s law constant, etc.) for a particular solute. The methods for identifying these parameters are described in detail, e.g., by Skaggs et al. (2002).

2.5 Root water and nutrient uptake

The sink term, $S$, in Eq. (1) represents the volume of water removed per unit of time from a unit volume of soil due to plant water uptake. The macroscopic approach of Feddes et al. (1978) is used in HYDRUS to account for root water uptake. This approach first distributes potential transpiration across the root zone, depending on the spatial root distribution, to obtain potential root water uptake as a function of depth. Potential root water uptake is then reduced due to various stresses (e.g., saturation and salinity) present in the root zone to obtain actual root water uptake. Integration of actual root water uptake over the entire root zone then gives actual transpiration. Root water uptake can be either non-compensated or compensated, i.e., reduced uptake from a stressed part of the root zone is compensated by an increased uptake from a non-stressed part of the root zone (Šimůnek and Hopmans, 2009).

The root solute uptake model implemented in HYDRUS was developed by Šimůnek and Hopmans (2009). A similar macroscopic approach as the one described above for root water uptake is also used for root solute uptake. Root solute uptake is defined as the sum of passive and active root solute uptakes. Passive uptake is simulated by multiplying root water uptake by a dissolved nutrient concentration for concentration values below a priori-defined maximum uptake concentration ($c_{\text{max}}$). The solute dissolved in water is taken up by plant roots when $c_{\text{max}}$ is large (larger than the dissolved concentration $c$), while no solute is taken up when $c_{\text{max}}$ is equal to zero. Active solute uptake is activated when passive solute uptake is insufficient to satisfy the user-specified potential active nutrient uptake rate. Similar to root water uptake, active root solute uptake can be either non-compensated or compensated, with the latter having increased solute uptake.
uptake from parts of the root zone with higher solute concentrations compensating for insufficient uptake from parts of the root zone with low solute concentrations (Šimůnek and Hopmans, 2009).

The spatial extent of the root zone can be constant during the HYDRUS simulations, or various approaches can be used to describe the root growth as a function of time. One can use a logistic growth function or define an a priori the rooting depth at particular times. Options to simulate root growth directly using the HYDRUS software or its various couplings with crop growth or root growth models were reviewed by Šimůnek et al. (2018) and Hartmann et al. (2018).

3. Sprinkler irrigation

Sprinkler irrigation is one of the main methods of irrigation used around the world. In the US, it is the dominant irrigation type representing approximately 60% of all irrigation systems, with most of them being center pivots. Of all pressurized irrigation systems, sprinkler irrigation, in comparison to drip, costs less per unit of irrigated land (Amosson et al., 2021), particularly for large areas. There are several forms of sprinkler irrigation, but the two main ones involve water application as droplets of varying sizes or as thin streams of water emanating from the sprinkler nozzle. In practice, many sprinkler irrigation devices employ both techniques to varying degrees. The irrigation efficiency of sprinkle irrigation ranges between 60% and 90%, with an average of 75% (Gilley and Watts, 1977; Waller and Yitayew, 2016). To ensure efficient utilization of applied water, it is important that irrigation devices are properly installed and operated under design conditions and that there is a good understanding of soil properties/conditions and anticipated water flow within the profile. For the latter, the HYDRUS model (Šimůnek et al., 2008, 2016b) has been widely applied to simulate soil water dynamics under irrigation, using various methods (e.g., drip and surface/flood) and management scenarios. This section discusses the application of HYDRUS for sprinkler irrigation modeling.

3.1 Existing HYDRUS applications for sprinkler irrigation

Sprinklers are usually designed to apply uniform amounts of water across the entire soil surface or crop canopy. Except for variable rate irrigation systems, in well-implemented sprinkler irrigation systems, there is less concern about the occurrence of vastly uneven water application across a field.
compared to a system such as drip irrigation. The question of soil water redistribution under sprinkler irrigation has been examined by studies such as Martello et al. (2015) and Oker et al. (2021). Martello et al. (2015) used HYDRUS (2D/3D) to simulate the effect of canopy interception and stem flow in maize on soil moisture redistribution following sprinkler irrigation or rainfall. Even though sprinklers are designed to apply water uniformly across the whole surface, canopy interception distorts the default water application pattern, significantly affecting irrigation uniformity and efficiency across a field. Oker et al. (2021) used HYDRUS (2D/3D) to simulate soil water distribution under a Low Elevation Spray Application (LESA) sprinkling system and compared it to that of a Mobile Drip Irrigation (MDI) nozzle package installed on a center-pivot system.

HYDRUS has also been applied to model the interactions between soil salinity dynamics and its management using sprinkler irrigation (Phogat et al., 2018; Wang et al., 2017b; Yang et al., 2019). In many parts of the world, soil salinity is a growing problem (Hopmans et al., 2021). Yang et al. (2019) used HYDRUS-1D to assess the effectiveness of sprinkler irrigation in leaching salts from the root zone of an almond orchard and compared the results against those from drip irrigation. Their study showed that sprinkler irrigation is more efficient than drip for leaching salts from the root zone. Phogat et al. (2018) used HYDRUS-2D to model water and salinity dynamics in sprinkler-irrigated almonds exposed to varying salinity levels at different growth stages. In this study, less saline irrigation water was substituted for recycled irrigation water in three phenologically different almond growth stages to better understand soil water and salinity dynamics under almonds irrigated with waters of varying salinity levels. The study found that: (1) irrigation with saline water decreased seasonal almond evapotranspiration by 10% and increased salinity by 54%; (2) winter rainfall, or non-saline water substitution, was insufficient to reduce soil salinity below the 1.5 dS/m almond tolerance level and: (3) drainage beyond a 2-m root zone was irregular and varied significantly during the growth season.

Beyond soil water redistribution and salinity, HYDRUS has also been applied to study other physical phenomena and interactions in the vadose zone. Naghedifar et al. (2018) used HYDRUS-1D to assess groundwater return flow from a sprinkler irrigation system and compared it with flood irrigation. Their study found that return flow from the sprinkler irrigation system was negligible, whereas that from flood irrigation was 13.3%. Wang et al. (2015) coupled HYDRUS-1D with the EPIC crop model to assess
the irrigation management in sprinkler-irrigated wheat in China. Alves de Oliveira et al. (2019) used HYDRUS-2D to simulate the transport of atrazine in the soil profile under sprinkler irrigation.

3.2 An example of a HYDRUS-2D application to sprinkler irrigation

Center-pivot sprinkler irrigation is one of the most commonly used methods of pressurized irrigation for field crop production, and these systems are usually fitted with sprinkler or spray nozzle packages (hereafter, the term “sprinkler” is used to refer to both sprinkler and spray nozzles). In operation, a sprinkler mounted on a center pivot travels along a circular path across a field, as opposed to a stationary or fixed one. Therefore, each point of the soil surface along the sprinkler path is subjected to a varying water application rate as the center pivot advances towards and away from that point. In contrast, the application rate of fixed sprinkler devices is relatively constant. A unique variation of sprinkler technology also used in center-pivot systems, the LEPA bubbler (Low Energy Precision Application) (hereafter, bubbler), is designed to concentrate water application on the soil surface area directly underneath the nozzle.

A case study of applying HYDRUS (2D/3D) to model soil water redistribution following irrigation using a sprinkler and bubbler, both mounted on a center pivot, is presented below (the Sprinkler and Bubbler examples in Table A). The key assumptions are: (1) both the sprinkler and the bubbler are mounted 80 m from the pivot point, and nozzle spacing is 1.5 m; (2) sprinkler and bubbler-wetted diameters are equal to 3 and 0.762 m, respectively; and (3) irrigation application depth is 2.54 cm, and pivot travel time is 44 h per revolution.

For both devices, soil water redistribution up to a depth of 1.8 m is simulated. The representative application rate of the sprinkler is shown in Fig. 1. Two soil types were considered: loamy sand and silt loam. Their soil hydraulic properties were taken from the HYDRUS database (Carsel and Parrish, 1988). The initial conditions (Fig. 2A) represent an unsaturated soil profile, similar to usual field conditions before an irrigation event. The sprinkler irrigation is implemented in HYDRUS-2D as an “atmospheric” boundary condition at the top of the model domain (soil surface). The sprinkler application rate, shown in Fig. 1A, is implemented using HYDRUS-2D’s “Time Variable” boundary conditions. For simplicity, the graph is discretized into 25-time steps, and corresponding application rates are computed. Because of approximation errors introduced by the temporal
discretization, the estimated irrigation depth is 3.08 cm. The bubbler is also implemented as an atmospheric boundary condition over two lengths of 38.1 cm each, on the right and left sides of the top of the model domain. Fig. 1B shows the application rate of the bubbler. A “free drainage” boundary condition is implemented at the bottom of the model domain (depth of 183 cm), and a “no flux” boundary condition is used one the right and left sides. Soil water redistribution is simulated for a period of 24 h (Fig. 3). Fig. 2 shows the initial and final water contents in loamy sand and silt loam soils in the HYDRUS-2D simulation of soil water redistribution following sprinkler irrigation.

![Graph](image1.png)

**Fig. 1** Application rates of a sprinkler (A) and LEPA bubbler (B), both located 80 m from the center of a pivot and applying an irrigation depth of 2.54 cm, with corresponding infiltration rates for loamy sand and silt loam soils.

![Graph](image2.png)

**Fig. 2** (A) Initial and (B) final ($t = 24$ h) water contents in loamy sand and silt loam soils in the HYDRUS-2D simulation of soil water redistribution following sprinkler irrigation.
and silt loam in the middle of the domain, while Fig. 3 shows the final water contents in loamy sand and silt loam at different locations of the transport domain. Infiltration rates for the loamy sand and silt loam soils are plotted against the sprinkler and bubbler application rates (Fig. 1). As shown in Fig. 1A, the infiltration rate of the loamy sand matches the sprinkler application rate at every time step, resulting in no surface runoff. For the bubbler, however, the infiltration rate of the loamy sand matches the application rate up to $t=0.01\,\text{h}$, after which runoff is generated. For the silt loam, the infiltration rates increase in tandem with the sprinkler and bubbler application rates till $t=0.07$ and $0.01\,\text{h}$, respectively, after which they begin to decrease. Subsequently, the difference between the application and infiltration rate is equivalent to potential runoff. In general, potential runoff occurs much more quickly for the bubbler because it has a significantly higher water application rate than the sprinkler (Fig. 1B). Figures Fig. 4A and B show cumulative infiltration and potential runoff for the loamy sand and silt loam soils following irrigation. As expected, the simulation results show that silt loam has the highest potential runoff of 1.85 and 2.08 cm for sprinklers and bubblers, corresponding to losses of 60.1% and 81.9%, respectively. The potential runoff for the LEPA application on loamy sand is 1.4 cm (55.1%).
In a well-drained and managed field, the potential surface runoff would manifest as ponded water, eventually infiltrating into the soil. The two-dimensional module of HYDRUS does not facilitate the accumulation of ponded water on the soil surface. Instead, computed surface runoff is instantaneously removed. However, an option to accumulate ponded water on the soil surface is available in HYDRUS-1D. If runoff is assumed to be negligible, implying that all applied water should infiltrate into the soil profile, then both sprinkler and bubbler irrigation can be implemented in HYDRUS-2D as a “time-variable flux” that is lower than the saturated hydraulic conductivity of the soil. A representative application time should then be computed to ensure that only the desired irrigation depth is introduced into the model domain. This implies that the actual application of the sprinkler, or bubbler, is not considered but rather translated to a “time-variable flux.”

4. Furrow irrigation

Despite being replaced by pressurized irrigation in developed countries, surface irrigation systems, such as furrows and basins, remain widespread among farmers in developing regions (FAO, 2011). Water (and sometimes also solutes) is conveyed by gravity flow to sections of a field that is either leveled (border-dyke irrigation) or prepared with parallel ridges and
furrows (furrow irrigation). In the process, water moves over dry soil, generating a front that transports water and nutrients along the field and simultaneously into the soil via infiltration. When correctly designed, these systems can simultaneously minimize deep drainage and leaching below the crop root zone, maximize water and nutrient distribution to the ridges (where the plants are growing), and uniformly irrigate the field, thus leading to optimal crop yields (Fahong et al., 2004; Horst et al., 2005; Šimůnek et al., 2016a; Siyal et al., 2012). Yet, the interacting surface and subsurface transport processes involved make their design and implementation a challenging and complex task.

Ubiquitously, this problem is tackled by using models that can predict and/or explain the system’s behavior under different operating conditions at different levels of complexity. Setting aside data-driven models (Mattar et al., 2015), numerical models provide a theoretical and transferrable framework to explain and predict physical processes involved in surface irrigation, which can be used to design and optimize these systems. Several models have been developed in the literature to simulate the coupled surface-subsurface transport. Earlier attempts used zero-inertia and kinematic wave approximations of the shallow water equation coupled with a modified Kostiakov function to simulate infiltration (Katopodes and Strelkoff, 1977; Oweis and Walker, 1990; Strelkoff and Katopodes, 1977; Walker and Humpherys, 1983). Later, the advection-dispersion equation was added to simulate solute transport (Abbasi et al., 2003b; Perea et al., 2010). Despite their good predictive performance, these models generally oversimplify subsurface transport processes.

To overcome this limitation, analytical or numerical zero-inertia formulations were coupled with the Richards equation to mechanistically describe transport processes in the subsurface (Ebrahimian et al., 2013; Tabuada et al., 1995; Wöhling et al., 2004; Wöhling and Schmitz, 2007; Zerihun et al., 2005; Köhne et al., 2011). Of particular relevance are the pseudo-3D models developed by Tabuada et al. (1995) and Wöhling et al. (2004), which provide a 1D and 2D description of surface and subsurface water flow along the channel, respectively. This approach has an important utility as it allows assessing the irrigation uniformity in different 2D cross-sections along the furrow. Nevertheless, while accurately simulating water flow, neither of the above models considered solute transport in surface and subsurface domains. Furthermore, their use of a Lagrangian approach poses significant numerical challenges (Wöhling et al., 2006).
4.1 Existing HYDRUS applications to furrow irrigation

While the HYDRUS model (Šimůnek et al., 2016b) has been quite widely used to simulate water flow and solute transport under furrow irrigation systems, it has typically been used only to simulate processes in the two-dimensional transport domain perpendicular to furrow without considering the flow and transport dynamics in the furrow itself (Bristow et al., 2020; Šimůnek et al., 2016a; Siyal et al., 2012; see also many more references listed in (Šimůnek et al., 2016b) and on the HYDRUS website).

Recently, Brunetti et al. (2018b) developed a hybrid Finite Element-Finite Volume pseudo-3D model to simulate the coupled surface-subsurface water flow and solute transport in blocked and open-ended furrows. The model combines the two-dimensional Richards-based Finite-Element solver, HYDRUS-2D, with a one-dimensional Finite-Volume discretization of the zero-inertia and advection equations. The model has been successfully validated in synthetic and experimental scenarios. Its main advantages are its computational efficiency, mass conservation performance, and the detailed description of water flow, solute transport, and root water and solute uptake along the entire furrow channel. To increase its usability and widespread use among scientists and practitioners, the model has been equipped with a GUI and embodied an add-on module in the newly released HYDRUS 5 software suite (https://www.pc-progress.com/en/Default.aspx?h3d2-Furrow). Details about the model and the GUI can be found in Brunetti et al. (2018b) and Brunetti et al. (2019c).

4.2 An example of the HYDRUS furrow module in multiple modeling scenarios

Selected modeling scenarios are used to demonstrate the potential applicability of the HYDRUS Furrow module for fertigation designing purposes. As pointed out by Siyal et al. (2012), there is a need to improve water, fertilizer, and soil surface management strategies to increase irrigation efficiency and reduce nitrogen losses due to leaching into groundwater. Most of the existing research has focused on fertilizer placement (Mailhol et al., 2007; Siyal et al., 2012; Waddell and Weil, 2006) and irrigation management (Abbasi et al., 2003b; Mailhol et al., 2007), while only a few studies have investigated the effect of soil surface management to reduce leaching and maximize fertigation efficiency (Bristow et al., 2020; Šimůnek et al., 2016a; Siyal et al., 2012). In particular, Šimůnek et al. (2016a) used HYDRUS-2D to examine the effect of compacting the
bottom of the furrow or placing a plastic sheet on the bottom of the furrow on the fertigation uniformity and efficiency. While results reported in these studies were promising, numerical simulations neglected the complex interacting surface–subsurface processes that occur during the water advance–storage–recession phases that are typical for furrow fertigation. The analysis was limited to two-dimensional vertical infiltration, which neglects the differences of the longitudinal distribution of water and solute in the field hat result from furrow fertigation. A similar approach was used, and similar limitations were encountered in the recent work of Pahlevani et al. (2021).

Therefore, in the present study, the HYDRUS Furrow module is used to simulate the influence of different soil management strategies on the fertigation of a 100 m-long blocked-end furrow (Table A). A non-reactive solute is considered in the analysis. The geometric characteristics of the furrow and input data are reported in Table 1. In particular, the effect of the plastic sheet ($S_p$) and soil compaction ($S_c$) is analyzed (Fig. 5) against a baseline scenario ($S_0$). The soil hydraulic parameters of loamy sand soil considered in this simulation are taken from the HYDRUS soil catalog (Carsel and Parrish, 1988) and reported in Table 1. For the $S_c$ scenarios, the saturated hydraulic conductivity of the top 2 cm of the soil is decreased to 1/10th of the original uncompacted value. Soil compaction in the field can be achieved by tractor wheels or with the Eversman v-shaped wheel (Siyal et al., 2012).

The subsurface vertical domain is discretized into 2049 triangular elements and 1078 nodes. The distribution of boundary conditions for different soil management scenarios is shown in Figure. The groundwater table is assumed far below the domain of interest, and thus a “Free Drainage” BC is assigned to the bottom nodes, while an “Atmospheric” boundary condition is set for the furrow ridge. Due to symmetry, the nodes representing the left and right boundaries of the subsurface domain are set as “no-flow” boundaries because no water flow or solute transport occurred across these boundaries. A hybrid Dirichlet/Neumann (variable pressure/zero flux) BC is assigned to the border of the trapezoidal channel to simulate variations of the water depth in the furrow. Finally, a “Third Type” Cauchy BC was set on top and bottom of the numerical domain to simulate the concentration flux along the boundaries. Plastic placement on the bottom of the furrow ($S_p$) is simulated by setting a no-flow boundary condition at the bottom of the furrow, so that infiltration can occur only through the sides of the furrow.
Figs. 6 and 7 show the simulated distributions of soil water contents and nitrate concentration, respectively, at time $t = 5400$ s at different locations along the furrow for the baseline ($S_0$), compacted ($S_c$), and plastic ($S_p$) scenarios. Simulation results show that the distribution of water contents and solute along the furrow in the baseline scenario is not perfectly homogeneous. Water and solute mostly accumulate in the first part of the furrow, where they percolate toward deeper soil horizons, while their penetration into the furrow ridge decreases along the furrow. This leads to an

<table>
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<tr>
<th>Table 1 Geometric characteristics, soil hydraulic properties, and other input parameters used in theoretical validation.</th>
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<td><strong>Bottom-end boundary condition</strong></td>
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<tr>
<td>Furrow length, $L$ (m)</td>
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<tr>
<td>Bottom width, $b_w$ (cm)</td>
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<tr>
<td>Side slope, $SS$ (—)</td>
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<td>Maximum depth, $h_{\text{max}}$ (cm)</td>
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<td>Bed slope, $S_0$ (—)</td>
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<td>Manning’s coefficient, $m$ (s/m$^{1/3}$)</td>
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<tr>
<td>Residual water content, $\theta_r$ (m$^3$/m$^3$)</td>
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<tr>
<td>Saturated water content, $\theta_s$ (m$^3$/m$^3$)</td>
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<td>Retention function shape parameter, $\alpha$ (1/cm)</td>
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<td>Retention function shape parameter, $n$ (—)</td>
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<td>Saturated hydraulic conductivity, $K_s$ (cm/s)</td>
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<td>Tortuosity, $l$ (—)</td>
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<tr>
<td>Initial water content, $\theta_0$ (m$^3$/m$^3$)</td>
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<tr>
<td>Inflow rate, $Q_{ir}$ (l/s)</td>
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<tr>
<td>Solute injection rate, $Q_{inj}$ (l/s)</td>
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<td>Inflow concentration, $C_{inj}$ (g/l)</td>
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<td>Longitudinal dispersivity (cm), $D_L$</td>
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<td>Transverse dispersivity (cm), $D_T$</td>
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<td>Irrigation cutoff time, $t_w$ (min)</td>
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<td>Solute cutoff time, $t_s$ (min)</td>
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</table>
Fig. 5 A schematic of the boundary conditions for different soil surface management scenarios.

Fig. 6 Simulated distributions of soil water contents at time $t = 5400$ s at different locations along the furrow (horizontal direction) for the original ($S_0$), compacted ($S_c$), and plastic ($S_p$) scenarios.
inhomogeneous fertigation scheme with the upper part of the furrow receiving more water and solute and thus expected to have higher crop yields (or larger nutrient losses by leaching) than the lower part of the furrow, more exposed to potential root water and nutrient stresses. The situation radically changes when the soil at the bottom of the furrow is compacted. The reduction of the soil hydraulic conductivity diminishes infiltration and increases velocities of the waterfront traveling in the furrow, thus leading to a more homogeneous distribution of the irrigation water along the field (and thus, potentially, to more uniform crop yield). Furthermore, the lower soil hydraulic conductivity of the bottom of the furrow increases the water level in the channel and favors the infiltration into the ridge.

Interestingly, Fig. 6 shows that, at the end of the recession phase, the final part of the furrow is slightly moister in the compacted ($S_c$) scenarios. This is mainly due to the alteration of the infiltration patterns between the sides and the bottom of the furrow for this management strategy. Nevertheless, solute remains well distributed (Fig. 7). The placement of a plastic sheet at the bottom of the furrow overcomes this problem and presents the greatest

![Fig. 7 Simulated distributions of solute concentration at time $t = 5400$ s at different locations along the furrow (horizontal direction) for the original ($S_0$), compacted ($S_c$), and plastic ($S_p$) scenarios.](image)
benefits. The irrigation and fertigation homogeneity increases, similarly as water and solute infiltration into the furrow ridge. The amount of water and fertilizer that leaches under the furrow bottom is lower compared to other analyzed scenarios.

The analysis shows how the HYDRUS Furrow module can be used to design efficient fertigation strategies by providing a comprehensive and realistic description of overland and subsurface transport processes.

5. Drip irrigation

5.1 Existing HYDRUS applications to drip irrigation

Drip irrigation is the most common method for high-value crops but is also very common for irrigating staple food crops in water-limited environments. This method has many advantages, including optimal control over the amount of irrigation water and the concentration of fertilizers given to the plant, so farmers have widely adopted the method. Previous studies have found that the same amount of water given at different timings can yield different crop yields (Or and Hanks, 1993). According to Rawlins and Raats (1975), the high water content in the root zone causes high soil water pressure head and hydraulic conductivity and, therefore, an increase in water availability to the plant. Stansell and Smittle (1989) argued that high water content in the root zone has a direct effect on the rate of transpiration and stomatal conductance, and therefore frequent irrigation will increase the efficiency of water use, photosynthesis, and yield.

Effective design and management of drip irrigation systems lead to the effective delivery of water and nutrients to the root zone resulting in higher water use efficiency and improved yields. Many design and management decisions involve understanding the wetted zone pattern around the emitter (Bresler, 1978; Lubana and Narda, 2001) and its relation to the root system structure and function. Water distribution in the soil is affected by many factors, including soil hydraulic characteristics, initial conditions, emitter discharge rate, application frequency, root characteristics, evaporation, and transpiration. HYDRUS (2D/3D) (Šimůnek et al., 2016b) has been previously used to successfully simulate water flow for surface and subsurface drip irrigation systems (e.g., Skaggs et al., 2004; Gårdenäs et al., 2005, Kandelous and Šimůnek, 2010; Honari et al., 2017; Domínguez-Niño et al., 2020a,b; see many more references listed on the HYDRUS website: https://www.pc-progress.com/Documents/Jirka/Drip_irrigation_papers.pdf).
In both surface and subsurface drip applications, irrigation is often modeled using a constant water flux across a boundary with fixed dimensions. However, the soil’s infiltration capacity depends on the initial conditions and the soil hydraulic properties. When the prescribed boundary flux is larger than the soil’s infiltration capacity, the model will force the water to infiltrate into the soil at a rate higher than this capacity, which will cause the pressure head at the boundary to rise to unphysical values, with consequences on the flow and soil water patterns. To overcome such problems with unphysical boundary pressure heads, various system-dependent boundary conditions (e.g., dynamic surface wetting for surface drip irrigation or drip characteristic function for subsurface drip irrigation) were implemented in the HYDRUS code (see Section 2) to facilitate proper physical characterization of the flow field around the surface and subsurface drippers.

Another system-dependent boundary condition is used to trigger irrigation when certain predetermined conditions in the system are reached (Dabach et al., 2013; Müller et al., 2016). This condition initiates irrigation whenever the matric head at a predetermined observation point drops below a certain pressure head threshold.

5.2 Surface drip irrigation

First, simulations of surface drip irrigation can be made using the boundary condition accounting for dynamic surface wetting (Gärdenäs et al., 2005). This condition allows the spatial distribution of the discharge rate at the soil surface to change with time. A ponded zone around this point is created when water is applied at a constant rate to a point on the soil surface. The ponded area increases with time at the beginning of irrigation, but later approaches a constant circular area (Shani et al., 1987). Fig. 8 demonstrates dynamic wetting of the soil surface for surface drip irrigation of two soils of different textures (soil hydraulic parameters for loam and sandy loam were taken from the HYDRUS soil catalog). In this example (the SurfaceDrip examples in Table A), 4L were applied at the dripper discharge rate of 2L/H using the system-dependent boundary condition accounting for dynamic surface wetting. Fig. 8 shows different responses in the two soils. While in the soil with higher saturated hydraulic conductivity (i.e., sandy loam), the radius reached a steady state in a relatively short time, in the heavier soil (i.e., loam), this process took much longer, showing the need for this system-dependent boundary condition.
In recent years, low flow rate emitters with flow rates of 0.4–0.6 L/H have been developed, even with pressure regulation. The effect of the discharge rates on soil water flow and root water uptake by plants was studied by Assouline (2002) using HYDRUS-2D. The simulated results showed that lowering the emitter flow rate from 2 L/H to 0.25 L/H increased the soil water content in the upper layer of the root zone and root water uptake, diminishing the reduction of potential transpiration. However, these results were greatly affected by the description of the root system, which was considered uniform between irrigations. Another study found that when irrigating the soil with the same amount of water at different flow rates, no differences were found in the water content distribution after the redistribution process (Skaggs et al., 2010). It should be noted that this study was done without plants that can change the soil wetting pattern because of the interaction between soil moisture, emitter flow rate, and root system structure and function.

Further attempts to describe water flow in the soil at low flow rates using HYDRUS (2D/3D) were made by Lazarovitch et al. (2009). These numerical experiments were performed without the presence of plants, and the conclusions are thus suitable only for the first stages of plant growth, in which root water uptake is minimal. The following examples illustrate how the root structure and response to water stress influences the plant’s ability to uptake water while surface-drip-irrigated with a continuous low flow rate (the DripPlant examples in Table A). The simulation duration was 1 week, and the discharge rate was 0.4 L/H (()). The critical stress index \( \omega_c \), which accounts for root water uptake compensation in the root water
uptake model, was set either equal to 1, i.e., no compensation, or to values smaller than 1, accounting for root water uptake compensation (i.e., reduced uptake from one part of the domain is compensated by increased uptake from other parts). The maximum rooting depth, $Z_m$, was set to 20 or 30 cm. Fig. 9 shows ratios between actual transpiration, calculated by the model, and potential transpiration for different values of the critical stress index and two maximum rooting depths. It can be seen that the issue of compensation in root water uptake is very important and has implications for a reliable description of deficit-irrigated systems, particularly for shallow root systems. There are currently insufficient data to better understand the compensation in root water uptake, and more studies are needed in that direction.

5.3 Subsurface drip irrigation

Second, simulations of subsurface drip irrigation can be made with a system-dependent boundary condition that describes the effect of back pressure on the dripper discharge rate while considering the source characteristics, inlet pressure, and the effects of the soil hydraulic properties (Lazarovitch et al., 2005; Naglic et al., 2014). When a predetermined discharge of a subsurface emitter is larger than the soil infiltration capacity, the pressure head in the source outlet increases and becomes positive. The built-up pressure head may significantly reduce the source discharge rate.

One of the challenges in developing these models is the ability to accurately describe the uptake of water and nutrients by roots under different growing conditions. The HYDRUS (2D/3D) model can simulate water flow and the transport of nutrients when the space is two- or
three-dimensional, as in drip irrigation, or one-dimensional, as in sprinkler irrigation. This model reduces potential root water uptake due to saturation (i.e., dryness) and salinity stresses (van Genuchten, 1987) and allows for passive and active nutrient uptake (Šimůnek and Hopmans, 2009). The root absorption functions have a number of parameters without which reliable simulations cannot be performed. These parameters cannot be evaluated directly due to the inability to maintain constant water content or nutrient concentrations in the root zone during the experiment.

5.4 Inverse problem

Another option for evaluating the parameters is to solve the inverse flow and transport problem that includes the uptake of water and nutrients by roots (Vrugt et al., 2001a,b; Hupet et al., 2002, 2003). In this approach, the plant traits are estimated by assuming a deterministic model and calculating the parameters of the selected model. The assumption, in this case, is that the characteristics of the plant can be described using a deterministic model that contains a relatively small number of parameters typical of each plant. Estimation of plant properties is obtained by optimizing the deviations between results calculated by numerically solving the flow and transport equations and measured flow variables, such as pressure heads, water contents, fluxes, or nutrient concentrations, at relevant times and space locations.

A calibrated numerical model can then be used to optimize system variables, leading to an optimal irrigation and fertilization regime that will maximize profit for the farmer and preserve the environment. Questions regarding the optimal emitter flow rate or spacing between the emitters can be answered with the help of the numerical model.

5.5 Geometrical description

In the inverse problem method, the model has to be executed several times, and for the high accuracy of the results, fine spatial and temporal discretization is required. For drip irrigation problems, it is almost impossible to run the optimization problems on a regular computer. In this situation, there is a constant attempt to find symmetry lines in the system to reduce the computational load and streamline the process. One symmetry line exists in the center of a subsurface emitter if the soil and the root zone look similar on both sides of the emitter. Another line of symmetry can be found at half the distance between emitters. A line of symmetry is equivalent to a no-flow
boundary since water contents and pressure heads are the same on both sides of the hypothetical line of symmetry, resulting in zero pressure head gradients perpendicular to this boundary. Kandelous et al. (2011) simulated subsurface drip irrigation as a two-dimensional (i.e., infinite line source), axisymmetric two-dimensional (i.e., a point source), and three-dimensional (i.e., a full description of the drip line geometry) problem, and discussed when and under what conditions each of these approaches should be used.

Fig. 10 shows the simulated results for two alternative ways of describing water flow around a subsurface emitter. Water flow is simulated in a fully three-dimensional domain (Fig. 10A) or a two-dimensional domain exhibiting radial symmetry around the vertical axis (Fig. 10B). Fig. 10C shows the soil water contents at three locations 5, 15, and 25 cm away (radially) from the dripper. These simulations (the Drip3D examples in Table A)

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**Fig. 10** The spatial distribution of water contents in a three-dimensional domain (A), an axisymmetric domain (B), and at three observation points (5, 15, and 25 cm away from the dripper) as a function of time (C).
depict two cycles of subsurface drip irrigation and redistribution. Initially, there is irrigation for an entire day, and then there is a cessation of irrigation for 4 days. It is clear that the water content response with time is almost identical in both domains, and the line of symmetry between emitters can be used. The simulation duration (the CPU time) for a three-dimensional domain was 679s, and for an axisymmetric domain, 11.8s. This significant time reduction (orders of magnitude) allows for faster evaluation of complex problems involving entire growing seasons and the use of the inverse problem to estimate parameters.

6. Fertigation

The HYDRUS software has been used over the years in many studies evaluating the fate and transport of various chemicals used in irrigated agriculture, including nitrogen species. Due to its flexible boundary conditions and well-designed graphical user interface, the HYDRUS model has been widely used to capture soil nitrogen dynamics, especially for different irrigation and fertilization strategies (Chen et al., 2020b,c; Mekala and Nambi, 2017; Mekala et al., 2017; Phogat et al., 2013). It has been used, for example, to quantify processes such as N leaching, transformation (e.g., mineralization, nitrification, denitrification, volatilization, and assimilation), and root uptake under different management conditions (e.g., mulching, tillage), different irrigation scenarios (e.g., furrow or drip irrigation, different irrigation rates), and different planting systems (e.g., monoculture or intercropping systems). This section reviews these HYDRUS applications.

6.1 Soil nitrogen transformation

Nitrogen, one of the most abundant elements in the atmosphere, plays a critical role in plant photosynthesis and primary production in natural terrestrial ecosystems (Makino, 2010; Sorrell et al., 2013). In general, biogeochemical transformations of nitrogen in the soil-plant-atmosphere continuum mainly include internal and external cycles. The external cycle refers to nitrogen transport among different ecosystems. The internal cycle refers to nitrogen transformations among different pools in the same ecosystem. These transformations can include mineralization (i.e., nitrogen fixation), assimilation, nitrification, denitrification, and volatilization (Fig. 11). High crop yield and sustainable agricultural ecosystems can be achieved only when the internal nitrogen cycle is well understood (Subbarao et al., 2012).
The HYDRUS model has been widely used to simulate nitrogen transformations under different environmental conditions, such as different soil textures, different irrigation methods, or different mulching scenarios (Azad et al., 2020; Salehi et al., 2017; Pahlevani et al., 2021; Castaldelli et al., 2018). Apparent differences in nitrogen transformations can be found in different scenarios and conditions. For example, the nitrification rate in sandy soils is faster than in clay and sandy loam soils, while nitrogen assimilation in clays is significantly higher than in the other two soils. Mekala and Nambi (2017), Mekala et al. (2017) evaluated the impact of different soil textures on nitrogen transformations using the HYDRUS model. They found that nitrification in sandy soil is significantly higher than in sandy loam soil. On the other hand, denitrification can become a dominant nitrogen transformation process in sandy loam soils, especially at saturations higher than 96%. Berlin et al. (2015) illustrated that nitrification in soils with high clay content was lower than in soils with low clay content and that the nitrogen peak
displayed hysteresis. The reason may be attributed to the difference in soil organic matter of different soil textures. Usually, the assimilation rate (i.e., the transformation from inorganic nitrogen to organic nitrogen) increases in response to an increase in soil organic matter, which results in a reduction in the soil NH$_4$-N concentration and a corresponding nitrification rate.

Nitrification is an important process of releasing energy in the nitrogen cycle, and it includes autotrophic nitrification and heterotrophic nitrification (Langergraber and Šimůnek, 2005). Autotrophic nitrification refers to the process of oxidizing soil NH$_4$-N to NO$_3$-N by autotrophic microorganisms. Heterotrophic nitrification refers to transforming nitrogen into oxidized nitrogen using organic carbon as a carbon source under the mediation of heterotrophic microorganisms. There are also apparent differences in nitrification among differently irrigated fields, especially between dry and flooded fields (Eltarabily et al., 2019; Halvorson et al., 2016; Mo’allim et al., 2018). In general, denitrification is the primary transformation process in flooded fields (Becker et al., 2007), in which high saturation in the surface soil layer results in an anaerobic soil environment. Meanwhile, anaerobic bacteria use NO$_3$-N as the final electron acceptor for respiration in an anaerobic soil environment to reduce NO$_3$-N to N$_2$O and N$_2$. Volatilization of nitrogen gases (N$_2$O and N$_2$) produced by denitrification is the main cause of low nitrogen use efficiency in agricultural production. However, nitrification is still stronger than denitrification in flooded fields with good drainage. For example, Li et al. (2018a) evaluated nitrogen transformation mechanisms in different soil layers of paddy farmland using the HYDRUS model and found that nitrification was about 25% higher than denitrification. Similarly, nitrification is the main transformation process in dry farming fields due to their high soil pore oxygen content. For example, Chen et al. (2020b) found using the HYDRUS model that average nitrification in a drip-irrigated corn field reached 31.2 kg ha$^{-1}$. Also, the nitrification rate gradually increased with a decrease in the irrigation depth (Zeng et al., 2017). In general, soil nitrification and denitrification are mainly affected by soil’s physical and chemical properties, e.g., soil temperature, soil moisture, and soil pH (Mekala and Nambi, 2017; Mekala et al., 2017; Herman et al., 2007; Scherger et al., 2021).

Nitrogen transformations also show apparent differences under different mulching treatments due to differences in mulching ratios. Compared with no mulching, plastic film mulching can increase soil temperature, promote the activity of soil microorganisms, accelerate the nitrogen denitrification
rate, and increase N$_2$O emissions (Lee et al., 2022). Furthermore, the nitrification rate increases in response to a decrease in the mulching ratio (Chen et al., 2020b).

The HYDRUS model is also often used to evaluate the mechanism of nitrogen transformation in fields with different tillage technologies (Colombani et al., 2020; Shafeeq et al., 2020; Miranda-Velez et al., 2022). According to simulation results, N$_2$O emissions in the no-till field were significantly limited compared with the conventional tillage field (Yoo et al., 2016; Tellez-Rio et al., 2015; Chatskikh et al., 2008). This phenomenon is mainly related to different soil structures under different tillage technologies. Conventional tillage technology can decrease soil porosity while significantly increasing oxygen content in soil pores. Thus, the nitrification rate can be promoted in conventional tillage fields. Compared with a conventional tillage field, the surface soil bulk density increased due to soil compaction in the no-tillage field, resulting in a reduction in N$_2$O emissions.

Mineralization can also be accurately quantified using the HYDRUS model. For example, Shekhar et al. (2021) compared mineralization rates under different soil moisture conditions and found that mineralization under moderate and severe water stress treatments decreased by 44.9% and 36.5% compared to a no-stress treatment, respectively. Organic macromolecular compounds (such as proteins, amino sugars, and nucleic acids) are decomposed into biomonomers via hydrolysis of microbial enzymes, and the biomonomers are then further ammoniated to ammonium nitrogen. Therefore, soil microbial activity is an important factor affecting nitrogen mineralization. In the study of Shekhar et al. (2021), the transformation of soil organic nitrogen to inorganic nitrogen was inhibited due to low soil microbial activity under water stress conditions.

### 6.2 Soil nitrogen movement

It is crucial to accurately capture the nitrogen transport to formulate reasonable fertilization application strategies, improve nitrogen use efficiency, avoid non-point source pollution, and promote sustainable agricultural development (e.g., Mekala and Nambi, 2017). Iqbal et al. (2016) compared the distribution characteristics of soil nitrogen in differently sized furrow-irrigated fields and found that soil nitrogen accumulation significantly increased in the field with a 2:1 ridge-ditch ratio compared to the
1:1 ridge-ditch ratio. Azad et al. (2018) evaluated differences in soil nitrogen dynamics under different irrigation rates and illustrated that the leaching amount of soil NO$_3$-N could be effectively decreased during the fertilization application period when the irrigation rate is 0.8 L h$^{-1}$. Tao et al. (2021) studied the effect of an improved underground drainage system on soil NH$_4$-N and soil NO$_3$-N dynamics using HYDRUS. They reported that the largest decrease in soil nitrogen mass consistently occurred in the filter profile, and soil NH$_4$-N in the 0–20 cm soil layer and soil NO$_3$-N in the 60–80 cm soil layer increased with the prolongation of irrigation duration. Karandish and Šimůnek (2017) evaluated the effects of 176 different water and nitrogen management strategies on soil water and nitrogen dynamics and showed that the 200 kg ha$^{-1}$ N-fertilizer application is the optimal amount, which can reduce nitrogen leaching by 12–99%.

The HYDRUS model has also been commonly used to evaluate soil nitrogen transport under different planting systems. For instance, Chen et al. (2020c) revealed the distribution characteristics of soil nitrogen in the corn-tomato intercropping field and found that soil NO$_3$-N concentrations in the tomato’s root zone were significantly higher than in the corn’s root zone. Moreover, the soil solute flux in the horizontal direction occurred mainly from the tomato’s root zone to the corn’s root zone. Doltra and Muñoz (2010) studied the soil NO$_3$-N distribution in the sweet pepper-cauliflower-Swiss chard rotation field and illustrated that the surface soil NO$_3$-N concentration first increased and then decreased with the crop growth.

Since the HYDRUS model has flexible upper boundary conditions to represent different mulching scenarios, the model can accurately capture the soil nitrogen dynamics under different mulching scenarios. Chen et al. (2020b) compared differences in the soil nitrogen distribution under biodegradable film mulching (BM), polyethylene film mulching (PM), and non-mulching (NM) scenarios. They showed no significant differences in soil NO$_3$-N concentrations under BM and PM in the early crop growth stage. However, soil NO$_3$-N concentrations under BM were higher than under PM 80 days after sowing due to an increase in the disintegrated area of the biodegradable film. Overall, the HYDRUS model can capture the soil nitrogen dynamics in different crop growth stages at the field scale and accurately quantify the nitrogen distribution characteristics for a long time series in large-scale regions (Nasta et al., 2021).
6.3 Soil fertilizer leaching

Fertilizers have been applied in large quantities as one of the effective ways to increase crop yields. However, irrational fertilizer applications cause waste and lead to non-point source pollution of agricultural soils (Guo et al., 2010). Nitrogen leaching can significantly damage surrounding environments, including surface and groundwater bodies, affecting ecological security (Bouraoui and Grizzetti, 2011). Recently, many researchers have used the HYDRUS model to carry out high-precision simulations of N transport and transformations under different soil textures and agronomic measures (Pare et al., 2006; Zhou et al., 2006), providing effective guidance and helping to optimize fertilization schemes and enhance the N use efficiency of crops under different conditions to ensure food-ecological security (Azad et al., 2018; Guo et al., 2013; Siyal et al., 2012).

Most previous studies have applied HYDRUS models to simulate water-N dynamics under specific soil conditions (Clement et al., 2021; Miranda-Velez et al., 2022; Singh et al., 2019). Soil texture varies significantly from region to region and is an important factor that directly affects the water-N transport processes and the amount of N leaching from the soil. Bi et al. (2003) used the HYDRUS model to simulate the vertical transport of water and NO3-N in two soils (yellow moist soil and eolian sandy soil) in the Huang-Huai-Hai Plain of China. Based on this, Rees et al. (2020) constructed six reclaimed coarse-textured soil profiles consisting of two cover soils (peat-mineral mix and forest floor mineral mix) and simulated nutrient leaching from these six profiles, using the simplicity of HYDRUS customizable soil profile properties of each layer. Results revealed that the peat-mineral mix retained 44% of the initial inorganic N within the surface 20 cm of the reclaimed soil profiles after heavy rainfall, while 84% of the inorganic N was leached from the forest floor mineral mix.

Taking advantage of the HYDRUS models’ ability to customize soil profiles using different soil characteristics, soil N leaching under different long-term conditions could be simulated to provide data to support the development of the best irrigation and fertilization scenarios. Azad et al. (2018) used a two-stage optimization approach and a calibrated HYDRUS model to develop an optimal water and fertilizer management program for maize fields for the soil reclaimed for growing crops. Azad et al. (2018) simultaneously optimized the irrigation flow rate, application starting time, and fertilizer application duration to minimize NO3-N
leaching in a fertigation cycle. Correspondingly, the fertilizer amount at each crop growth stage was optimized throughout the growth season by comparing multi-scheme simulations based on the optimized irrigation rate. HYDRUS-simulated results provided insight into how cover crops affect N leaching losses, helping optimize the design of a soil cropping system to minimize N losses.

Anthropogenic agronomic measures significantly affect root zone leaching of soil NO3-N (Arbat et al., 2013; Shaygan et al., 2018a,b). Shafeeq et al. (2020) investigated the effects of several conservation agriculture practices (conventional tillage, permanent broad beds (PBB), zero tillage (ZT), PBB with residues, and ZT with residues) on the spatial-temporal distribution of soil moisture and NO3-N during the wheat growth stages, inversely optimized the relevant reaction parameters (i.e., nitrification rates, and the distribution coefficient), and predicted daily variations of NO3-N in the soil profile. Based on the HYDRUS simulation results, this study recommended using PBB with residues for wheat cultivation in the maize-wheat cropping system to improve water and N use efficiency and reduce water and N losses.

To address the problem of water and nutrient leaching below the root zone in light-textured soils due to the position of subsurface drip lines and/or poor management of the irrigation system, El-Nesr et al. (2014) used the HYDRUS model to evaluate the effectiveness of three anti-leaching techniques (a physical barrier, a dual-drip system with concurrent irrigation, a dual-drip system with sequential irrigation) applied in bare and vegetated soils. Results showed that the dual-drip system with sequential or concurrent irrigation is very efficient in limiting the downward leaching of nutrients and that these systems can be applied in actual production to reduce the risk of environmental pollution.

Since current regional-scale groundwater models, such as MODFLOW, tend to simulate the fate of solutes in the saturated zone by greatly simplifying the near-surface hydrologic processes, their simulations often lead to poor results. Lyu et al. (2019) coupled the one-dimensional vadose zone flow model HYDRUS-1D and the groundwater model MODFLOW to provide a feasible method for simulating the fate and transport of salt and N in the subsurface and for assessing the long-term effects of irrigation with reclaimed water. The HYDRUS model can be coupled with other models to simulate various biogeochemical processes under different conditions, providing an effective tool for improving simulation accuracy and rationality.
Fig. 12 demonstrates soil NO$_3$-N leaching in sandy loam for surface drip irrigation with three different irrigation depths (15, 22.5, and 30 mm; the N application duration of 5 days), three different durations of fertilizer application (5, 10, and 15 days; the irrigation depth of 30 mm), and the same N-fertilizer application (2.1 mg cm$^{-2}$) (the NLeach example in Table A). In this example, the longitudinal dispersivity ($D_L$) was considered to be 50 cm within the 0–100 cm soil layer, and the transverse dispersivity ($D_T$) was assumed to be one-tenth of $D_L$ (Cote et al., 2003). The molecular diffusion coefficients of NH$_4$-N and NO$_3$-N in free water were set to be 0.064 and 0.068 cm$^2$ h$^{-1}$, respectively (Cote et al., 2003; Nakamura et al., 2004). The distribution coefficient $K_d$ for NH$_4$-N and NO$_3$-N were assumed to be 3.5 and 0 cm$^3$ g$^{-1}$, respectively (Hanson et al., 2006). This study also assumed that NH$_4$-N transforms directly into NO$_3$-N since nitrification of NO$_2$-N to NO$_3$-N is relatively fast. The soil bulk density is 1.5 g cm$^{-3}$, and the nitrification rate (transformation of NH$_4$-N to NO$_3$-N) in the liquid and solid phases in the sandy loam were set to 0.12 and 0.28 d$^{-1}$, respectively (Castaldelli et al., 2018). These values lead to an approximate retardation factor for NH$_4$-N of about 22.9 and a half-life of about 3–6 d. NH$_4$-N was assumed to be initially present in the top 10 cm of the soil profile and additionally applied with the irrigation water. Both NH$_4$-N and NO$_3$-N were assumed to be passively taken up by plant roots (rooting depth of 80 cm and rooting radius of 40 cm). The third-type Cauchy boundary condition was used for solute transport along all boundaries with specified water fluxes (at the top boundary), while the second-type Neumann boundary condition was used at the bottom.

Fig. 12 Actual and cumulative NO$_3$-N leaching at a depth of 40 cm in scenarios with (A) different irrigation depths ($I = 15, 22.5, and 30$ mm; the N application duration of 5 days) and (B) different durations of the fertilizer application ($D = 5, 10, and 15$ days, the irrigation depth of 30 mm) and the same N-fertilizer application of 2.1 mg cm$^{-2}$. 

![Graph](image-url)
boundary. In the HYDRUS model, the N-fertilizer application mass equals the product of the irrigation water volume \((L^3)\) and the solute concentration \((ML^{-3})\) in irrigation water. Thus, the solute concentration of irrigation water (input value) was determined by dividing the N-fertilizer application mass by the irrigation water volume. In this example, the first topdressing mass and the irrigation water depth are \(0.63\, mg\, cm^{-2}\) and \(3\, cm^3\, cm^{-2}\), and thus the solute concentration of irrigation water is \(0.21\, mg\, cm^{-3}\). Since \(NH_4-N\) was greatly retarded in the soil profile, Fig. 12 only shows actual and cumulative solute fluxes for \(NO_3-N\) for different scenarios. The simulation results showed that soil nitrogen leaching increased in response to an increase in the irrigation depth, while it decreased with an increase in the duration of the fertilizer application.

### 6.4 Crop root N uptake

Optimization of N fertilizer applications is needed to prevent the negative impacts of these fertilizers on the environment. Such optimization requires considering complex interactions between root water and N uptake and their implications for crop production (Azad et al., 2020; Groenveld et al., 2021). The transfer of N from the soil solution into the plant can be described using active or passive mechanisms, which refer to the mass flows of N into roots with water taken up for transpiration or against energy gradients, respectively (Groenveld et al., 2021). The passive and active root N uptake functions implemented in the HYDRUS models have been widely used to optimize N fertilizer applications in agricultural production.

All principles and parameter settings of passive/active root nutrient uptake implemented in HYDRUS are described in detail by Šimůnek and Hopmans (2009) and in the model’s technical and user manuals (Šimůnek et al., 2022a,b; Šejna et al., 2022). Root passive N uptake is simulated by multiplying water uptake (compensated or uncompensated) by the dissolved N concentration for concentration values below an a priori-defined maximum concentration \(c_{max}\), the maximum allowed solution concentration for uptake. All nutrients dissolved in water are taken up by plant roots when \(c_{max}\) is large (larger than the dissolved concentration \(c\)), while no nutrients are taken up when \(c_{max} = 0\), with only active uptake remaining in this case. The maximum solution concentration for passive root uptake, \(c_{max}\), thus controls the relative proportion of passive root water uptake to total uptake. Using this flexible formulation, uptake mechanisms can vary between specific nutrients. For example, Na uptake can be
excluded by setting \( c_{\text{max}} = 0 \), passive Ca uptake can be limited by defining a finite \( c_{\text{max}} \) value, or all of the soil solution available P or N can be allowed to be taken up passively by setting \( c_{\text{max}} \) to a very large value.

Ranjbar et al. (2019) calibrated and validated the HYDRUS model parameters for root passive N uptake using data from two maize experiments over the 2015 and 2016 growing seasons. Simulations showed that HYDRUS was reasonably accurate in estimating total N uptake at harvest, although it could not simulate cumulative N uptake during various growth stages with high accuracy. The authors hypothesized that some neglected processes, such as active N uptake, caused an underestimation of the N uptake rate during the vegetative stage when the corn reached its maximum growth rate. Azad et al. (2019) used the HYDRUS model (water-solute transport, root water/N uptake, and root growth) to simulate N uptake in a sandy clay/sandy loam soils under a surface drip irrigation system and calibrated various parameters to optimize nitrogen use efficiency. Azad et al. (2019) compared root N uptake for two fertilizer application frequencies with the maize N requirements during various maize growth stages. Results showed that reducing the number of irrigation fertilizer applications in sandy clay loam soils increased the NO\(_3\)-N uptake by plants. However, fewer irrigation-fertilization events in sandy loam soils decreased the NO\(_3\)-N uptake.

The HYDRUS model has also yielded meaningful results about active root N uptake, another important process. When optimizing N fertigation, Groenveld et al. (2021) considered the effects of water and N stress on the plant size and corresponding feedback on potential transpiration and N uptake. To accomplish this, Groenveld et al. (2021) modified HYDRUS to consider the reduction of potential transpiration due to N uptake limitation. The model was then calibrated and validated using a dataset consisting of three NO\(_3\)-N concentrations and six irrigation levels, i.e., using 18 treatments to fertilize cucumber plants grown in the evaporator. The model was validated by testing its ability to accurately reduce potential N uptake and transpiration in the presence of water and N deficiency.

Li et al. (2015c) observed and simulated (using HYDRUS-1D) N transport and transformations in an experimental direct-seeded-rice (DSR) field in the Taihu Lake Basin of eastern China for two consecutive seasons. The calibrated and validated HYDRUS model indicated that NH\(_4\)-N was the predominant form (74% of N uptake on average) for crop N uptake, and NH\(_4\)-N uptake represented 32.1% and 30.8% of total N input over the
2008 and 2009 seasons, respectively. Similarly, Sharmiladevi and Ravikumar (2021) also improved the accuracy of root N uptake simulation by the HYDRUS model through intensive field experimentation, where various fluxes of urea, NH$_4$-N, and NO$_3$-N under drip irrigation were quantified to develop the N fertilizer application schedule for the entire rice growth period. In soil improvement, Mazloomi and Jalali (2019) studied NH$_4$-N uptake and transport in sandy loam soils for different application rates (2%, 4%, and 8%) of vermiculite, nano clay, and zeolite amendments. The HYDRUS model indicated that the application of inorganic amendments to sandy loam soils reduced NH$_4$-N transport and increased the effective utilization of N fertilizer in agricultural systems. HYDRUS simulations helped to identify the best fertigation management to reduce N leaching and increase root uptake. It is necessary to investigate different fertigation strategies for different soils and growing seasons to increase the efficiency of N uptake by plants.

The example used above to assess N leaching (the NLeach example in Table A) also provides information about root NH$_4$-N and NO$_3$-N uptake for different simulated scenarios, i.e., different irrigation depths (15, 22.5, and 30mm) and different durations of fertilizer application (5, 10, and 15 days) with the same N-fertilizer application (2.1mg cm$^{-2}$) (Fig. 13). The maximum allowed solution concentration ($c_{max}$) for passive uptake for NH$_4$-N and NO$_3$-N were set as 1.0 and 0.4mg cm$^{-3}$, respectively (Chen et al., 2020b). In general, root NO$_3$-N uptake was significantly higher than NH$_4$-N uptake in different scenarios during the simulation period since NH$_4$-N was relatively quickly nitrified into NO$_3$-N. Moreover, in different irrigation depth scenarios, root NO$_3$-N or NH$_4$-N uptake increased in response to an increase in the irrigation depth. However, an interesting result was obtained in the scenario with different durations of the fertilizer application. The highest root NO$_3$-N or NH$_4$-N uptake occurred for the application duration of 10 d, which showed that soil nitrogen could be easily taken up by plant roots in this scenario.

Another example (the NUptake example in Table A) is used to demonstrate the modeling of active and passive crop nitrogen uptake and sprinkler irrigation. This example includes three different N-fertilizer application levels (2.8, 2.1, and 1.4mg cm$^{-2}$) and three different soil textures (sandy, sandy loam, and loam). In this example, the transformation of NH$_4$-N to NO$_3$-N was neglected, and NO$_3$-N was directly applied with the irrigation water. The dispersivity ($D$) was considered to be 10cm, the
The maximum allowed solution concentration ($c_{\text{max}}$) for passive uptake was set as 0.4 mg cm$^{-3}$, and the potential active solute uptake rate was set as 0.1 mg cm$^{-2}$ day$^{-1}$. The Michaelis-Menten constant was set to 0.5 mg cm$^{-3}$. It was also assumed that potential solute uptake was reduced due to reduced root water uptake. A concentration flux boundary condition was set at the top and bottom boundary, and 20% of the N-fertilizer application was assumed to be initially present in the top 10 cm of the soil profile.

**Fig. 13** Root NH$_4$-N and NO$_3$-N uptake in scenarios with (A) different irrigation depths ($I = 15, 22.5, \text{ and } 30 \text{ mm, with an N application duration of 5 days}$) and (B) different durations of the fertilizer application ($D = 5, 10, \text{ and } 15 \text{ days, with an irrigation depth of 30 mm}$) and the same N-fertilizer application of 2.1 mg cm$^{-2}$. 

maximum allowed solution concentration ($c_{\text{max}}$) for passive uptake was set as 0.4 mg cm$^{-3}$, and the potential active solute uptake rate was set as 0.1 mg cm$^{-2}$ day$^{-1}$. The Michaelis-Menten constant was set to 0.5 mg cm$^{-3}$. It was also assumed that potential solute uptake was reduced due to reduced root water uptake. A concentration flux boundary condition was set at the top and bottom boundary, and 20% of the N-fertilizer application was assumed to be initially present in the top 10 cm of the soil profile.
The results showed that the crop nitrogen uptake rate increased after fertilization applications, while the cumulative crop nitrogen uptake decreased in response to a decrease in nitrogen-fertilizer application levels (Fig. 14). Additionally, an apparent difference in the crop nitrogen uptake rate was also found for different soil textures. In general, cumulative crop nitrogen uptake is different in different soil textures, and it increases from sand to sandy loam and loam.

Fig. 14 Actual and cumulative root nitrogen uptake rate in scenarios with (A) different N-fertilizer application levels (2.8, 2.1, and 1.4 mg cm$^{-2}$; sand) and (B) different soil textures (sand, sandy loam, and loam, with an N application of 2.8 mg cm$^{-2}$).
7. Salinity and sodicity

A major challenge for irrigated agriculture, particularly in arid and semi-arid regions, is irrigation-induced salinization of land and water resources (U. S. Salinity Laboratory Staff, 1954; Shainberg and Shalhevet, 1984; Wallender and Tanji, 2012). Many irrigation projects, both ancient and modern, have struggled or failed over time due to the degradation of soils and waters (Jacobsen and Adams, 1958; Ghassemi et al., 1995; Hopmans et al., 2021). The pervasiveness of soil salinity and sodicity in irrigated agriculture is such that salt management has been identified as a key motivation for early fundamental studies in soil science (Letey, 1984).

HYDRUS was initially developed at the USDA-ARS U.S. Salinity Laboratory (Šimůnek et al., 2008), and it has always had strong capabilities for modeling salinity under irrigation. HYDRUS has been widely used to evaluate the impacts of irrigation and salinity management on soil and water quality and crop yields.

Two approaches are available to model irrigation in salt-affected lands. The simpler method is to evaluate soil salinity in terms of the total salt concentration of the soil solution. The concentration $c$ in Eq. (2) is treated as a non-reactive tracer, equal to the total aqueous salt concentration. With this approach, it is possible to simulate salt additions, accumulation, and leaching in the soil profile, as well as to evaluate the impact of salinity on crop productivity via the HYDRUS root water uptake features.

More detailed assessments of irrigation and salinity are possible using the HYDRUS UNSATCHEM module (Šimůnek and Suarez, 1993; Suarez and Šimůnek, 1993; Šimůnek and Suarez, 1994; Šimůnek et al., 1996; Gonçalves et al., 2006; Ramos et al., 2011). The module includes capabilities for simulating multiphase transport of CO$_2$, transport of major ions (Ca$^{2+}$, Mg$^{2+}$, Na$^+$, K$^+$, SO$_4^{2-}$, and Cl$^-$), major ion chemistry including complexation, cation exchange, precipitation and dissolution (e.g., of calcite, gypsum, and dolomite), and water quality effects on hydraulic conductivity.

A search of “HYDRUS” and “salinity” on Google Scholar locates hundreds of journal articles and other texts documenting HYDRUS applications to soil salinity problems using both approaches discussed above. Here we offer a selective overview of representative projects.
7.1 Crop-water simulations for salinity management

All irrigation waters contain some amount of salt. As crops grow and extract water from the soil, salt is left behind in the root zone, where it will accumulate over time unless the applied irrigation and/or rain exceeds crop water requirements by an amount that is sufficient to flush salts into the deeper subsurface and maintain the rootzone salt balance. The fraction of applied water that passes below the root zone is known as the leaching fraction (LF); the LF required to keep root zone salinity at acceptable levels for a given crop is called the leaching requirement (LR). While LF and LR are valuable management concepts, their utility in operational management has been questioned (e.g., Corwin et al., 2007; Letey et al., 2011; Oster et al., 2012). Traditional LR analyses have been criticized for overestimating the impact of salinity on crop growth, thereby encouraging over-irrigation. Limitations identified in LR analyses include steady-state and one-dimensional flow assumptions and neglect of salt precipitation and dissolution reactions.

An alternative is to simulate a growing season(s) using HYDRUS, evaluating the impacts of water quality and irrigation practices on crop water uptake using the HYDRUS solute transport and root water uptake features. Among others, Corwin et al. (2007) found that differences in leaching requirements derived from transient and steady-state models were relatively minor, whereas accounting for salt precipitation led to significantly different recommendations. Similarly, Oster et al. (2012) found that with higher salinity irrigation waters, yields predicted using UNSATCHEM were greater than yields predicted with other models due to UNSATCHEM’s ability to account for salt precipitation, as well as the nonlinear relationship between salt concentration and osmotic potential.

As an illustration, consider the following scenario, which is based on one assessed by Oster et al. (2012) and Skaggs et al. (2014). Forage corn is grown over a 20-week season. Multiple seasons having the same time-varying atmospheric boundary conditions are simulated back-to-back. By the final season, the simulated system has approached a quasi-steady state with respect to seasonal water uptake and dynamics.

Four model setups, each for two irrigation regimes, are evaluated (the Salinity examples in Table A). The first is a HYDRUS simulation that does not include salinity. Second is a HYDRUS simulation with an irrigation water salinity of 3 dS/m. The last two are UNSATCHEM simulations.
with irrigation water salinities of $\approx 3$ dS/m but differing in chemical compositions, one a chloride-dominated water and the other having higher levels of sulfate and alkalinity.

Table 2 gives model results for two simulated irrigation regimes, one a deficit irrigation scheme in which seasonal applied water ($I_{irr}$) is less than the seasonal potential transpiration ($T_p$), $I_{irr}/T_p = 0.9$, and the other in which applied water is in excess of potential transpiration, $I_{irr}/T_p = 1.1$. The presented results are the final seasonal leaching fraction (LF), evaluated as the ratio of cumulative water flux at the bottom of the root zone to the seasonal applied water, and the final seasonal relative yield, evaluated as the ratio of seasonal actual and potential transpiration.

The results in Table 2 demonstrate that relationships between applied water, water quality, leaching fraction, and crop yield are straightforward only when salinity is neglected (as is done with classical LF and LR assessments). Among the tested models featuring salinity, a range of outcomes was obtained. The UNSATCHEM model with chloride water generated higher yields and lower leaching fractions than the HYDRUS model with salinity because, in the former simulation, calcite precipitation in the upper

<table>
<thead>
<tr>
<th>Model</th>
<th>$I_{irr}/T_p$</th>
<th>$I_{irr} = 0.9$</th>
<th>$I_{irr} = 1.1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>HYDRUS, no salinity</td>
<td>90</td>
<td>0</td>
<td>100</td>
</tr>
<tr>
<td>HYDRUS, $EC_{iw} = 3$ dS/m</td>
<td>77</td>
<td>14</td>
<td>88</td>
</tr>
<tr>
<td>UNSATCHEM, $EC_{iw} = 3$ dS/m, chloride</td>
<td>79</td>
<td>12</td>
<td>90</td>
</tr>
<tr>
<td>UNSATCHEM, $EC_{iw} = 3$ dS/m, sulfate</td>
<td>82</td>
<td>8</td>
<td>93</td>
</tr>
</tbody>
</table>

$EC_{iw} =$ irrigation water salinity; $I_{irr} =$ seasonal irrigation; $T_p =$ seasonal potential transpiration.
part of the root zone removed salt from the solution and reduced the effective root zone salinity. Similarly, the UNSATCHEM simulation with higher sulfate and alkalinity produced the highest yields and lowest leaching because significant amounts of calcite and gypsum were precipitated in the root zone. If the simulations were done with higher irrigation water salinities, the differences between model outcomes would become more pronounced. Fig. 15 illustrates the root zone salinity profiles at the midpoint of the final simulated season for each model.

### 7.2 Salinity under micro-irrigation

Micro-irrigation systems (drip, micro-sprinkler, etc.) create relatively complex, spatially varying patterns of water and salinity in irrigated soils (e.g., Burt and Isbell, 2005). HYDRUS (2D/3D) has been used in many studies investigating leaching and water requirements in micro-irrigated systems. Among others, Hanson et al. (2008) showed that a conventional or water balance approach for estimating leaching fractions predicted little or no leaching when applied water was less than the potential evapotranspiration, whereas field data and HYDRUS modeling showed considerable leaching around the drip lines. Raij et al. (2016) used HYDRUS (2D/3D) and UNSATCHEM to study spatial leaching patterns in soil lysimeters and

![Fig. 15 Rootzone salinity profiles at the midpoint of the growing season for two irrigation levels (Irr = 0.9 Tp and 1.1 Tp) and three modeling scenarios (the standard HYDRUS and the UNSATCHEM model with chloride- and sulfate-dominated water). The plot on the right shows the root uptake density distribution.](image-url)
different methods for evaluating leaching fractions. Yang et al. (2019) compared leaching in 1D (sprinkler-irrigated) and 2D (drip-irrigated) systems, finding that leaching fractions were higher under drip than under sprinkler, and that sprinkler was a more efficient means for maintaining salt balance.

7.3 Sodic soil reclamation

Irrigated soils (particularly heavy-textured clay soils) with a high exchangeable sodium percentage usually possess undesirable physical characteristics such as low permeability and surface crusting. Reclamation of sodic soils generally involves replacing sodium on the exchange surfaces with calcium. Typically, calcium is introduced to the soil through the addition of amendments such as gypsum, although native soil minerals can also be a source. Standard formulas exist for calculating the required calcium or amendment needed to reduce the exchangeable sodium percentage to desirable levels, typically less than 10% (e.g., James et al., 1982; Loveday, 1984). Sodic soil reclamation is relatively complicated owing to the interactions of sodicity, salinity, and permeability; one must take care not to worsen an infiltration problem by introducing an amendment solution with a low electrolyte concentration. Further, sodic soil reclamation can be expensive due to the cost of amendments.

Many researchers have used UNSATCHEM to study sodic soil reclamation with the goal of improving efficiency and reducing costs (e.g., Šimůnek and Suarez, 1997; Kaledhonkar et al., 2006; Reading et al., 2012; Wang et al., 2016a; Shaygan et al., 2018a,b). Among others, Suarez (2001) used UNSATCHEM to investigate alternative reclamation strategies and concluded that for soils possessing native calcite, “green manuring” (i.e., incorporating fresh organic matter into the soil to boost soil CO₂) can be used to reclaim soil without gypsum additions and with less water. More recently, Phogat et al. (2020a) assessed the impact of annual gypsum additions on maintaining acceptable sodicity and salinity levels.

7.4 Shallow groundwater

In addition to irrigation water additions and native soil minerals, root zone salinization can occur due to the upward movement of shallow, saline groundwater. HYDRUS has been used in a number of studies to evaluate the impact of shallow groundwater. For example, Forkutsa et al. (2009) modeled irrigated cotton production as affected by salinity and shallow groundwater in the Aral Sea Basin. Karimov et al. (2014) assessed the impact
of salinity and shallow groundwater on winter wheat production in the Fergana Valley (Central Asia). Li et al. (2015a) modeled soil water and salt dynamics as influenced by shallow groundwater in the Heihe River Basin. Narjary et al. (2021) evaluated the effects of water table depth and evaporative flux on soil salinity.

### 7.5 Recycled and produced water

The disposal of recycled or produced water to irrigate agricultural crops is another interesting application of the HYDRUS and UNSATCHEM models (e.g., Mallants et al., 2017; Phogat et al., 2020a,b, 2021). Produced water is water that comes out of the wells during fracking operations, coal seam gas production, or crude oil production. Produced water contains soluble and non-soluble oil/organics, suspended solids, dissolved solids, and various chemicals used in the production process. The application of produced water as irrigation water (possibly after blending with fresh water) is associated with many problems, such as salinity and sodicity risks and associated changes in soil physical and chemical properties (e.g., reduction of hydraulic conductivity), which can be assessed using the HYDRUS model and its modules (e.g., UNSATCHEM).

### 8. Chemigation

Modern irrigation systems are used, besides delivering water, also for transporting agrochemicals (e.g., pesticides and herbicides) to benefit plant health. The chemicals are injected into the irrigation system (Chemigation) and transported directly into the plant environment (Taha, 2022). Each agrochemical has its own chemistry and unique interactions with the soil matrix. Each solute can be involved in several processes, such as transport, adsorption, degradation, volatilization, or even interactions with other solutes (Spurlock et al., 2013a). Besides the ability to improve the scheduling of chemical applications to allow for their maximum utilization, numerical models also can track the fate of applied solutes and their metabolites in the root zone and their transport below the root zone into groundwater, which in general could be harmful to the environment.

#### 8.1 Historical developments

Modeling of solute transport in soil systems has been practiced for several decades, initially using the ADE’s analytical solutions and later numerical
solutions. The analytical solutions typically require complete decoupling of water flow and additional simplifications such as uniformity of soil properties and are, therefore, very limited. In most cases, they are also limited to strict linearity, zero- or first-order reactions, and full decoupling of the solutions for different solutes (as well as the decoupling of the water flow from the solute transport). A large number of the ADE’s analytical solutions (e.g., van Genuchten, 1985; van Genuchten and Wierenga, 1976; van Genuchten and Wagenet, 1989) and programs evaluating these solutions (e.g., CFITM, CFITIM, CXTFIT, 3DADE, N3DADE, and CHAIN) were implemented in the public-domain Windows-based STANMOD (STudio of ANalytical MODels) computer software package (Šimůnek et al., 1999), which can be considered to as belonging to the HYDRUS family of software packages.

Numerical solutions are more flexible in many aspects mentioned above and, therefore, gained popularity over the years, with HYDRUS playing a major role in that popularity. The vast majority of numerical applications of solutions to water flow and solute transport in soil systems were of an agricultural orientation (e.g., tracking the fate of fertilizers, pesticides, or salinity), but numerous applications for environmental problems soon followed, looking at nutrient leaching to groundwater, contaminant transport from landfills, and more. In the following, we present several examples of such applications.

8.2 Standard modules and their predecessors

Šimůnek et al. (1992) were among the first to add solute transport capabilities to the numerical solutions of the Richards equation (then SWMII, a predecessor of HYDRUS). The ADE used at the time included advection, dispersion, and a very limited range of reactivity processes (linear adsorption (i.e., constant retardation factor) and zero- and first-order reactions in both the liquid and solid (sorbed) phases). The code gained increasing popularity starting mostly at the end of the 1990s, with the advancement of personal computation and the stability of the code as it developed from SWMII to SWMS_2D to the early HYDRUS packages in one or more dimensions (Šimůnek et al., 2008). In that relatively limited approach, linear sorption (assuming equilibrium) is considered in Eq. (2) using \( s = k_{dfc} \), and the sink/source term \( \phi \) includes zero \( (k_0) \) and first \( (k_1c) \) order reactions, and parallel terms for the solid (sorbed) phase. Note that in most cases, sorption is mathematically represented as a retardation factor that comes in front of the left-hand side of (2) and is constant for linear sorption.
Examples of early applications include De Vos et al. (2000), who used SWMS_2D to model nitrate leaching (i.e., as an inert solute). Persicani (1996) used HYDRUS (and three other models) to check the sensitivity of pesticide leaching in soil profiles. Vanderborght et al. (1998) modeled advection-dispersion (ignoring diffusion) in heterogeneous soils and compared their results to the particle tracking approach. Yang et al. (1996) considered linear adsorption in their 2D stochastic simulation framework (with the hydraulic conductivity and the adsorption constant being the stochastic variables). Boateng and Cawfield (1999) conducted an extensive sensitivity analysis of the Richards-ADE system to contaminant transport, considering most parameters of the Richards equation (with van Genuchten–Mualem parameters), considering advection, dispersion, first-order sorption, and zero- and first-order reactions. These and many other earlier references to HYDRUS packages and their predecessors can be found here.

An example of a relatively advanced application of the classic HYDRUS model for solute transport is seen in Hanson et al. (2006). They considered drip irrigation in two geometrical configurations (one of which is axisymmetric), where fertilizers (urea, ammonium, and nitrate) were applied with the water (fertigation). In their model, they considered sequential first-order reactions (hydrolysis of urea and nitrification) and linear adsorption (of ammonium). Denitrification was not considered (as in the experiment associated with the model, it was negligible), and volatilization and gas transfer were ignored. This represents a classic agronomic study that looks into the fate of fertilizer in the subsurface. However, for more complex cases when oxygen may be absent at times or in regions of the subsurface, such a modeling approach that relies only on a sequence of first-order reactions may be insufficient.

In later versions of HYDRUS and other codes that solve similar problems, more sophisticated reactions evolved over the years. Clearly, the space is too limited to review them all, and we will only mention several, referring the reader to the HYDRUS manual and website for further elaboration and presentation of specific equations. For example, Kodešová et al. (2004) studied chlorotoluron transport in a soil profile and modeled it using both Freundlich and Langmuir isotherms. Pal et al. (2014) used HYDRUS-1D to model phenol breakthrough experiments in soil columns using the three classical sorption isotherms (linear, Freundlich, and Langmuir). Pot et al. (2005) and Köhne et al. (2006) used HYDRUS-1D to model herbicide transport using the dual-permeability model with two-site non-equilibrium sorption. Chotpantarat et al. (2011) studied the
transport of several heavy metals in soils and used HYDRUS-1D to model non-equilibrium sorption, considering Langmuir isotherm and two-site sorption. Finally, Köhne et al. (2009a,b) provided a comprehensive review of HYDRUS applications involving transient water flow and tracer and pesticide transport in structured soils.

8.3 Specialized add-on modules

The next level of complexity in modeling solute transport is using a higher complexity of reactions, which typically involve more than a single reactive species and coupling of the different reactions. In the HYDRUS framework, several specific tools were developed over the years for specific applications and environments (e.g., UNSATCHEM, Suarez and Šimůnek, 1997). Goldberg et al. (2007) provide a comprehensive overview of both existing models and their applications, mostly related to surface complexation. Later on, a more generic solution to the need emerged by coupling the PhreeqC code (Parkhurst and Appelo, 1999) with HYDRUS (Jacques et al., 2006) to form HP1. For example, Jacques et al. (2008a) studied aqueous phase complexation and ion exchange (competitive sorption) for several major ions and heavy metals, including cadmium and zinc. The use of PhreeqC in HP1 allows great flexibility in modeling complex biogeochemical processes. For example, Ben Moshe et al. (2021) used this flexibility to model carbon and nitrogen processes in the context of soil aquifer treatment using multi-Monod-type reactions.

An interesting development in solute transport codes, HP1 included, is their use in modeling the transport of non-solutes. This is increasingly practiced to study colloid and nanoparticle transport, considering processes such as attachment and detachment, straining, and more. Makselon et al. (2017) provide an example of such a model considering silver nanoparticles. Many references involving HYDRUS applications to simulate the fate and transport of various types of particles are listed on the HYDRUS website (i.e., https://www.pc-progress.com/Documents/Jirka/Particles_Transport_Papers.pdf).

8.4 HP1 example

The following example is used to demonstrate in more detail the ability of the HP1 code to track more complex biogeochemical processes beyond the capability of the conventional ADE with first-order reactions (The HP1 example in Table A). Jacques et al. (2008b) demonstrated the modeling
of uranium transport in soil following fertilizer applications. Their model considered annual fertilizer applications with inorganic phosphate contaminated by elements from the uranium decay chain. The soil profile comprised seven (7) layers to a total depth of about 1 m. The numerical solution considered 14 different species (C, Ca, Cl, F, Mg, N(V), Na, P, S(VI), and U(VI), O, and H) and a liquid-phase charge (to be balanced by the solid phase surface charge). Three types of geochemical equilibrium reactions were considered, including aqueous speciation reactions, cation exchange reactions on organic matter, and surface complexation reactions on Fe oxides. The reactions were strongly pH sensitive (i.e., protons, hydroxides, and surface hydrolysis were also considered). Carbon dioxide was not considered, as the pH range in the system was 3.5–4.5. Most reactions (including surface complexation ones) involve more than a single species; therefore, first-order reactions cannot be used. The results of this model showed a very good fit to experimental data, which could not be achieved using the more conventional models.

A different example (Liu, 2020) looked at the root zone’s total carbon and nitrogen cycle (specifically, the goal was to explore these processes under varying irrigation frequencies). She considered not only the classic nitrification and denitrification but also mineralization, decomposition of soil organic matter, dissolved organic carbon, and nitrogen, as well as microbial biomass and its growth or decay, and oxygen transfer between the liquid and gas phases. The considered processes are shown in Fig. 16, including the differentiation of the process direction for oxic and anoxic conditions.

Fig. 17 shows a sample of the results obtained by this complex model, looking at nitrification rates for three different irrigation regimes (see captions). Above all, this model considers oxygen levels in the soil, and accordingly, the reaction rates and the microbial dynamics are adjusted. One can easily note the influence of water quality and irrigation frequency on the biochemical processes. For example, nitrification rates in the upper 30 cm are higher in treatment TL than TH, primarily because of the higher aeration allowed between irrigation events. At the same time, FH rates are lower than TH because the concentration of organic nitrogen and carbon is lower.

The flexibility that is associated with HP1 seems endless. Nevertheless, the number of reported applications, especially in the agricultural context, is relatively small. While no statistical significance test was conducted, apparently, most of the applications of HP1 are in more environmentally related
**Fig. 16** Schematic of biochemical cycling in the root zone and microbial communities.

**Fig. 17** Spatio-temporal distributions of nitrification (i.e., ammonium transformation to nitrate) rates in different fertigation regimes (weekly cycles, for TH and FH irrigation on days 2, 4, and 7; for TL irrigation on days 3 and 7; water quantities adjusted; TH and TL use treated wastewater and FH uses freshwater).
research. The reason for this is not clear, but we suspect that this is related, in part, to the complexity of the model and the lack of a graphical user interface, even if minimal, dedicated to specific scientific environments.

9. Spatial variability

Efficient irrigation management decisions require a good understanding of temporal variations in root water uptake and spatial variations in soil hydraulic properties, which inherently impact water dynamics, solute transport, root distribution, and plant growth (Dabach et al., 2015). The soil–plant system of irrigated crops can be simulated by considering various model complexities, such as defining 1D, 2D, or 3D transport domains, describing homogeneous, layered, or fully heterogeneous soils in a single simulation, or by running a series of simulations representing measured or estimated variability in soil hydraulic properties. Additionally, spatial variation in irrigation inputs will cause water content heterogeneity in the irrigated field. Therefore, understanding different levels of spatial variability in the irrigated root zone can help with various decisions, such as selecting sensor locations for optimal triggered irrigation scheduling, providing information on the expected levels of variability in the measured data, or optimizing irrigation application methods that rely on non-uniform applications or involving different soil textures or materials. This section provides an overview of different levels of spatial variability, how they have been addressed using HYDRUS, and additional examples and guidance on how to apply them in various scenarios.

9.1 Irrigation system uniformity

The HYDRUS code can be used to study the effects of different levels of irrigation uniformity on drainage and solute leaching. Irrigation uniformity levels can be simulated by running Monte Carlo simulations with discharge rates sampled from a selected distribution associated with the desired irrigation uniformity. Such an approach can be applied to several drippers in a multi-dimensional simulation (Raij et al., 2018), to individual simulations, each with a discharge in a defined distribution, or a series of simulations representing variable emitter discharge rates along an irrigation line due to pressure head loss (Guan et al., 2019; Wang et al., 2016b). In a 3D study, it was found that lower irrigation uniformity in drip-irrigated lysimeters caused higher drainage variability than the observed variability in chloride...
concentrations (Raij et al., 2018). On the other hand, in 2D studies, it was found that increased irrigation uniformity decreased drainage amounts and nitrate loads (Guan et al., 2019; Wang et al., 2016b). Fig. 18 demonstrates how various levels of irrigation uniformity, i.e., with a coefficient of variation (CV) of 2%, 4.4%, and 9%, affect soil water contents at different locations relative to a dripper, as simulated in 500 runs. The simulation domain was the same as in the Drip Plant project (Section 5—Drip irrigation, Table A). Sandy loam and loamy soils were considered (Figs. 18A and C and 18B and D, respectively). Daily irrigation events from a surface irrigation area with a radius of 20 cm were simulated for four days. The irrigation discharge rate was randomly sampled 500 times from a normal distribution with the same mean but varying standard deviations, according

![Fig. 18](image-url)
to the selected CV (Fig. 18E). The Matlab code used to create these simulations can be found in this link. Water contents in three observation nodes (Fig. 18F) varied in 500 simulations because of different imposed discharge rates. As expected, the higher the CV of the irrigation discharge rate, the higher the variability in the soil water content, especially during irrigation events (Figs. 18A and B). As a result, values of the water content CV during the irrigation events were higher than the irrigation CV (Figs. 18C and D).

### 9.2 Deterministic spatial variability

Vertical heterogeneity due to soil layering, for example, in alluvial soils, can be simulated in HYDRUS by defining each soil layer’s hydraulic parameters and assuming horizontal homogeneity (Botros et al., 2012). If enough data is available, the depth of each layer can vary in any dimension accordingly (Bednorz et al., 2016). Botros et al. (2012) simulated water flow and nitrogen transport in an irrigated nectarine field with a 3D domain with horizontal soil layers of varying depths in the east-west direction but homogeneous in the north-south direction. Water fluxes below the root zone and nitrate concentrations in the deep vadose zone, simulated using the layered approach, were comparable to stochastic simulations using either a Miller-Miller approach or a measured spatial correlation of the van Genuchten hydraulic parameters (Botros et al., 2012). 3D transport domains can be used to simulate water contents and solute distributions in complex irrigated systems such as a drip-irrigated cotton field with partial plastic mulch on the growing beds (Li et al., 2018b) or rainfed banana plants grown on Andisol with a complex canopy geometry (Sansoulet et al., 2008). In addition, simulations using 3D domains can help explain processes of the wet bulb and salinity overlap that are underestimated in 2D conventional models assuming symmetry (Kandelous et al., 2011). When 2D or 3D domains cannot be used due to computational constraints, 1D simulations can be carried out at the field or regional scale, and the results can be ensembled to include and describe the spatial differences. For example, soil properties, weather, slope, and land use maps can be used to create unique combinations of 1D simulations, which can then be integrated spatially to describe water and solute fluxes, as well as solute and water content distributions in the landscape (Turkeltaub et al., 2018; Henri et al., 2020, 2021; Qiu et al., 2020; Sprenger et al., 2016; Sela et al., 2012; Lai and Ren, 2016).
Fig. 19 presents two examples of layered soils where the first has a sandy loam layer in a loam domain (Fig. 19A, the Drip3D2L1 example in Table A), and the second has a loam layer in a sandy loam domain (Fig. 19B, the Drip3D2L2 example in Table A). These simulations use the same boundary conditions as the Drip3D examples in Section 5—Drip irrigation (Table A). Following an irrigation event during day 1, the volumetric water content is lower in the sandy loam layer than in the loam layer. This approach has been used to describe naturally occurring variability. In addition, induced soil profile variabilities, such as capillary barriers utilized to modify and control soil water distribution or irrigation using properties of porous materials, have been simulated with HYDRUS (2D/3D) for optimizing such systems (e.g., Ben-Gal et al., 2004; Siyal and Skaggs, 2009; Ityel et al., 2011; Sao et al., 2021).

9.3 Stochastic spatial variability
The effects of the spatial variability caused by the randomness of specific soil hydraulic properties, such as saturated hydraulic conductivities or porosities,
can be simulated using the HYDRUS code by first generating the spatial distribution of this parameter (using a theoretical (Guan et al., 2019; Wang et al., 2016b; Martinez et al., 2014) or measured (Hu et al., 2007) probability distribution of this property) and then running sequential simulations with a range of this parameter’s values. Theoretical distributions can be generated by defining a mean and coefficient of variation (CV) or standard deviation for the variable of interest (Guan et al., 2019; Martinez et al., 2014; Bossa and Diekkrüger, 2014) by generating a range of textures and bulk densities as inputs to Rosetta (Wang et al., 2016b), or by using means and standard deviations reported by Rossetta3 (Zhang and Schaap, 2017; Raij-Hoffman et al., 2022). Such simulations can optimize irrigation amounts to minimize leaching, not at a specific point in the field but as a probability density function (Hu et al., 2007). Additionally, different levels of hydraulic parameters’ heterogeneity can be studied, and their effects on water fluxes and solute loads can be described (Guan et al., 2019).

Fig. 20 presents the average and 95% confidence intervals of water contents during two irrigation events at an increasing lateral distance from a sub-surface dripper obtained from 187 simulations. Simulations were carried out for a homogeneous soil profile with varying $K_s$ values for two soil textures reported in Rosetta3. The mean and standard deviation of $K_s$ (on a log scale with base 10) were used to randomly sample $K_s$ values for each simulation. These simulations use the same boundary conditions as the Drop3D1 example in Section 5—Drip irrigation (Table A). The confidence bounds for time-variable water contents at each location in each soil demonstrate the uncertainty associated with using pedotransfer functions when only soil texture is known. While the uncertainty of the water content remains high during the two irrigation events, the variability of the flux at the bottom boundary decreases with time in this example. Considering measured or estimated variability in soil properties or irrigation systems can provide information on their effect on the uncertainty of different model outputs (in this case, water content and bottom boundary fluxes). This information can be used to evaluate model-to-measurement fit and a choice of type, method, and frequency of measurements.

In addition to non-dimensional parameter uncertainty (as discussed above), the measured or assumed spatial correlations of any selected hydraulic parameter can be considered in HYDRUS simulations. Correlation lengths in different directions can be used to generate a spatially correlated parameter space (Botros et al., 2009). Significant differences in 3D N fluxes
were observed in simulations considering the spatial correlation of soil hydraulic properties, as opposed to those using uncorrelated scaling factors or deterministic layered heterogeneities. On the other hand, water fluxes in the field with spatially correlated soil hydraulic properties were similar to those in the deterministic layered profile and different from those in the field with uncorrelated scaling factors. This was due to the nature of the highly horizontally correlated alluvial soil presented in Botros et al. (2009, 2012).

An additional option offered by HYDRUS is to generate stochastic distributions of hydraulic conductivity ($\alpha_K$) and pressure head ($\alpha_h$) scaling factors using the Miller-Miller similitude approximation (Miller and Miller, 1956), where these two scaling factors are correlated. The stochastic distribution requires a mean $K_s$, a standard deviation of $\log_{10}$ value of $\alpha_K$, and horizontal ($X$) and vertical ($Z$) correlation lengths. Additional numerical

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**Fig. 20** Average and 95% confidence intervals for 187 simulations with varying $K_s$ values for loam and sandy loam soils. Water contents at observation points located at depths of 20 cm (vertical) (dripper depth) and 5 cm (A), 15 cm (B), and 25 cm (C) away (horizontal) from the dripper. Time-dependent water fluxes at the bottom boundary (D).
experiments were performed to explore the influence of stochastic heterogeneity during an irrigation event using the flow domain in the DripPlant1 example in Section 5—Drip irrigation (Table A) with a sandy loam soil for a homogeneous soil profile, and heterogeneous soil profiles with a standard deviation of \(\log_{10}(\alpha_K) = 0.5\) cm and (a) a vertical correlation length \(Z = 5\) cm, (b) a horizontal correlation length \(X = 10\) cm, and (c) horizontal and vertical correlation lengths \(X = 10\) cm and \(Z = 5\) cm, respectively. Fig. 21A presents representative water content soil profiles for a homogeneous domain, and heterogeneous domains with vertical, horizontal, and both vertical and horizontal heterogeneities. Fig. 21B presents water contents at three observation nodes and the fluxes at the bottom boundary. The results demonstrate the significant variability of water contents in heterogeneous domains compared to the homogeneous one, with higher variability of both water content and bottom boundary fluxes for the vertical and horizontal heterogeneity than the combined heterogeneities. Similarly, water fluxes at the bottom boundary were more variable when only one directional heterogeneity was simulated rather than both directions combined. Examples of horizontal heterogeneity can be found in highly layered alluvial soils, and vertical heterogeneity is found in cracked soils with/or soils with preferential flow paths. In either case, the extent of the spatial correlations will depend on the soil profile’s specific properties. These results demonstrate the importance of considering heterogeneity, especially for contaminant flow and transport studies. Scaling factors can also be generated externally and imported into HYDRUS domains. An example can be found in Raij et al. (2018) or Botros et al. (2009), where three-dimensional distributions of scaling factors for unsaturated hydraulic conductivity were externally generated and imported into HYDRUS-3D.

9.4 Estimation of soil hydraulic parameters for heterogeneous soils

Various laboratory and field methods and in-situ soil sensors and devices are used to estimate soil hydraulic properties, and water flow and solute transport dynamics during irrigation. However, identifying optimum locations of sensors for a given spatial heterogeneity is critical for efficient irrigation water management. For example, the wetting front resulting from drip irrigation will be affected by the spatial heterogeneity of the soil between the dripper (with and without geotextile membrane) and the tensiometer. As a result, the wetting front will not reach tensiometers located at the same distance from the dripper at the same time. Dabach et al. (2013) used
a system-dependent boundary condition in HYDRUS that triggers irrigation of a fixed duration when a specified soil water matric head threshold is reached at a predetermined point in the soil profile. This boundary condition represents a demand-based irrigation system that directly depends on plant water uptake. HYDRUS simulations showed that the optimal location...
of tensiometer placement is near the subsurface dripper, resulting in a low CV of matric head measurements and applied irrigation water, high sensitivity to irrigation, and lower drainage below the root zone (Dabach et al., 2015). Zeng et al. (2012) compared the centrifugal, tensiometer, soil core, disc infiltration, and inverse solution methods to estimate soil hydraulic parameters for a drip-irrigated heterogeneous gravel soil. The two-dimensional HYDRUS inverse simulation produced the best result even though a slight overestimation of soil moisture was present, which revealed a problem of underestimating water movement with the disc infiltration approach compared to the soil core method.

Similarly, Abbasi et al. (2003a) used the Levenberg–Marquardt optimization algorithm implemented in HYDRUS to estimate soil hydraulic and solute transport parameters of several soil horizons below experimental furrows. Their results showed only minor improvements in model predictions with optimized parameters. A two-step method, i.e., sequential estimation of the soil hydraulic parameters followed by the estimation of the transport parameters, was used to improve the model predictions further. Despite implementing a scaling procedure for the unsaturated soil hydraulic properties, variability in the optimized longitudinal dispersivity values for the layered soil profiles was found to be higher than for the homogeneous soil profile due to the variations in soil water retention curves of the different soil horizons.

The Miller–Miller scaling approach implemented in HYDRUS was used by Weihermüller et al. (2006) to assess the variability in solute breakthrough curves in suction cups. Weihermüller et al. (2006) demonstrated that mean pore water velocities and dispersivities ranged by a factor of 1.6 and 1.5, respectively, for different heterogeneous structures. In addition, the suction cup sampling area, deformation of streamlines, and the flow channels were also found to have an influence, and numerical simulations indicated that about 20 suction cups were required for calculating a mean breakthrough curve in the chosen heterogeneous flow field (Weihermüller et al., 2006).

Similarly, lysimeters are widely used for closing water mass balances by monitoring the storage in the soil profile, drainage, and solute leaching at the bottom. Raij et al. (2018) investigated the influence of local heterogeneity in soil hydraulic conductivities and dripper discharge rates on drainage and chloride concentrations using 100 HYDRUS three-dimensional simulations per treatment. Different random spatial realizations of the conductivity scaling factor were generated, assuming a log-normal distribution
Their result demonstrated that irrigation caused higher variability in drainage amounts than soil heterogeneity, while soil heterogeneity caused higher variability in drainage concentrations than irrigation heterogeneity.

Most of the studies mentioned above used numerical simulations to demonstrate the influence of spatial heterogeneity on sensors. Domínguez-Niño et al. (2020a,b) investigated the sensor-to-sensor variability due to uncertainties in the measurement process plus the natural variability in the actual soil water dynamics by comparing 57 capacitance-type soil moisture sensors in the field and HYDRUS-3D virtual sensors under drip irrigation. However, the HYDRUS-3D model was used to simulate soil water dynamics only in a homogeneous soil and uniform root distribution and did not account for heterogeneous soil and root distributions, macropores, and soil irregularities. The results demonstrated that the HYDRUS-3D simulations successfully reproduced the soil water dynamics and patterns of daily amplitude, but compared to the sensors, simulations were less variable, underestimated root water uptake, and overestimated the influx of irrigation water. Overall, these results demonstrated that various soil sensors could be too sensitive to local variations in soil texture and the presence of gravel, stones, roots, macropores, or small compacted soil parts.

Understanding field wetting patterns during irrigation and fertigation can provide helpful information for efficiently managing these systems. In the past decade, advanced, minimally invasive geophysical tools, such as electromagnetic induction, cosmic ray sensors, ground penetrating radar, and electrical resistivity tomography (ERT), have been used for 2D mapping of wetting patterns and solute distributions for various irrigation systems (Algeo et al., 2016; Cassiani et al., 2015; Coppola et al., 2016; Han et al., 2016; Hardie et al., 2018). For example, Hardie et al. (2018) compared the drip irrigation wetting patterns and nitrate distributions using ERT, dye tracer, and HYDRUS-2D modeling. The results showed some variability in observed, measured, and predicted infiltration patterns and nitrate transport across the three approaches due to the preferential flow processes in the field. However, simultaneous ERT, dye tracer, and modeling studies can be used to understand water flow and solute transport in an irrigation field.

9.5 Challenges, recommendations, and future opportunities

All the processes described above can be simulated simultaneously, and different levels of variability can be considered simultaneously to study
complex processes (e.g., irrigation, soil hydraulic parameters, and scaling factors, Guan et al., 2019; Raji et al., 2018). The global problem of non-point source pollution from irrigated agriculture needs to be assessed at the regional scale, even though the processes occur at the field/local scale. One approach is to use an ensemble of one-dimensional HYDRUS simulations, including all combinations of soils and crops occurring in the area of interest (Henri et al., 2020; Turkeltaub et al., 2018). Then, each combination of water and solute loading is assigned to various spatial locations and either fed into a groundwater model or used as potential groundwater loadings. Qiu et al. (2020) studied landscape-level ecosystem services, including agricultural landscapes, using a biophysical model coupled with HYDRUS-1D and found that “time” components were more important than “space” drivers in such landscapes.

Emerging technologies, such as electrical resistivity tomography (Hardie et al., 2018; Peddinti et al., 2020), are increasing the opportunity to use spatially distributed data at larger scales than traditional measurements (i.e., Skaggs et al., 2004). Therefore, combining field monitoring, virtual monitoring, and validation of observed sensor data using representative HYDRUS simulations can provide great insight into local heterogeneity. Future studies should include a combination of multiple sensors for collecting a range of parameters and site-specific soil characterization to better understand the effects of spatial heterogeneity on irrigation management. Such efforts will also provide additional opportunities to fill the data gaps further and refine the model.

10. Model calibration

Numerical models are mainly developed to describe and predict the behavior of physical systems. When the deviation between model predictions and actual observations (e.g., soil moisture patterns or water depths in the furrow channel) is acceptable, then the model can complement or even replace real experiments. The model’s predictive accuracy depends on the adequacy of the model structure, as well as on a proper (and physically realistic) definition of model parameters. The process by which the model structure is selected and parameters are adjusted to minimize the distance between model predictions and measurements is broadly defined as model calibration. This procedure is generally accomplished by combining the model with iterative statistical and numerical optimization techniques.

HYDRUS is internally coupled with the gradient-based Levenberg-Marquardt search method (Marquardt, 1963), which solves a nonlinear least
squares optimization problem to calibrate various model parameters using transient observations. The algorithm is robust when the response surface of the calibration problem is unimodal, which is generally the case for well-posed inverse problems. Being supported by the HYDRUS GUI, the algorithm has been used in several irrigation-related studies to inversely estimate soil hydraulic and/or transport parameters. This has been generally accomplished by comparing simulated and observed soil water contents at different depths in drip-irrigated fields (Bufon et al., 2012; Chen et al., 2021; Gonçalves et al., 2015; Li et al., 2015b; Nayebloie et al., 2022; Patel and Rajput, 2008; Qi et al., 2018; Rana et al., 2022; Selim et al., 2013; Zhang et al., 2018), furrow channels (e.g., Abbasi et al., 2004; Dialameh et al., 2022; Ebrahimian et al., 2013; Ranjbar et al., 2019; Zhang et al., 2013), or other irrigated areas (e.g., Arbat et al., 2008; Bethune et al., 2008; Deb et al., 2013; Er-Raki et al., 2021; Hou et al., 2017; Li, 2020; Mokari et al., 2019; Rai et al., 2019; Rezayati et al., 2020; Saefuddin et al., 2019; Salehi et al., 2017; Tan et al., 2014).

The main limitation of the Levenberg-Marquardt algorithm is its local search capability, which makes its use questionable for high-dimensional inverse problems that use different types of measurements. In these circumstances, the response surface tends to be complex, noisy, and characterized by multiple local minima. To address this problem, several studies have externally coupled HYDRUS with global optimization algorithms such as the Particle Swarm, Genetic, and Shuffled Complex Evolution Optimization algorithms (Azad et al., 2018, 2019; Brunetti et al., 2018a; Erazo-Mesa et al., 2022; Kumar et al., 2022; Peddinti et al., 2018, 2020; Schneider et al., 2013; Vrugt et al., 2008; Zhou et al., 2007, 2012) or with the PEST calibration suite (Carlos et al., 2022; Liu et al., 2021, 2022). Despite requiring external tools, advanced programming skills, and significantly more computational resources, the results of these studies show that the use of global optimization algorithms can improve the HYDRUS calibration procedure and better diagnose model structural inadequacies when estimated parameters assume physically unrealistic values.

### 10.1 Uncertainty assessment

**Uncertainty analysis** complements model calibration and represents a valuable tool for assessing the model’s structural adequacy and predictive accuracy. Despite being frequently applied in combination with HYDRUS for vadose zone hydrological modeling, its use in irrigation-related studies
remains rather limited. Brunetti et al. (2018a) coupled HYDRUS-1D and the Global Sensitivity Analysis-Generalized Likelihood Uncertainty Estimation technique (GSA-GLUE) to calibrate and assess the uncertainty of the soil hydraulic and thermal parameters of an irrigated extensive Green Roof (GR). Recently, the Bayesian inference was used to statistically compare one conceptual and three HYDRUS-based mechanistic parameterizations (e.g., unimodal, bimodal, and dual porosity) of an irrigated GR at the laboratory scale (Brunetti et al., 2020). In another study, Brunetti et al. (2021) coupled HYDRUS-1D and the multimodal Nested Sampling algorithm (Feroz et al., 2009) to reproduce observations from three GRs irrigated with wastewater and simultaneously assess the uncertainty of inversely estimated soil hydraulic and solute transport parameters. The Bayesian inference was also applied by Guo et al. (2020), who used two surrogate-based uncertainty assessment techniques to calibrate the HYDRUS model against measurements from field irrigation experiments. Albeit limited, the results of these studies highlight the beneficial role of uncertainty assessment in combination with HYDRUS to (1) assess how the model’s predictive uncertainty affects model outcomes, which is of crucial importance when delivering model results to decision-makers, (2) verify whether the informational content of calibration measurements is sufficient to constrain model predictions, or update the prior belief of the modeler, and (3) compare multiple model parameterizations and avoid the use of data-unjustified complex model structures that tend to overfit measurements.

### 10.2 Sensitivity analysis

Along with uncertainty assessment, *sensitivity analysis* is a fundamental tool for model diagnostics, as it can be used for both predictive and explanatory purposes. In the first case, it can complement model calibration and uncertainty assessment by providing a statistical basis to quantify how different model parameters affect, alone and/or jointly, the fitting accuracy. Uninfluential parameters can then be excluded from the calibration, thus reducing the dimensionality of the inverse problem. When used for explanatory intentions, it can identify factors that most influence a certain variable of interest (e.g., root water uptake, nutrients leaching, etc.), thus guiding the experimental design (e.g., specific complementary laboratory measurements). Sensitivity analyses are generally divided into two groups: local one-factor-at-a-time (LSA) and global sensitivity analysis (GSA).
By varying only one factor at a time, LSA is easy to implement and computationally cheap. It has been used in several studies in combination with HYDRUS to assess the influence of soil hydraulic and transport parameters on water flow and nutrient transport in irrigated fields (Beyene et al., 2018; Geza et al., 2021; Jiménez-Martínez et al., 2009; Kadyampakeni et al., 2018; Reading et al., 2012; Rocha et al., 2006; Sun et al., 2022; Xu et al., 2019; Yang et al., 2017). However, LSA neglects the effects of parameters’ interaction, which is known to play an important role in environmental models. To overcome this limitation, GSA explores a large portion of the parameters’ space to identify combined or individual parameter effects. This frequently requires thousands of model executions to achieve stable estimates of the sensitivity indices, thus significantly increasing the analysis’s computational burden. Techniques such as the Morris screening scheme (Morris, 1991), the Sobol’ sequence (Sobol’, 2001), or the E-FAST method (Saltelli et al., 1999) have been successfully coupled with HYDRUS in multiple studies (Brunetti et al., 2018a; Li et al., 2012; Liang et al., 2017; Liu et al., 2022; Peddinti et al., 2018; Skaggs et al., 2014; Tao et al., 2021; Zhou et al., 2012).

The literature review suggests that GSA should be preferred when the computational cost of a single HYDRUS execution is low (e.g., seconds), as it provides statistically meaningful information about the most influential parameters and their interaction, which can be used to prioritize experiments (i.e., explanatory setting) or reduce the dimensionality of the inverse problem (i.e., predictive setting). Instead, LSA should be used when the model is computationally intensive to assess its sensitivity to small changes in specific parameters’ values. Ideally, for predictive purposes, this should be performed around the global optimum identified during the calibration procedure to check the model sensitivity near its most probable values. A prognostic use before calibration could lead to misleading conclusions if the LSA starting point lies in low-fitting regions. Similarly, for explanatory purposes, it is advisable to perform the LSA in regions of the parameters’ space identified as probable based on the literature review, prior information, and the modeler’s expertise.

### 10.3 Irrigation optimization

Model calibration, uncertainty assessment, and sensitivity analysis are all fundamental steps to obtain a model that can robustly predict the physical behavior of the system under investigation. Once this objective is achieved,
the model can be used for multiple purposes, among which the most important in irrigation management is the optimization of the irrigation system. This includes establishing the irrigation schedule (e.g., water/nutrients injection timing and duration) and defining locations and types of sensors (e.g., tensiometer, soil moisture sensors) and actuators (e.g., pumps, valves). The latter are key components of real-time systems, which are becoming very popular due to their capability to dynamically adapt the irrigation strategy depending on soil status. In this direction, the HYDRUS model includes a system-dependent boundary condition, which initiates irrigation whenever the matric head at a predetermined location drops below a certain threshold (Dabach et al., 2013). This enables the modeler to design and optimize a real-time sensor (i.e., tensiometer)—actuator (e.g., valve) irrigation system tailored to the specific soil.

In any case, regardless of the irrigation system type, the irrigation strategy should be designed to maximize crop yield while simultaneously minimizing the environmental footprint and installation and maintenance costs. This leads to a complex multi-objective optimization problem that can be solved by coupling the model with various numerical optimization techniques. For example, Kandelous et al. (2012) coupled HYDRUS-2D with the multi-objective optimization algorithm AMALGAM (Vrugt and Robinson, 2007) to derive the Pareto front and explore tradeoffs between water applications, irrigation system parameters, and crop transpiration, and to evaluate the best management practices for subsurface drip irrigation systems in alfalfa. Similarly, Roy et al. (2019) obtained the Pareto front by combining HYDRUS-2D with an evolutionary multi-objective optimization procedure to minimize water utilization and maximize crop yield prediction. Both studies prove that coupling HYDRUS with multi-objective search techniques can provide decision-makers with multiple tradeoffs for physically based irrigation strategies. However, more research is needed to demonstrate the benefits of this type of analysis and include the economic costs as an additional objective function, which would lead to a 3D Pareto surface.

Despite being a valuable tool, the multi-objective optimization of the irrigation system can be computationally intensive and requires specific programming and numerical skills that are not widespread among irrigation managers. Hence, a huge portion of the literature body has simplified the multi-objective optimization problem by focusing only on using HYDRUS to optimize a single objective function (e.g., water and nutrients use efficiency, root water uptake, etc.) (Akhtar et al., 2013; Brunetti
et al., 2018a; Fontanet et al., 2020, 2022; García Morillo et al., 2017; Karandish and Šimůnek, 2018; Lena et al., 2022; Müller et al., 2016; Ning et al., 2021; Qin et al., 2016; Seidel et al., 2015; Xu et al., 2019; Yi et al., 2022). The results of these studies are encouraging and show that the mechanistic framework provided by HYDRUS enables the modeler to obtain irrigation management strategies that are hydrologically functional, agriculturally efficient, and, more importantly, physically realistic. Nevertheless, the optimization procedure can still be improved by: (1) performing multi-objective optimization searches, in which the economic costs are included, as this is a crucial choice criterion in real applications, (2) propagating the effects of model uncertainty in the optimization procedure, as this would provide more honest predictions to decision-makers, and (3) taking into account dynamic changes in model structure (e.g., tillage effects on soil hydraulic properties) over medium-to-long term simulation periods.

11. Special irrigation methods

Over the last few years, the HYDRUS software has also been used to evaluate multiple traditional and/or experimental special irrigation methods. These applications include dual-drip irrigation (El-Nesr et al., 2014), pitcher irrigation (Siyal et al., 2009), irrigation using clay pipes (Siyal and Skaggs, 2009; Siyal et al., 2013), capillary wick irrigation (Al-Mayahi et al., 2020; Kamal et al., 2019), irrigation from ring-shaped emitters (Saefuddin et al., 2019; Noguchi et al., 2021), irrigation systems with a capillary barrier (Al-Mayahi et al., 2020; Ityel et al., 2011; Noguchi et al., 2021; Sao et al., 2021 and Wongkaew et al., 2018), vertical line source irrigation (Fan et al., 2018a,b, 2021a,b, 2022; Kanda et al., 2020a,b), film hole irrigation (Chen et al., 2020a; Fan et al., 2019a,b, 2021a; Hou et al., 2014; Jie et al., 2020), and many others (e.g., Fan et al., 2018c; Ji et al., 2015; Li et al., 2013; Pan et al., 2021; Wang et al., 2017a; Zemni et al., 2022; Zhou et al., 2017).

11.1 Dual-drip

El-Nesr et al. (2014) used HYDRUS (2D/3D) to evaluate three novel technologies enhancing a spatial distribution of water and solutes in the root zone while limiting downward leaching. These technologies included (a) a physical barrier under a dripper and a dual-drip system with (b) concurrent and (c) sequential irrigation. Numerical simulations showed that applying a
dual-drip system or installing a physical barrier could significantly alter the wetting pattern and spatial distribution of applied solutes. The simulations also showed that the physical barrier and the dual-drip systems are more suitable for coarse-textured soils than fine-textured soil. A dual-drip irrigation system with two emitters that can be operated sequentially allows controlling which solute is retained in the root zone and which one is leached by simply altering the operation of the two drippers.

11.2 Pitcher

Siyal et al. (2009) used HYDRUS-2D to evaluate the functioning of pitcher irrigation, an ancient but very efficient irrigation system used in many arid and semiarid regions, such as in Northern Africa, Iran, China, India, Pakistan, Brazil, Indonesia, and Zimbabwe (Fig. 22; see also references in Siyal et al., 2009). Siyal et al. (2009) investigated the water content distributions around small, medium, and large pitchers buried in fine- and coarse-textured soils and with different saturated hydraulic conductivities of the pitcher material. Water content distributions simulated by HYDRUS-2D were found to be in close agreement with the experimental results, indicating that HYDRUS-2D is a suitable tool for investigating and designing pitcher irrigation systems. Simulated and experimental results

![Fig. 22 Photographs illustrating pitcher irrigation and the axisymmetric finite element mesh diagram used by Siyal et al. (2009) to simulate water infiltration from a buried pitcher (Photo credits: Altaf Siyal).]
also showed that a large pitcher, double the size of a smaller one but with half the hydraulic conductivity, will produce approximately the same wetting front as the smaller pitcher. Fig. 23 illustrates the impact of the pitcher wall’s saturated hydraulic conductivity, for large pitchers, on simulated infiltration into an initially dry loam soil (the Pitcher example in Table A).

11.3 Clay pipe
HYDRUS (2D/3D) was used by Siyal and Skaggs (2009) and Siyal et al. (2013) to evaluate soil wetting patterns and solute transport under porous clay pipe subsurface irrigation, respectively. Subsurface irrigation using porous or perforated clay pipes, similar to pitcher irrigation discussed above, has been practiced since ancient times. It can still represent an efficient, water-saving irrigation method for many less developed countries in arid and semiarid regions. Siyal and Skaggs (2009) successfully compared experimental and simulated soil wetting patterns for subsurface pipe systems.
operating at different water pressures. They also simulated the irrigation system’s function in different soil textures (sand, sandy loam, loam, silt), as well as in layered soils (sandy loam over loam or loam over sandy loam). Siyal et al. (2013) expanded their study by additionally simulating salt accumulation near the soil surface from a subsurface clay pipe irrigation system during the growing season of okra. Their results showed that proper management of salt accumulation is vital for sustainable crop production whenever subsurface irrigation systems are being implemented.

11.4 Capillary wick

Capillary wick irrigation systems were analyzed using HYDRUS models by Kamal et al. (2019) and Al-Mayahi et al. (2020). Low-pressure wick irrigation systems represent energy-efficient systems that can play an important role in smallholder greenhouse crop production or home gardens by ensuring higher water use efficiency than most traditional approaches. Al-Mayahi et al. (2020) extended the analysis of the wick irrigation system by also considering a capillary barrier to prevent the leaching of irrigation water from the root zone.

11.5 Capillary barrier

The functioning of a capillary barrier under various irrigation systems has been studied using HYDRUS-1D and HYDRUS (2D/3D) by Ityel et al. (2011), Wongkaew et al. (2018), Al-Mayahi et al. (2020), Noguchi et al. (2021), and Sao et al. (2021). While Wongkaew et al. (2018) considered surface-applied irrigation (sprinkler), Al-Mayahi et al. (2020) considered capillary wick irrigation, Noguchi et al. (2021) considered subsurface drip irrigation (using ring-shape emitters), and Sao et al. (2021) considered uniform, line-source, and plant-targeted surface irrigation. All these studies showed that if properly designed, the capillary barrier can keep water in the root zone by preventing its leaching to deeper soil layers.

11.6 Ring-shaped emitters

Saefuddin et al. (2019) used HYDRUS (2D/3D) to evaluate the functioning of a subsurface drip irrigation system using a ring-shaped emitter. A ring-shaped emitter (made from a standard rubber hose) is a low-cost subsurface irrigation system developed and introduced for subsurface irrigation in Indonesia for small-scale farmers who have scarce water resources. The three-dimensional version of HYDRUS (2D/3D) was used to evaluate
the performance of the ring-shape emitter, including multiple alternative
designs with different numbers of holes (in the rubber hose) and changes
in the covering method. Numerical results were successfully compared
against experimental data collected during experiments with the original
ring-shaped emitter.

11.7 Other irrigation methods

11.7.1 Vertical line source irrigation

Fan et al. (2018a,b, 2021b, 2022) used the HYDRUS-2D software and
laboratory experiments to evaluate the performance of the vertical line
source (moistube) irrigation system. Vertical line source irrigation is a
water-saving method developed for deep-rooted fruit trees in the arid
regions of China to enhance direct water and nutrient delivery to the root
zone while reducing soil evaporation and improving water and nutrient use
efficiency. Fan et al. (2018a,b) performed multiple HYDRUS-2D simula-
tions to identify the main influencing factors (e.g., soil texture, initial water
content, pressure head, moistube length, and buried depth) for this irrigation
system on the soil wetting pattern.

11.7.1.1 Moistube Irrigation

HYDRUS (2D/3D) was used in a study by Kanda et al. (2020a,b) to eval-
uate the performance of moistube irrigation (MTI), a subsurface irrigation
technology that uses a semipermeable membrane to emit water continuously
into the soil in response to soil water potential and applied pressure. Kanda
et al. (2020a) evaluated how soil texture (loamy sand and sandy clay loam)
influences the soil water dynamics of MTI using laboratory experiments and
numerical simulations. Kanda et al. (2020a) evaluated how the moistube
placement depth influences the soil water dynamics and root water uptake
of cowpea. The goal was to determine the optimal depth of placement of
moistube tapes in cowpea production to minimize water losses via drainage
and soil evaporation and thereby improve water use efficiency.

11.7.2 Film hole irrigation

Film hole irrigation (FHI) was investigated using the radially symmetrical
option of the HYDRUS (2D/3D) software by Hou et al. (2014), Chen
et al. (2020a), Fan et al. (2019a,b, 2021a), Jie et al. (2020), and Pan et al.
(2021). This irrigation method is used mainly in the arid regions of
China, where plastic film mulch is widely used to prevent evaporation
and weeds growth. Water flows on the plastic film and infiltrates through
crop holes and special irrigation holes. Film hole irrigation is thus similar to point source irrigation. Compared to traditional surface irrigation methods, film hole irrigation significantly improves water use efficiency. According to Fan et al. (2021a), there are two types of film hole irrigation, i.e., film hole free infiltration (FHFI) and film hole interference infiltration (FHI), depending on whether the soil wetting fronts under the two neighboring film holes are independent or interfere with each other during FHI. In general, HYDRUS proved to be a robust and useful tool in evaluating this type of irrigation.

### 11.7.3 Additional irrigation methods

Many other irrigation techniques have been numerically evaluated using HYDRUS (2D/3D), mainly in the literature from China. For example, negative-pressure irrigation has been studied by Ji et al. (2015), Zhou et al. (2017), and Wang et al. (2017a), bubbled root irrigation by Li et al. (2013), buried diffuser irrigation (a special type of subsurface drip irrigation method) by Zemni et al. (2022), and horizontal moistube-irrigation by Fan et al. (2018c). HYDRUS (2D/3D) proved to be an ideal tool for evaluating the performance of these various irrigation techniques.

### 12. Summary and outlook

The use of HYDRUS is widespread today in many areas related to irrigation. In this work, we have reviewed the software’s capabilities and demonstrated them using numerous examples. The model is still being continuously developed, and new features that better describe processes in the irrigated root zone are being added. HYDRUS can help design irrigation systems and determine the optimal irrigation and fertilization regimes. Since the model can examine flow and transport processes in and under the root zone, it can also be used to examine the sustainability of various irrigation regimes. Correct use of the model may optimize applications of water and other agrochemicals, such as fertilizers and pesticides. Future agriculture will have to look closely at the transport of agrochemicals through the vadose zone and into groundwater.

Computational power advances every day, but simultaneously, there is a need to evaluate many processes using a very high spatial and temporal resolution. While using finer spatial and temporal discretizations may reduce numerical errors, the computational demand may, at the same time, increase dramatically. The number of discretization nodes usually increases by a
power of two when the problem’s dimensionality increases. While personal computers can perform complex simulations, the calculation duration may be too long, reducing our ability to estimate model parameters or optimize irrigation scheduling. Parallel calculation tools can take advantage of the existing capacity of computers with multiple cores or processors and significantly speed up time-consuming simulations, especially those requiring many finite elements. Examples of such tools are the HyPar module (Šimůnek et al., 2016b) or the ParSWMS model (Gohardoust et al., 2021; Hardelauf et al., 2007). Today it is also possible to perform calculations in the cloud, which can significantly speed up the simulations and allow HYDRUS users to carry out comprehensive stochastic simulations (e.g., Sasidharan et al., 2019).

Another alternative and promising approach is using emulators to perform computationally intensive tasks. An example of such an emulator can be found in Neuro-Drip (Hinnell et al., 2010). This study combines an artificial neural network with a statistical description of the spatio-temporal distribution of added water from a single drip emitter to provide easily accessible, rapid illustrations of the spatial and temporal subsurface wetting patterns. These cheap-to-run surrogate models can be trained to rapidly emulate the response of the mechanistic model to changes in a finite number of parameters, thus enabling the modeler to perform complex model calibration and irrigation optimization tasks on standard personal computers. However, the applicability of such surrogate tools is limited to a relatively low number of parameters (e.g., 10) as the training phase becomes computationally expensive in higher dimensions. Another possibility is to hybridize HYDRUS with machine learning methods to reduce the computational cost of expensive parts of the code (e.g., reaction). Surrogate and hybrid modeling for physically based irrigation analysis is certainly a topic worthy of future investigation.

The HYDRUS ability to simulate crop growth is still relatively limited. The standard HYDRUS modules account for crop growth only externally by inputting potential evaporation and transpiration fluxes (or the leaf area index in 1D to separate potential evapotranspiration into potential evaporation and transpiration). HYDRUS also allows users to externally prescribe a time-variable rooting depth (and width) using the logistic growth function or in a tabulated form. The HYDRUS models do not allow the rooting zone’s spatial extent to change actively due to certain environmental conditions and stresses (e.g., Hartmann et al., 2018). While there have been attempts to provide HYDRUS the ability to simulate crop growth
None of these implementations is currently available in the HYDRUS software, and only the models of Hartmann et al. (2017) are directly available from the HYDRUS website as non-standard HYDRUS modules (i.e., not fully supported by the HYDRUS GUI). Alternative approaches (e.g., Couvreur et al., 2012, de Jong van Lier et al., 2009, 2013) to the macroscopic model of Feddes et al. (1978) to account for various root water uptake stresses would also be a desirable new feature of the HYDRUS models.

The environmental conditions of the irrigated root zone can change rapidly due to irrigation and soil drying. Soil water contents, temperatures, and salt concentrations and their composition can affect soil hydraulic and solute transport (e.g., degradation) parameters. Since the model dynamically and spatially calculates the environmental variables, it can simultaneously update model parameters that depend on them. Some of these connections are already implemented in HYDRUS, such as the dependence of the hydraulic conductivity on the chemical composition of the soil solution (e.g., sodium adsorption ratio, SAR, and electric conductivity, EC) (Suarez and Šimůnek, 1997), the dependence of soil hydraulic properties (via viscosity and surface tension) on solution concentrations (e.g., Silva et al., 2020), or the dependence of solute reaction parameters (i.e., degradation) on changes in water contents and temperatures. More complex interactions between the environmental variables and model parameters can be considered using the HP1 model (e.g., Jacques et al., 2008a,b). Introducing additional relationships between environmental factors and model parameters (e.g., clogging, i.e., a reduction of the hydraulic conductivity as a function of cumulative infiltration of water and/or solute/bacteria) would further increase the applicability of the HYDRUS models.

Stable water isotopes are increasingly used as environmental tracers to investigate flow processes in the unsaturated zone in both bare and planted soils (e.g., Stumpp et al., 2012), to quantify water and nutrient travel times, and to identify water sources for root water uptake and the age of these sources (e.g., Zhou et al., 2021, 2022). Only the 1D computational version of the HYDRUS model can currently simulate the fate and transport of stable water isotopes subject to no (Stumpp et al., 2012) or constant fractionation during evaporation. This contrasts with the standard formulation of solute transport in HYDRUS during evaporation, where solutes concentrate at and near the soil surface when water evaporates. However, ignoring the evaporative enrichment, as done in this 1D model, leads to
underestimating $^2$H and $^{18}$O concentrations in the topsoil, which may be more significant in regions with higher evaporative losses (Sprenger et al., 2018). This evaporative enrichment, as well as its dependence on environmental factors (e.g., temperature and tension), has been recently implemented into the computational module of HYDRUS-1D by Zhou et al. (2021, 2022), but it has not yet been included in the HYDRUS GUI or its higher dimensional modules. The ability to simulate the fate of environmental tracers (and related issues, such as travel times and water age) would be another desirable feature of future HYDRUS releases.

Modern agriculture often uses various types of mulching to reduce evaporative losses and prevent weed growth. While traditional mulching has been done using plastic films (e.g., Li et al., 2015b, 2018b), more environmentally friendly alternatives, such as biodegradable (e.g., Chen et al., 2019, Chen et al., 2020b,c) or sprayable (e.g., Filipović et al., 2020) mulches, are being intensively investigated. While HYDRUS has been used in many of these applications, its ability to fully describe dynamic boundary conditions associated with the application of biodegradable and sprayable mulches and their temporarily changing properties is still rather limited, and further developments are needed.

While considerable efforts have gone into developing the HYDRUS models to account for irrigation practices, we also understand that model development, calibration, and validation are never-ending processes. Today, the model can consider various physical, chemical, and biological processes and their interrelationships. While the model development for irrigation practices is progressing considerably, the progress in sensing the agricultural field is limited. Although there are many point sensors that describe the state of water (water content or potential) in the field in a temporal manner, the spatial variation in the soil-plant system still limits their use in model calibration. Undoubtedly, the development of non-intrusive methods can improve the spatial description of the water status in the soil. Even today, there are only a very few methods that can continuously quantify the chemical composition of soil water, and thus, the model calibration is done with the help of a general but continuous measure of the bulk electrical conductivity or tests that usually require human intervention (soil sampling, suction cups). Regarding biological tests, the situation is even more complex, and today, very few methods can evaluate the root system structure and functions under field conditions.
## Appendix

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h1d—HYDRUS-1D, version 4.x; h3d3—HYDRUS (2D/3D), version 3.x; hyd5—HYDRUS, version 5.x.
References


