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HYDRUS Software Applications to Subsurface Flow and Contaminant Transport Problems

March 21-22 2013

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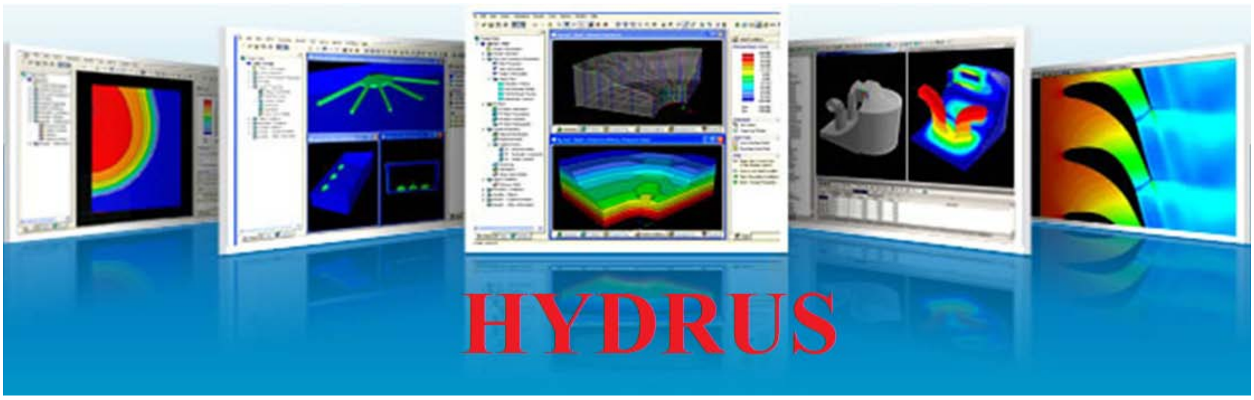

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Preliminary Program

Thursday, March 21, Morning session:
Variably-Saturated Water Flow and Transport of Contaminants

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9:30-9:45	Kalin, J., B Petkovšek, P. Montarnal, A. Genty, E. Deville , and J. Krivic, Comparison of two numerical modeling codes for hydraulic and transport calculations in the near field. (Slovenia and France)
9:45-10:00	Pontedeiro, E. M., V. O. Almeida de Sousa, and M. Th. van Genuchten, HYDRUS-1D modeling applications to waste disposal problems in Brazil. (Brazil)
10:00-10:15	Xiao, H., J. Böttcher, and J. Šimůnek, Simulation of heavy metal transport in unsaturated soil: Use of scale factors to quantify variable sorption isotherms. (Germany)
10:15-10:30	Schwen, A., G. Bodner, and W. Loiskandl, Temporal variations of soil hydraulic properties and its effect on soil water simulations. (Austria)
	Coffee Break
11:00-11:15	Grinevskiy, S. O., and S. P. Pozdniakov, The use of HYDRUS-1D for groundwater recharge estimation in boreal environments. (Russia)
11:15-11:30	Kanzari, S., M. Hachicha, R. Bouhlila, and J. Battle-Sales, Characterization and modeling of water movement and salts transfer in a semi-arid region of Tunisia. (Tunisia)
11:30-11:45	Kurinova, N., Sensitivity of recharge evaluation results using HYDRUS to parameters and boundary conditions variations. (Russia)
11:45-12:00	Filipović, V., R. Kodešová, and D. Petošić, Numerical modeling of water flow and nitrate dynamics on zero tension plate lysimeters using HYDRUS-2D. (Croatia)
12:00-12:15	Pozdniakov, S., P. Wang, S. Grinevskiy, and J. Yu, Simulation of groundwater evapotranspiration with HYDRUS-1D in desert environments. (Russia)
12:15-12:30	Elmi, A., Phosphorus leaching potentials from re-constructed soil columns using HYDRUS-1D model. (Kuwait)
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Thursday, March 21, Afternoon Session: Inverse Problems, Nonequilibrium Flow

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2:30-2:45	Diamantopoulos, E., and W. Durner, Dynamic non-equilibrium water flow in variably saturated porous media. (Germany)
2:45-3:00	Kébré, M. B., F. Ouédraogo, F. Cherblanc, and F. Zougmoré, Transfer at low water content: new and simple experimental approach for inverse determination of van Genuchten transport coefficients. (France, Burkina Faso)
3:00-3:15	Léger, E., A. Saintenoy, and Y. Coquet, Inverting saturated hydraulic conductivity from surface ground-penetrating radar monitoring of infiltration. (France)
3:15-3:30	Glæsner, N., and H. H. Gerke, Single- and double-porosity modeling of solute transport in intact soil columns – effects of texture, slurry placement, and intermittent irrigation. (Denmark, Germany)
3:30-3:45	Turkeltaub, T., O. Dahan, and D. Kurtzman, Investigation of recharge fluxes under different land-uses with calibrated models to transient deep vadose zone data. (Israel)
3:45-4:00	Anlauf, R., and P. Rehrmann, Simulation of water and air distribution in growing media. (Germany)
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9:30-9:45	Morvannou, A., N. Forquet, M. Vanclooster, and P. Molle, Which Hydraulic Model to Use in Vertical Flow Constructed Wetlands? (France)
9:45-10:00	Karlsson, S. C., H. Jönsson, S. Dalahmeh, and C. Lalander, Hydraulic properties and reduction of COD, phosphorus and nitrogen in sand filters used for greywater treatment – simulation and verification. (Sweden)
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11:45-12:00	Leterme, B., and D. Jacques, Hg modelling in soil systems using HP1. (Belgium)
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12:15-12:30	Sandhu, C., T. Fichtner, I. Hasan, and P.-W. Graeber, Predicting the impact of treated wastewater on groundwater recharge by simulating reactive transport in the unsaturated zone. (Germany)
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2:30-2:45	Dabach, S., J. Šimůnek, A. Ben-Gal, J. Shi, and N. Lazarovitch, Optimization of triggered irrigation using a system dependent boundary condition in HYDRUS 2D/3D. (Israel)
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3:15-3:30	Ramos, T. B., J. Šimůnek, M. C. Gonçalves, J. C. Martins, A. Prazeres, and L. S. Pereira, Modeling water and nitrogen fate in plots with sweet sorghum irrigated with fresh and blended saline waters using HYDRUS-2D. (Portugal)
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4:00-4:15	Arye, G., and J. Šimůnek, Modeling surface-active solute transport with HYDRUS. (Israel)
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4:45-5:00	Yurtseven, E., J. Šimůnek, S. Avci, and H. S. Öztürk, Comparison of ion(salt) movement in the soil profile subject to leaching with the HYDRUS-1D simulations. (Turkey)
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List of Abstracts

Invited Keynote Presentations:

Volunteered Abstracts:

Please reference the abstracts as follows (adjust highlighted text as needed):
Authors, Title, *The 4th International Conference "HYDRUS Software Applications to Subsurface Flow and Contaminant Transport Problems"*, Book of Abstracts edited by J. Šimůnek and R. Kodešová, March 21-22, 2013, Dept. of Soil Science and Geology, Czech University of Life Sciences, Prague, Czech Republic, ISBN: 978-80-213-2368-1, pp. ??, 2013.

Some General Thoughts about Modeling Flow and Transport Processes in Soils and Groundwater

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Numerical models have become indispensable tools in both research and engineering to obtain a better understanding and prediction of subsurface water flow and solute transport processes. The HYDRUS codes in particular have seen many applications as evidence by the broad range of topics being discussed at this conference. The increased use of HYDRUS and related models is spurred by the introduction of increasingly powerful computers, advanced numerical methods, improved descriptions of the basic flow and transport processes involved, and simultaneous progress in the development of improved technologies for estimating much-needed model parameters. These advancements cannot be fast enough in view of the tremendous environmental challenges facing this planet, including water, food and energy security issues. At the same time it is important also for us to appreciate the limitations of even the most advanced numerical models. For example, we continue to struggle with such very basic issues as how best to capture observed flow and transport processes in usable equations for modeling purposes, how to characterize subsurface heterogeneity (including preferential flow) at a range of scales, and how best to integrate all pertinent physical and biogeochemical information into predictive tools for management and engineering applications. The main message of this introductory presentation is to keep pressing further development and testing of our simulation and measurement technologies. This must include further improvements in the conceptual basis of our models, and developing better methods to integrate or fuse modeling expertise and hard and soft data into practical protocols to more effectively address our environmental problems. Some of the opportunities and challenges are illustrated by three different HYDRUS applications: (1) estimating subsurface radionuclide transport from a uranium mining site, (2) phytoremediation processes, and (3) the subsurface transport of selected radionuclides in phosphogypsum when applied as an amendment in agricultural operations.

New Features and Developments in HYDRUS Software Packages

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The capabilities of the HYDRUS (2D/3D) software package have been substantially expanded by new modules accounting for processes not available in the standard HYDRUS version. These new modules include the **DualPerm**, **C-Ride**, **HP2**, **Wetland**, and **UnsatChem**. All these modules simulate flow and transport processes in two-dimensional transport domains and are fully supported by the HYDRUS graphical user interface. Additionally, the **DualPerm** module implements the dual-permeability modeling approach of Gerke and van Genuchten (1993) simulating preferential flow and transport. The **C- Ride** module implements colloid transport and colloid-facilitated solute transport (Šimůnek et al., 2006), the latter often observed for many contaminants, such as heavy metals, radionuclides, pharmaceuticals, pesticides, and explosives. **HP2** is a two-dimensional alternative of the HP1 module (Jacques and Šimůnek, 2005), currently available with HYDRUS-1D, that couples HYDRUS flow and transport routines with the PHREEQC geochemical model of Parkhurst and Appelo (1999). The **Wetland** module includes two alternative approaches (CW2D of Langergraber and Šimůnek (2005) and CWM1 of Langergraber et al. (2009)) for modeling aerobic, anaerobic, and anoxic biogeochemical processes in natural and constructed wetlands. Finally, the **UnsatChem** module simulates the transport and reactions of major ions in a soil profile. A brief description and several demonstrative applications of each module will be presented. Many processes included into these specialized modules of HYDRUS (2D/3D) are currently also available as part of HYDRUS-1D. Further development of these modules, as well as of several other new modules (such as Overland Flow, Slope Stability, and Meteo), is still envisioned. Continued feedback from the research community is encouraged.

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Reactive Transport Modeling of Subsurface Flow Constructed Wetlands using the HYDRUS Wetland Module

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Constructed wetlands (CWs) are engineered water treatment systems designed to remove various types of contaminants. A large number of processes simultaneously contribute to water quality improvement in CWs. During the last decade, there has been a wide interest in the understanding of complex "constructed wetland" systems, including the development of numerical process-based models describing these systems. A number of process-based numerical models for subsurface flow (SSF) CWs have been developed during the last few years. However, most of them are either in a rather early stage of development or are available only in-house. The HYDRUS wetland module is the only implementation of a CW model that is currently publicly available. Version 2 of the HYDRUS wetland module includes two biokinetic model formulations simulating reactive transport in CWs: CW2D and CWM1. In CW2D, aerobic and anoxic transformation and degradation processes for organic matter, nitrogen and phosphorus are considered, whereas in CWM1, aerobic, anoxic and anaerobic processes for organic matter, nitrogen and sulphur are taken into account. In this paper, we describe the HYDRUS wetland module, as well as its two biokinetic models. We further present simulation results for horizontal flow CWs obtained using both biokinetic models. Compared with the CWM1 implementation in the RETRASO code, the HYDRUS implementation is able to simulate fixed biomass, which is of high importance for obtaining realistic predictions of the treatment efficiency of CWs. We also compare simulation results for horizontal flow CWs obtained using both CW2D and CWM1 modules that show that CWM1 produces more reasonable results since it also considers anaerobic degradation processes. The influence of wetland plants on the simulation results is also demonstrated. Simulated biomass profiles in the filter are completely different when considering oxygen release from roots, thus indicating the importance of considering plant effects.

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The HPx Reactive Transport Models: A short Overview of Development and Possibilities

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The HPx reactive transport codes are developed to consider coupled flow and transport processes in variable-saturated porous media with a variety of low-temperature geochemical processes. They consist of the HYDRUS models for water flow and solute transport (HYDRUS-1D, version 4.16 and HYDRUS (2D/3D), version 2.02) with the generic thermodynamic and kinetic model PHREEQC-2.17. As such, HPx, now available for one- (HP1) and two-dimensional (HP2) flow and transport problems, expand significantly the capabilities of the individual codes.

Recent developments and applications are:

- Gas diffusion. One important application of this process is CO_2 sequestration in soils. HPx gives a large flexibility in defining different kinetic networks with rate coefficients depending on temperature, water content, or any other variable. Such implementation is illustrated using parts of the model of Porporato et al. (2003).
- Extension to two-dimensional flow problems.
- Inverse optimization of geochemical parameters. An example is given, in which soil hydraulic, solute transport, and cation exchange parameters are optimized using data from water and solute absorption experiments (Jacques et al., 2012).
- Feedback between changes in geochemical variables and transport properties. As an example, leaching of a cementitious material and the progression of pH and porosity fronts is discussed.
- Benchmarking of several of these new developments with other reactive transport codes.

HPx is a flexible tool which can handle complex flow and transport problems combined with rather complex geochemistry models. A typical example is geochemistry of mercury, which is present in a (contaminated) soil in different forms and phases.

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Selected Applications of HYDRUS Models to Evaluate Uniform and Nonequilibrium Flow in Structured Soils.

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Water flow and contaminant transport in structured soils are frequently influenced either by water and solute temporal immobilization inside soil structure elements (e.g. concept of mobile and immobile water) or by bypassing the soil matrix due to enhanced water flow and contaminant transport in macropores (e.g. preferential flow). Such nonequilibrium flow may occur and can be visualized at macro- and microscales using a dye tracer (Kodešová et al., 2012). Both phenomena may be simulated using either the dual-porosity or dual-permeability models implemented in HYDRUS programs, which assume two continuums (domains) within a simulated flow region. Using these models require assessing fractions and hydraulic properties of both domains and characteristics describing mass exchange between these domains. Equilibrium and nonequilibrium water flow and herbicide transport within the soil profile (3 different soil types) under field conditions and in the undisturbed soil samples (taken from all diagnostic horizons of 3 soil types) under laboratory conditions was simulated using single-porosity model and both dual domains modules in HYDRUS-1D (Kodešová et al., 2008, 2009). Fractions of domains were in these studies evaluated using micromorphological images. Other properties were partly measured and partly optimized using the program. Great impact of parameters describing mass exchange between matrix and macropore domains on preferential flow character was documented using the radially symmetric dual-permeability model in HYDRUS 2D/3D (Kodešová et al., 2010). Interaction between domains is frequentaly influenced by clay and organic matter coatings, which slowdown water and solute transport between domains (Kodešová et al., 2012; Fér and Kodešová, 2012), and enhance preferential flow in structural soils (Kodešová et al., 2010).

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Investigating the impact of irrigation method on profitability of smallholder gardening: Incorporating HYDRUS-1D into a Decision Support System

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Dry-season irrigation in remote areas of tropical developing regions provides many households with both nutritional and monetary supplements. Often, smallholders depend on traditional (unimproved) water sources for meeting their irrigation needs, which are highly seasonal and many times unreliable throughout the length of the season: dams, natural ponds in ephemeral streams, or hand-dug shallow wells. Optimizing profits from these small-scale gardens is complicated by the unpredictability of water amounts available through the season as well as the time, labor and capital constraints common to subsistence livelihoods. Millions of smallholder farmers face these challenges daily.

The HYDRUS-1D numerical model was incorporated into a Decision Support System (DSS) for investigating these dynamics of smallholder irrigation. In this case, revenue from field-grown tomato was modeled. Transpiration levels for a range of irrigation rates and water salinity levels were obtained using the HYDRUS-1D code. These transpiration results were then translated into actual crop yields according to the yield-transpiration relationship for field-grown tomato. In addition, various measures of time availability in the garden were input into the DSS, in order to introduce labor constraints into the decision process. For each irrigation and salinity level, total agricultural costs, comprised of capital and operation costs, were output alongside yields and benefits. This was done for both hand watering and drip irrigation in order to provide a comparative measure of the two irrigation approaches in relation to smallholder economies.

Results of this investigation suggest that, due to the tradeoff between capital costs and time-savings, drip irrigation does not always result in optimal net revenue as compared to hand-watering. We identified a linear relationship between the rate of revenue earned and the ratio between water and time availability for both irrigation methods. While these relationships are nearly identical, they reach a unique threshold value after which water becomes a limiting factor. The value of this threshold is lower for hand watering because the amount of water applied per unit of time working is less, thus labor becomes a limiting constraint at lower water supply levels. Drip irrigation allows labor to earn higher revenue at sufficient water supplies. Thus, it should be promoted where labor is relatively limiting.

Simulation of Water and Air Distribution in Growing Media

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Water and particularly air content in growing media in plant containers is important information for the grower. To optimize crop growth, the relative importance of substrate type and irrigation strategy on water uptake of growing media must be known. Describing water uptake and distribution in the container with a dynamic simulation model may overcome the disadvantages of static parameters such as container capacity and air capacity.

Water uptake and redistribution was investigated for an ebb-and-flow irrigation system with two different growing media, a coarse white peat and a fine seedling substrate, two flooding depths (1 and 4 cm) and three flooding durations (5, 10 and 15 min).

The results were used to evaluate the use of HYDRUS-1D to describe water uptake and redistribution. The hydraulic functions water retention curve and hydraulic conductivity needed for the simulation model were determined in the laboratory.

Hysteresis becomes especially important in irrigation systems where the water is applied from the bottom of the container, such as ebb-and-flow irrigation. Preliminary simulations with HYDRUS-1D made clear that hysteresis of the water retention curve must be taken into account for growing media to get reliable simulation results. Water retention drying curves were determined by standard sand box apparatus. Wetting curves were determined with equipment where the water content in growing media was measured in an experimental container with a constant flooding depth. Under the assumption that the water content at equilibrium is analogous to the water retention curve, the water content of the growing media above the water surface will correspond to distinct pF values. Drying and wetting curve were parameterized to be used in HYDRUS-1D.

The simulation was divided into a flooding cycle with a constant head lower boundary condition and a drainage cycle with a seepage phase boundary condition. The simulated water content at the end of the flooding cycle was used as initial condition for the drainage cycle.

The results show that substrate properties and flooding height are the main parameters determining water uptake during ebb-and-flow irrigation while flooding time has a minor effect only.

HYDRUS-1D is able to describe water uptake and redistribution in containers filled with growing media sufficiently well, but only if the hysteresis of the water retention curve is taken into account. This correct representation of the water balance in plant containers is an important basis for future work on oxygen concentration changes in growing media.

Application of the HYDRUS (2D/3D) Inverse Solution Module for Evaluation of the Soil Hydraulic Parameters of a Quaternary Complex in Northern Bulgaria

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The characterization and numerical modeling of the unsaturated zone is among the key factors in the prognostic fate and transport studies of the contaminants migration in the environment. The paper deals with the use of the HYDRUS (2D/3D) (Šimůnek et al., 2006) code for determination of hydraulic parameters of the 10-m deep vadose zone from borehole infiltration tests by inverse modeling. The investigated soil profile is located in the Pleistocene loess complex near the town of Kozloduy, Northern Bulgaria, in the vicinity of the Kozloduy Nuclear Power Plant (NPP).

Four constant-head infiltrometer tests were carried out at several meters below the ground surface to determine the unsaturated hydraulic properties of particular layers, namely silty loess, clayey loess, clayey gravel, and a highly carbonated zone. Infiltration tests provided data on cumulative infiltration and the movement of the wetting front in the initially unsaturated sediments surrounding the infiltrometer. A cylindrical time-domain reflectometry TRIME-IPH/T3 probe, operated by the TRIME-HD device, was used to measure water content variations with time during the movement of the wetting front. Special polycarbonate access tubes for the TRIME probe were installed at a distance of 0.3 to 0.5 m from the infiltrometers. An axisymmetric model was developed in HYDRUS (2D/3D) for each of the four infiltrometers. The vertical dimension of the model was limited to the soil layers that were immediately influenced by the infiltrating water. By means of an inverse optimization routine implemented in the finite element code HYDRUS (2D/3D), field-scale soil hydraulic parameters θ_r, θ_s, α, n, and K_s were derived for all layers of interest.

Apparently, the size of the affected volume of soil was large enough to reduce the effect of spatial variability and to produce average field-scale hydraulic parameters that are relevant for large-scale predictions of flow patterns and radionuclide migration pathways in the region of Kozloduy NPP.

Keywords: unsaturated zone, soil hydraulic parameters, field experiment, HYDRUS (2D/3D)

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Modeling Surface-Active Solute Transport with HYDRUS

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Surface active solutes (SAS) or surfactants are organic compounds that contain both hydrophilic and hydrophobic groups. When water is the solvent, the polar or ionic functional group imparts favorable solubility properties, whereas the nonpolar hydrophobic part distorts the solvent structure and promotes orientation at the interface. The result of this process is the reduction of surface tension at the water-air interface (γ_{LV}). Assuming that soil pores consist of bundles of capillary tubes of different sizes, the effect of γ_{LV} on the capillary pressure (Ψ) can be inferred from the *Laplace equation*. Accordantly, for a given unsaturated water content (θ) and contact angle (ε), a reduction in γ_{LV} will be associated with a similar relative reduction in Ψ. In a similar manner, for a given θ and γ_{LV}, Ψ is linearly proportional to cos(ε). Consequently, the capillary pressure saturation relationships, $\Psi(\Theta)$, can be significantly affected by these quantities.

Following the above concept, the overall working scheme of our modeling effort is:

$$\gamma_{LV}(C) \Rightarrow \varepsilon(\gamma_{LV}, \theta) \Rightarrow \Psi(C, \theta, \gamma_{LV}, \varepsilon) \Rightarrow \Psi\text{-gradient} \Rightarrow \text{unsaturated water flow}$$

$\boldsymbol{\gamma_{LV}(C)}$ represents the concentration (C) dependence of γ_{LV} during solute transport, namely, variations of γ_{LV} in time and space as a function of the SAS transport characteristics. In general, γ_{LV} is inversely related to C down to a point where no additional reduction in γ_{LV} occurs due to aggregation and/or precipitation of the SAS. A reduction in the dissolved SAS concentration can occur due to adsorption to the solid phase. As a result, the surface properties of the solid phase may change and, thus, may be expressed in a variation of ε.

$\boldsymbol{\varepsilon(\gamma_{LV},\theta)}$ emphasizes the dependency of ε on both γ_{LV} and θ. Specifically, for a given soil property, an increase in θ and/or the reduction in γ_{LV} reduces ε to a point where $\varepsilon = 0$.

$\boldsymbol{\Psi(C,\theta, \gamma LV, \varepsilon)}$ indicates that the reciprocal relations between all four quantities can be expressed by the value of Ψ. The ***Ψ-gradient*** – a driving force for unsaturated water flow in the porous media – is the result of the temporal and spatial variations in $\boldsymbol{\Psi(C, \theta, \gamma_{LV}, \varepsilon)}$.

To enable modeling of this complex system of processes, empirical and/or physically-based equations of $\Psi(\theta, \gamma_{LV}, \varepsilon, C)$ and $K(\theta, \eta$ (viscosity), $C)$ were incorporated into the HYDRUS-1D code (Šimůnek et al., 2008) for modeling transient water flow and solute transport in variably-saturated soils. In the current presentation, a sensitivity analysis probing the effects of the above quantities and their reciprocal relations on unsaturated water flow will be demonstrated.

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The Root System as a Hydraulic Architecture: Principles and Applications

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Many hydrological models including the process of root water uptake (RWU) do not consider the dimension of root system hydraulic architecture (HA) because explicitly solving water flow in such a complex system is too time consuming. However, they might lack process understanding when basing RWU and plant water stress predictions on functions of variables such as the root length density distribution.

On the basis of analytical solutions of water flow equations in a HA, we developed and validated a macroscopic model for both RWU distribution and plant water stress, which respects physical principles of water flow in root systems of any complexity. Rather than thousands of local parameters defined at the root segment scale, the new model has three macroscopic parameters defined at the plant scale: (i) the standard sink fraction distribution SSF, (ii) the root system equivalent conductance K_{rs} and (iii) the compensatory RWU conductance K_{comp}. It is simple, computationally light, clearly decouples the process of water stress from compensatory RWU, and its structure is appropriate for hydraulic lift simulation.

In a further study, the model was coupled to Richards' equation in the Windows-based computer software package HYDRUS-3D. A sensitivity analysis of soil water dynamics to RWU parameters was performed, and the feasibility of model inverse parameterization from synthetic soil water dynamics data, on different soil types, was questioned.

Using HYDRUS-HP1 to Estimate ^{226}Ra Transport in Soils Following the Use of Phosphogypsum in Agriculture

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Agricultural soils often require the use of fertilizers and soil conditioners to optimize production. In this study we provide an analysis of the subsurface transport of radionuclides released from phosphogypsum (PG) when used as a fertilizer or amendment in agriculture. PG (dihydrated calcium sulfate), a residue of the phosphate fertilizer industry, can contain relatively high amounts of impurities from the host rock, including heavy metals and radionuclides such as ^{238}U and especially ^{226}Ra. It is important to assess the environmental risks caused by the long-term use of PG in agriculture. During the phosphate production process, the naturally present radionuclides tend migrate to both the fertilizer (especially ^{238}U and ^{234}U) and phosphogypsum (^{226}Ra and ^{210}Pb).

Our study focused on the transport of ^{226}Ra when PG is applied annually to a typical soil profile in the Brazilian Cerrado. Expected water flow and solute transport processes were estimated first using the HYDRUS-1D software package assuming linear equilibrium transport, followed by similar simulations using the HP1 multicomponent transport module of HYDRUS-1D. Analyses with HP1 considered a range of geochemical and physical parameters affecting ^{226}Ra transport in the vadose zone. We studied especially the effects of varying calcium concentrations on ^{226}Ra transport, showing that this variable is relatively important when making predictions. Several aspects related to the modeling approach, such as the use of daily versus monthly weather data and the influence of assuming different transport regimes in the vadose zone (e.g., transient versus long-term steady-state flow) are discussed also.

Optimization of Triggered Irrigation Using a System-Dependent Boundary Condition in HYDRUS (2D/3D)

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Water productivity and efficiency of irrigation systems can be improved by optimizing water application regimes. One way to do this is to automate irrigation such that application amounts and timing are a direct response to changes in soil water pressure head. Managers are challenged, when using in such systems, to correctly choose the sensor location and pressure head threshold values, especially in light of the spatial heterogeneity of soil-plant systems. Little work has been done to investigate the relationship between irrigation scheduling, soil water potential threshold values, water salinity, and an irrigation application volume, and their dependence on the sensor location and soil heterogeneity.

We propose that numerical modeling can be applied to quickly and accurately optimize the operational parameters required in automated feed-back irrigation scheduling. A system-dependent boundary condition, which initiates irrigation whenever the matric head at a predetermined location drops below a certain threshold, was implemented in the HYDRUS 2D/3D code. The model was used to evaluate experimental data and subsequently optimize the operational parameters.

Three field experiments were conducted to evaluate the effects of different potential transpiration rates, irrigation water salinity and irrigation management strategies on a triggered irrigation system. In all experiments, irrigation was controlled by a closed loop irrigation system linked to tensiometers. The results showed that HYDRUS 2D/3D predictions of irrigation events, matric heads and soil salinity were in good agreement with experimental data, and that the code could be used to optimize irrigation thresholds and water amounts applied, as a function of water salinity, to increase water productivity and maximize yield.

Results of HYDRUS 2D/3D simulations also indicate that the location of the sensor relative to the water source has a crucial effect on irrigation efficiency. Sensors that control the irrigation system should be placed very close to the water source to avoid the effect of heterogeneity of soil properties on water flow dynamics. The further away the sensor, the higher variability in the irrigation system operation. As plants grow and transpiration increases, the irrigation threshold needs to be adjusted in order to supply the increased water uptake. Increasing the water volume in each irrigation pulse might not be a good solution, since more water is wasted, especially in sandy soils. Irrigation duration should be based on water volume or time rather than measurements of pressure head since variability in measurements increases during irrigation. When irrigating with saline water, decreases in plant uptake result in higher matric head, hence fewer irrigations, which in turn may cause even higher salinity. Therefore, irrigation with saline water cannot be based on tensiometers alone but has to be complemented by soil salinity monitoring.

Dynamic Non-Equilibrium Water Flow in Variably Saturated Porous Media

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During the last 50 years, experimental observations have shown that the soil hydraulic properties estimated under static and dynamic methods can differ substantially. These observations are often described by the term "dynamic non-equilibrium" or "dynamic effects", and they occur under different experimental boundary conditions. For a given pressure head boundary condition non-equilibrium effects appear as a relaxation in the cumulative outflow data while the pressure head remains constant inside the soil column. For a given flux applied boundary condition, non-equilibrium effects appear as a relaxation of the pressure head over time, while the macroscopic water content distribution appears static. These effects are often attributed to various processes such as: air-water-interface reconfiguration, pore-water blockage, air entrapment, dynamic contact angles, among others.

We developed a simple non-equilibrium model to quantitatively describe these observations. The model considers two continua at the macroscopic scale: one continuum is described by the Richards equation and the second, associated with non-equilibrium water flow, by an extended Richards equation using the Ross and Smettem non-equilibrium approach. The new model was implemented by extending the Hydrus-1D code. This model can describe the dynamic effects occurring in transient flow experiments very well.

Dual-Drip Subsurface Irrigation System: Can it Act as a Hydraulic Barrier?

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Subsurface drip irrigation systems, compared to other irrigation systems, enhance delivery of water and chemicals directly into the root zone. However, in light-textured soils, certain quantities of water may percolate below the root zone due to the subsurface position of drip lines. The main objective of this paper is to evaluate three technologies to enhance a spatial distribution of water and solutes in the root zone and to limit downward leaching. The three technologies include a) a physical barrier, b) a dual-drip system with concurrent irrigation, and c) a dual-drip system with sequential irrigation. To achieve this objective, we performed computer simulations and field experiments. Numerical simulations were carried out using the HYDRUS (2D/3D) software for both bare and cultivated soils. The results indicate that the physical barrier is more efficient than dual-drip systems in enhancing the water distribution in the root zone while preventing downward leaching. On the other hand, the dual-drip system with sequential irrigation, followed by the dual-drip system with concurrent irrigation, is the most efficient in limiting downward leaching of solutes. The results of the study suggest that the system that combines the physical barrier with the hydraulic barrier due to sequential irrigation by a dual-drip system provides the largest benefits in terms of enhancing the spatial distribution of both water and solutes in the root zone and preventing their downward leaching.

Keywords: Drip Irrigation, HYDRUS (2D/3D), Leaching, Root Zone

Phosphorus Leaching Potentials from Re-constructed Soil Columns Using HYDRUS-1D Model

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Modern agricultural production uses phosphorus (P) extensively to meet the challenges of feeding rapidly growing population and changing lifestyles, making P a leading source of impairment for rivers and streams in Canada. Developing effective management strategies to reduce P losses from agro-ecosystems requires improved understanding of P transport pathways in the soil. The purpose of our study was to investigate vertical distribution and transport processes of phosphate (PO_4) in reconstructed soil columns using HYDRUS-1D model. Results obtained from field experiments were used to calibrate and validate the HYDRUS-1D model. The results showed that 98% of the total P applied was concentrated in the top 0.2 m of the columns, and decreased progressively with soil depth. The model over-predicted PO_4 adsorption, leading to a weak correspondence between the simulated and the measured results for PO_4. This is a suggestion that the HYDRUS-1D model could not account accurately for the different soil structures found in the undisturbed soil columns and the preferential flow that occurs in these columns. This may be due to the fact that Freundlich isotherm, which is part of the transport equations, could not adequately describe PO_4 adsorption onto the soil particles.

Using HYDRUS-1D for Estimating Hydraulic Conductivities of the Soil Aggregates and their Clay-Organic Coatings from Capillary Rise Data

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Soil aggregates are in some soils and their horizons covered by organomineral coatings, which may significantly influence water and solute transfer into the aggregates. Knowledge of a coating occurrence, their structure and hydraulic properties is required for a more precise description of water flow and contaminant transport in soils using dual-permeability models. The aim of this study was to describe hydraulic properties of clay and organic matter coatings in the iluvial (Bt2) horizon of Haplic Luvisol. Sets of 30 unsorted aggregates, 24 aggregates with mostly clay coatings and 24 aggregates with clay-organic coatings, respectively, were studied to evaluate an impact of various coating composition. The coatings were removed from a half of the aggregates of each set. First, the wetting soil-water retention curve was measured on all soil aggregates. Parameters of the soil-water retention curves were obtained using the RETC program. Then the capillary rise from the saturation pan into the multiple aggregates (set of 14 or 15 aggregates) at boundary pressure heads of -5 and -1 without and with coatings was measured. The saturated hydraulic conductivities of the aggregates, $K_{s,aggr}$, and their coatings, $K_{s,coat}$, were numerically optimized using the HYDRUS-1D program and the cumulative infiltration in time measured for the aggregates without and with coatings, respectively.

Data of the soil-water retention curves, measured on aggregates with and without coatings, did not allow distinguishing between retention curve parameters of the soil aggregates and their coatings. Therefore the same parameters were evaluated for both. Capillary rise into the soil aggregates without coatings was always faster than into the aggregates with coatings. As result the optimized saturated hydraulic conductivities, $K_{s,coat}$, of the clay and the organic matter coatings (the average values for unsorted, mostly clay and clay-organic coatings were 3.69 10^{-7}, 2.76 10^{-7} and 1.81 10^{-7} cm min^{-1}, respectively) were one to two order of magnitude lower than the saturated hydraulic conductivities, $K_{s,aggr}$, of the aggregates (the average values for corresponding aggregates were 3.87 10^{-6}, 6.52 10^{-6} and 1.11 10^{-5} cm min^{-1}, respectively). Slightly variable $K_{s,aggr}$ (or $K_{s,coat}$) values were obtained for different bottom pressure heads, and the lower $K_{s,aggr}$ (or $K_{s,coat}$) values were estimated from the second run of the tests compare to the first run of tests for each set of aggregates. No statistically significant differences between $K_{s,coat}$ values obtained for coatings of various compositions were found (Fér and Kodešová, 2012).

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Numerical Modeling of Water Flow and Nitrate Dynamics on Zero Tension Plate Lysimeters Using HYDRUS-2D

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Lysimeter experiments generally simulate actual field conditions and can be the closest to real field conditions. The efficiency of the zero tension plate lysimeters, which were implanted in silty-clay soils as well model (HYDRUS-2D) ability to simulate water flow and nitrate dynamics were evaluated. Low efficiency of lysimeters during the vegetation period was mostly caused by high crop water demand and possible water diversion to the sides when the groundwater table was low. The HYDRUS-2D model was able in some degree to reproduce observed outflows. Water and solute diverged from the plate towards the dryer unsaturated soil when groundwater table was low. Pressure head and nitrate concentration distributions simulated around the lysimeter plate illustrated that the lysimeter plate had a significant impact on the water regime and nitrate dynamics within the soil. This paper represent part of results which were published by Filipović et al. (2013).

Keywords: Zero tension plate lysimeter, water flow, nitrate dynamics, modeling, HYDRUS-2D

Reference

Filipović, V., and R. Kodešová, and D. Petošić, Experimental and mathematical modeling of water regime and nitrate dynamics on zero tension plate lysimeters in soil influenced by high groundwater table, *Nutrient Cycling in Agroecosystems*, DOI 10.1007/s10705-012-9546-5, *95*, 23-42, 2013.

Single and Double Porosity Modeling of Solute Transport in Intact Soil Columns – Effects of Texture, Slurry Placement, and Intermittent Irrigation

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We investigated the effect of injection and surface application of dairy slurry on leaching of nonreactive slurry components (Br tracer applied to slurry) and water flow (tritium tracer applied with irrigation water) for differently textured soils and irrigation regimes. The studies were performed on intact soil columns (20 cm diam., 20 cm high) from the plow layer of a loam, sandy loam, and loamy sand. The experiments were carried out during unsaturated conditions with low suction (5 hPa) applied at the lower boundary.

In the fine-textured soils, placing slurry within the soil matrix by injection reduced leaching of the Br tracer without influencing transport of the tritium tracer, indicating the mechanism of retention of slurry solutes in small pores (immobile region), inaccessible by the flowing water, as the active flow volume did not change as a result of the injection procedure. As transport occurred through a larger fraction of the loamy sand, no effect was observed in this more coarse-textured soil.

Irrigation interruptions during intermittent irrigation induced retention of the tritium tracer and increased leaching of the Br tracer in the slurry injected loam soil. We hypothesize increased mass exchange of solutes between mobile and less mobile pore regions as compared with steady flow during continuous irrigation for both tracers; meaning transport of the tritium tracer from mobile to immobile pore regions during interruptions, and transport of Br from immobile to mobile pore regions during interruptions.

These hypotheses and mechanisms were tested by simulations using single- and double porosity models implemented in HYDRUS-1D numerical code. Partitioning of the soil into two coupled pore domains for which separate hydraulic and transport properties are defined with mass transfer parameters for solute concentrations and water flow seem relevant for describing transport during intermittent irrigation.

The Use of HYDRUS-1D for Groundwater Recharge Estimation in Boreal Environments

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The well-known package HYDRUS-1D was used for groundwater recharge simulation based on long term meteorological data with daily resolution. For boreal climate, with a long winter period, initial meteorological data such as precipitation can't be used directly as the atmospheric boundary condition input file. This data must be preprocessed to take into account snow accumulation and snow melting, evaporation from snow and vegetation cover and soil freezing-defrosting processes. For this a special preprocessing code SurfBal for simulating surface water and energy balances and generating upper boundary for HYDRUS-1D was developed. SurfBal calculates using known daily values of precipitation, solar radiation and maximum and minimum temperature surface water balance including: interception by canopy, surface (leaf and snow) evaporation, snow accumulation, consolidation of snowpack and its melting and surface runoff as well as initial potential values of evaporation and transpiration and input water flow for HYDRUS-1D.

The results of water balance and groundwater recharge simulations using SurfBal and HYDRUS-1D for climate conditions of middle European part of Russia shows the principal role of spring-period surface-soil water budget for groundwater recharge under various landscapes and soil cover and due to different groundwater level depth.

Simulation of Uranium Tailing Leaching using VS2DRT

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Uranium contamination of surface and ground water from passive and active uranium tailing is a serious environmental problem in many industrialized nations like US. Reactive transport models can be used to predict the potential environmental impacts of new uranium tailing sites as well as to assess level of contamination from existing uranium tailing sites. Hence, reactive transport models are useful tools to visualize potential treats as well as emanate dangerous and to design preventive and remedial measures to protect and rehabilitate the water resources. In the present study a newly developed two dimensional multi-species coupled reactive transport model, VS2DRT, is used to simulate uranium tailing leaching. The problem is adapted from HYDROGEOCHEM-5 and HP2 manuals and deals with the release and subsequent migration of uranium from a uranium tailing pile towards the ground water and a river. The simulation does not involve redox reaction and shows the application of VS2DRT in simulating uranium migration in the subsurface.

Infiltration Into Stony Soils: Modeling of the Process Using the HYDRUS Codes

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Mountainous soils usually contain a large number of rock fragments (particle diameter ≥ 2 mm), which strongly influence the soil physical and hydrophysical properties and subsequently the movement of water in and through such soils. This work presents the results of the study evaluating the effects of rock fragments (quantitatively expressed as stoniness) on water infiltration into the soil and water percolation through stony soil layers into the relatively impermeable strata using the Darcy´s approach. Rock fragments as a part of stony soils significantly decrease their retention capacity as well as hydraulic conductivity. Stones simply decrease the effective cross-section of a more conductive soil matrix; the stones' hydraulic conductivity is negligible in comparison to the soil matrix (fine-textured particles).

Input data were measured in the field and in laboratory. The so-called effective parameters were estimated using the Darcy´s approach. It means that soil characteristics represent a bulk soil with both fine particles and rock fragments. To do this, all stony soil characteristics were evaluated using the representative elementary volume (REV), the dimension of which depends mainly on the size of the rock fragments and is orders of magnitude larger than sample volumes, used for the soil matrix (the Kopecky's cylinders). For a soil with stones of about 10 cm in diameter, the REV was estimated to be 1 m^3. Since it would be technically extremely difficult to measure hydraulic characteristics on a soil sample this big, we used the simulation model HYDRUS-2D (simulating the classical Darcy's approach) to estimate the saturated hydraulic conductivity using numerical experiments. Resulting data were then implemented in the simulation model HYDRUS-1D.

Simulation results of an infiltration process have shown the importance of stoniness in infiltration kinetics. However, the initial soil water content was found to be a dominant factor in this particular case (for a stony soil at Western Tatras, Slovakia). Soil skeleton decreases the effective hydraulic conductivity and retention capacity of stony soils. During infiltration with the rainfall rate lower than the saturated effective hydraulic conductivity, the penetration rate of the infiltration front in stony soils will be higher than through non-stony soils. From the above it follows that the formation of the subsurface runoff is being modified by soil stoniness. The higher stoniness, the earlier appearance of the surface runoff can be expected.

Simulation of Different Rainfall Intensities Impact on the Reactive Transport of Mine Tailing Metal Contaminants

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Contamination of the underling aquifer beneath a mining area is one of the environmental problems that can be modeled in order to minimize the contamination of groundwater and river flow systems. Interpreting the geochemistry and achieving a good understanding of the involved processes is necessary to mitigate the environmental damages. Extensive internal risk predication models often fail to predict where catastrophes will arise. In this study the potential risk of metals contamination around the mining sites is evaluated, and the metals reactive transport sensitivity to different leachate fluxes is estimated. The PHREEQC numerical model is applied to simulate the reactive transport of three metals (Cd, Ni and Mn) from Zanjan (Iran) Zinc leaching plant tailings, with variable leachate fluxes in 30 days. The simulation showed that different rainfall rates induce variable metal speciations. Decreasing water contents lowered the soil solution pH and produce new cation exchange conditions. The simulation results were generally in good accordance with the experimental results. Incompatibility in some scenarios may be attributed to PHREEQC linear cation retardation assumption. Of the three considered metals, the modeled Ni concentrations were the least compatible in different scenarios. We conclude that variations in water fluxes can significantly influence metals mobility and availability and hence, specific risk assessments for past and present hydrological regimes are highly suggested for mining disposal sites.

Investigation the Effect of Acidic Rain pH on Reactive Transport of Groundwater Metal Contaminants

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Multicomponent reactive transport in porous media is a complex process, owing to a combination of variability in the processes involved and the inherent heterogeneity of nature. In recent years, various multicomponent reactive transport models have been developed to study the mobility of potentially toxic heavy metals in the subsurface. Heavy metals and other contaminants might release from mining sites, especially from waste dumps or tailing ponds. Soil and groundwater contamination due to mining activities is a worldwide environmental problem. Among the inorganic toxicants of great concern in mine tailings, Pb^{2+}, Zn^{2+} and Cd^{2+} figure prominently due to their abundance and potential toxicity. This study investigated the effect of pH on the transport of these metals through Lakan (Iran) lead and zinc leaching plant tailings. The local equilibrium assumption (LEA) was adopted and HP1 model and PHREEQC database were employed to simulate heavy metals movement through saturated soil at the laboratory column scale, in a 15 days period. Not surprisingly, lower pH increased metal transport. However the simulation result generally agreed well with previously column study results, they indicate that physical and chemical parameters must be carefully determined and used in the simulation procedure. The use of 2D and 3D models and kinetic modeling approach is highly suggested to more accurately simulate the related reactions and to improve the results precision.

Comparison of Two Numerical Modeling Codes for Hydraulic and Transport Calculations in the Near Field

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In the past years the Slovenian PA/SA team has performed many generic PA/SA studies for the future Slovenian LILW repository, most recently a Special Safety Analysis (SSA) for the Krško site. The modeling approach taken was to split the problem into three parts: near-field (detailed model of the repository), far-field (i.e., geosphere) and biosphere. In the SSA the code used to perform near-field calculations was Hydrus2D.

Recently the team has begun a cooperation with CEA/Saclay and, as a part of this cooperation, begin investigations into using the Alliances numerical platform for near-field calculations in order to compare the overall approach and calculated results.

The article presents the comparison between these two codes for a silo-type repository that was considered in the SSA. We will present the physical layout and characteristics of the repository and develop and implement a hydraulic and transport model of the repository in Alliances. Some analysis of sensitivity to mesh fineness and to simulation timestep have been preformed and will also be presented. The compared quantity will be the output flux of radionuclides on the boundary of the model. We will compare the results and comment on differences/similarities.

Characterization and Modeling of Water Movement and Salts Transfer in a Semi-Arid Region of Tunisia

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The semi-arid region of Bou Hajla (Kairouan – Central Tunisia) is exposed to the risk of soils and aquifers salinization. A characterization of water movement through the use of TDR probes installed at up to 4 m in depth, and of salts transfer by soil sampling was conducted to highlight this risk. At the same time, climatic parameters were monitored. The results were gathered over the period of approximately one year (June 12, 2006 to May 08, 2007). The water movement and salts transfer were simulated by Hydrus-1d model, and inverse modeling was used to optimize the required hydrodynamic parameters. It was found that the simulated profiles of volumetric humidity and the electrical conductivity of soil are close to those measured. The calculated RMSE values are low, indicating the reliability of Hydrus-1d for the simulation of the hydro-saline dynamics in field conditions.

Keywords : Soil, Salinization, Hydrus-1d, Aquifer, Semi-arid region, Tunisia.

Characterization and Modeling of Water and Salt Dynamic in a Sandy Soil Under the Effect of Surface Drip Irrigation

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In a global context of water scarcity and salinization, there is a more pressing need for an efficient use of the irrigation management through alternative localized irrigation's techniques. Characterization and two-dimensional modeling of water movement and salts transport is important to manage such irrigation system. Nevertheless, that is not highly valued in most numerical modeling studies of two-dimensional flows and solute transport under drip irrigation. For this purpose, an experiment of two monoliths was implemented by a sandy soil equipped with TDR probes to monitor water content and Watermark sensors for monitoring soil pressure head. Soil salinity was measured according the method of the soil diluted extract (soil/water ratio of 1/5). Preliminary tests on small monoliths were carried to determine hydrodynamic parameters of this soil. The monoliths were saturated, one, with a distilled water and the other with a saline water (electrical conductivity = 4 dS.m^{-1}). Characterization results show a more important axial dynamic of water than lateral movement and the formation of a saline bulb around 20 cm in depth. Modeling of water movement and solute transport was performed with Hydrus-2D. Four types of hydrodynamic parameters were used for model calibration on the monolith irrigated with distilled water. The best calibration was obtained with the parameters estimated using RETC software from retention curve data measured by the evaporation method. Model validation was performed on the data obtained from the monolith irrigated with saline water. Modeling results showed a good agreement between measured and predicted values. A scenario highlighting the effect of significant evaporation (8 mm.day^{-1}) during an irrigation cycle revealed a potential soil salinization risk with the formation of a saline bulb of medium salinity (3.5 dS.m^{-1}) around the emitter. This bulb extends to 30 cm in depth. In the long-term, after several cycles of irrigation, salinity risk can be aggravated and affect the soil physical properties and, in consequence, crops production.

Key words: Soil, Salinization, Irrigation, Modeling, Hydrus-2D.

Hydraulic Properties and Reduction of COD, Phosphorus and Nitrogen in Sand Filters Used for Greywater Treatment – Simulation and Verification

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Greywater can, after suitable treatment, be a sustainable resource for irrigation, cleaning and strengthening the groundwater by infiltration. A vertical flow sand filter is a simple, effective and inexpensive system for treating greywater. The performance of sand filters treating artificial greywater was tested in the laboratory over a period of 113 days. The filters consisted of columns (0.2 m diameter) filled with sand to a height of 0.6 m. The hydraulic properties of the filters were measured as well as the inflow and outflow concentrations of COD, BOD_5, total and phosphate phosphorus and total-, ammonia- and nitrate nitrogen.

To get a better quantitative understanding of the treatment processes inside the filters, the HYDRUS-CW2D computer software was used to simulate the filters. The simulation of water flow through the filter could be well fitted to the measured flow by adjusting three model parameters: the air entry value; pore size distribution index and pore connectivity parameter.
For the COD reduction the simulated results agreed well with experimental data after adjustment of the microbial lysis parameters of HYDRUS-CW2D. The simulated reduction of COD was 65 % while 72 % reduction was measured for the filters in the lab. Simulated reduction of phosphorus in the sand filter effluent corresponded well to the measured reduction: the simulated reduction of phosphorus was 72 % while the experimental filters achieved a 79 % reduction. Also the simulated effluent concentration of nitrate compared quite well to the measured values. Almost no reduction (4 %) in total nitrogen took place in the experimental filters which agreed with the simulated reduction (0 %). For the phosphorus and nitrate components in HYDRUS-CW2D, so far no changes have been made to the default parameters.

Using HYDRUS-CW2D for running simulations has so far improved our understanding of our lab scale sand filters by pointing towards the possibility that some water passes by the filter by running along the filter column walls. The simulations also indicated that the biological activity and COD reduction mainly took place in the very top of the filter which agreed with experimental observations.

The laboratory setup includes also vertical filters with bark and charcoal as filter materials and our next challenge is to simulate their performance using HYDRUS-CW2D.

Predicting Soil CO_2 Dynamics in Arable Land of Andisol in Western Suburb of Tokyo

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Recently, carbon capture and storage at both shallow and deep soil layers is recognized as a function of agricultural fields. When discussing global warming mitigation such as proper agricultural practices and/or appropriate depth of incorporating composts in agricultural lands for carbon storage, prediction of not only CO_2 efflux but vertical distribution of CO_2 concentration of soil air phase is important. Few studies, however, had evaluated the model performance of simulated profiles of soil CO_2 concentration. The purpose of this study is to predict soil CO_2 dynamics which include both CO_2 flux from the surface and profiles of CO_2 concentration in arable bare lands using SOILCO2 in HYDRUS-1D.

The study site was Institute for Sustainable Agro-ecosystem Services of the University of Tokyo (ISAS-UT) in western suburb of Tokyo, where Andisol is distributed. For model validation, 10 m square bare area was prepared and continuous monitoring data of soil moisture, temperature and CO_2 concentration at depths of 10, 20 and 50cm has been obtained every 20 minutes from Aug. 2010 to Oct. 2011. CO_2 efflux from the surface was measured with closed chamber method in both summer and winter. Meteorological data was obtained from ISAS-UT and AMeDAS weather station located near the field.

Since there is no common way in determining parameters describing soil CO_2 production, we tried to determine the parameter of soil CO_2 production dependence with depth with the measured profile of dissolved organic carbon (DOC). Durner-Mualem model was employed for soil hydraulic function and parameters were determined by inverse analysis with evaporation experiments. In the inverse analysis, porosity of the field soil was employed as volumetric water content at saturation $\theta_{s,}$ since θ_s is an important parameter to predict diffusion of CO_2 through air filled pores in a variably saturated soil. This is very important for soil with large porosity such as Andisol.

Simulated results agreed with observed daily and seasonal variation of soil moisture, temperature and CO_2 concentration. Quick response of soil moisture and soil CO_2 concentration to rainfall, which observed in the field, was also well described. As well, predicted cumulative CO_2 flux for a year was comparable to the value which was estimated with observed data. We concluded that the parameter of CO_2 production dependence with depth were properly determined with measured profile of DOC concentration and soil CO_2 dynamics in arable bare land could be predicted by using SOILCO2 model.

Transfer at Low Water Content: New and Simple Experimental Approach for Inverse Determination of van Genuchten Transport Coefficients

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The unsaturated soil hydraulic properties (soil water characteristic curve and relative permeability) are key factors for soil sciences fields and civil engineering. Because of the strong dependence of these hydrodynamic parameters with water content, their determination is subject to considerable experimental and numerical problems. Difficulties increase when the soil tends to oven- dry situation, the state characteristic of arid and semi-arid areas. And costs (time, money) of the methods for determination of these properties are relatively high.
In this article, we present:

- In short review, the problem of the determination of the soil – water characteristic curve and relative permeability in all the range of soil water content: experiments, models of unsaturated soil hydraulic properties and associated numerical methods;
- A simple, robust and less costly experimental method for the inverse determination of hydrodynamic parameters. The principle of this experiment is to create a strong gradient of water content in a column of homogeneous soil under conditions of constant flux (null) on the extremities in a fairground temperature controlled. Ideally, a single transfer phenomenon namely liquid phase filtration should be predominant in the column.
- The numerical isothermal water transfer model and the formulation of the inverse problem (MINPACK's lmdif and lmder algorithms and Downhill simplex algorithm). The state variables chosen are the gravimetric water content and the vapor pressure.

The van Genuchten (1980) - Mualem (1976) model for soil - water characteristic curve and relative permeability is applied. ROSETTA code is used to determine initial values of VGM model parameters. Different scenarios on the model taking into account the residual water content (w_r), Mualem tortuosity parameter (L) and permeability parameter at saturation (K_s or K_0) will be simulated and discussed. A discussion is presented in consideration of water vapor flow in the soil under our experimental conditions and the validity of isothermal transport.

Key words: soil water characteristic; relative permeability; inverse problem; van Genuchten parameters

Root Water Uptake Under Deficit Irrigation: Model Calibration and Comparison

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Numerous sink functions for root water uptake: microscopic and macroscopic, empirical and mechanistic, compensatory and non-compensatory, are indiscriminately employed in research and referenced in the literature, indicating an absence of information regarding model relevance for specified boundary conditions. This research is an attempt at filling the information gap concerning root-water-uptake model robustness. We present results from a parallel comparison and evaluation of the performance of two empirical and one semi-mechanistic model in solving for root water uptake under optimal and deficit-irrigation conditions, in two soils: loess and fine sand, and with three crops: wheat, tomato, and sweet sorghum, each characterized by a unique root distribution.

A global optimization search algorithm was employed for model parameterization in conjunction with a numerical model for solving Richards' water transport equation. System variables, including the spatial and temporal soil water potential measured from cropped soil columns, served as input data. Model calibration was validated by comparing the measured transpiration of deficit-irrigated plants, cultivated in a rotating lysimeter system, to modeled transpiration values. Model performance under varying degrees of compensation was evaluated, along with the effect of initial soil water potential conditions.

The quality of algorithm convergence during the calibration stage was relied on for a preliminary evaluation of model robustness in predicting soil water dynamics. Algorithm convergence quality was compared using indices representing both the ratio between the 95% confidence interval parameter range and the corresponding most likely parameter value, as well as the error in the modeled soil water potential value, calculated with most likely parameter values, relative to observations. Indices revealed inter-model variation as well as inter-treatment variation in algorithm convergence quality, due to soil texture and plant type. The soil water dynamics of wheat grown in loess and sand were best predicted when the sink function of the Richards equation was solved with the modified Feddes (FD) and van Genuchten (vG) models, respectively. The same pattern was seen for tomato. The soil water dynamics of both sand and loess, cropped with sweet sorghum, were best predicted when the Nimah and Hanks (NH) model was incorporated into the sink function. Water stress was the most significant in sand columns cropped with sweet sorghum, which may indicate that the accuracy of NH increases as the soil water potential decreases, possibly due to NH's consideration of the unsaturated hydraulic conductivity, which expresses a highly, non-linear dependence on the soil water potential.

When calibrated models were validated in drought conditions, modeled transpiration values calculated with vG showed a good fit with measured values for both wheat and tomato. However, FD overestimated the transpiration of loess-grown wheat regardless of the initial soil water content, and overestimated the transpiration of loess-grown tomato in an initially hydrostatic profile. The difference in model performance is attributed to the soil textures for which they were tested.

The effects of compensation and the root distribution decreased with decreasing soil water content, and the initial conditions greatly affected modeled transpiration results. Transpiration 'overshoot' may be linked to the fact that potential transpiration values assigned to deficit-irrigated plants were taken from plants kept under well-watered conditions, and are therefore not representative of potential transpiration values for the smaller-sized plants that result under drought conditions.

We conclude that model performance was affected by soil texture, root distribution, and irrigation regimes. Therefore, a more mechanistic approach, able to account for such factors, should be incorporated into existing empirical models. In addition, continued testing should be carried out with the NH model in order to better-understand its limitations and work toward widening its applicability.

Sensitivity of Recharge Evaluation Results Using HYDRUS to Parameters and Boundary Conditions Variations

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We examine the dependence between the type of bottom boundary conditions using in model which describe different geolandscape elements and results of groundwater recharge simulations. Geolanscapes is the term emphasizing indicative types of environmental by plants and soil types, geological cross-sections and groundwater levels.

For our research we choose part of Moscow river valley which was nearby Zvenigorod town. There is located MSU geology research-station. Studied area is a part of Moscow syneclise. The geological cross-section from top to bottom consist of Quatenary sand and loam, Jurassic dark clay, laying with discrete location, and Carboniferous limestone. This cross-section is usual for Moscow region.

The groundwater recharge modeling have two part. First part is the atmospheric moisture transformation on surface (Grinevsky, Pozdnyakov, 2010), second – moisture transport in vadozone (Simunek, 2008).

Upper boundary conditions are described by result of modeling precipitation transformation on surface by program “sur_bal”. Application this program allow take into account such conditions as plant type, composition of soil (sand, sandy-loam, loamy), temperature, sun insolation, daily volume of precipitation. Bottom boundary conditions depend on the groundwater level depth. In this study we use the condition constant and variable pressure head. The second type of bottom conditions was defined by long-term monitor groundwater levels which take place in MSU geology research-station.

The findings in this study support the idea that the use variable pressure head conditions for definition bottom boundary conditions are significant for modeling processes of moisture transport and definition recharge part of water balance.

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Inverting Saturated Hydraulic Conductivity from Surface Ground-Penetrating Radar Monitoring of Infiltration

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Hydraulic properties of soils, described by the soil water retention and hydraulic conductivity functions, strongly influence water flow in the vadose zone, as well as the partitioning of precipitation between infiltration into the soil and runoff along the ground surface. Their evaluation has important applications for modeling available water resources and for flood forecasting. It is also crucial to evaluate soil's capacity to retain chemical pollutants and to assess the potential of groundwater pollution.

The determination of the parameters involved in soil water retention functions, 5 parameters when using the van Genuchten function, is usually done by laboratory experiments, such as the water hanging column. Hydraulic conductivity, on the other hand can be estimated either in laboratory, or *in situ* using infiltrometry tests. Among the large panel of existing tests, the single or double ring infiltrometers give the *field* saturated hydraulic conductivity by applying a positive charge on soils, whereas the disk infiltrometer allows to reconstruct the whole hydraulic conductivity curve, by applying different charges smaller than or equal to zero. In their classical use, volume of infiltrated water versus time are fitted to infer soil's hydraulic conductivity close to water saturation. Those tests are time-consuming and difficult to apply to landscape-scale forecasting of infiltration. Furthermore they involve many assumptions concerning the form of the infiltration bulb and its evolution.

Ground-Penetrating Radar (GPR) is a geophysical method based on electromagnetic wave propagation. It is highly sensitive to water content variations directly related to the dielectric permittivity. Thus it appears to be an accurate tool for wetting front infiltration monitoring.

In this study we used Hydrus-1D to simulate infiltration of water inside a ring infiltrometer during a certain time. We generated water content profiles associated with a saturated hydraulic conductivity value, knowing the other van Genuchten parameters, at each time step with Hydrus-1D. The water content profiles obtained by Hydrus-1D were converted to permittivities profiles using Complex Refractive Index Method relation. We then used GprMax suite programs to generate radargrams and follow the wetting front using arrival time of electromagnetic waves coming from GPR.

The synthetical inverse problem was made in the same way as presented above, generating water content profiles according to one unknown saturated hydraulic conductivity, convert them to permittivities and compute GPR monitoring using GprMax2D. By minimizing the misfit between arrival times, we inverted the saturated hydraulic conductivity.
Using this procedure we study the possibility to obtain other parameters (namely α and n), by MCMC inversion. By the means of sensitivity and misfit diagrams we try to conclude on links between those parameters and the possibility to obtain them our inversion method.

We carried out experiments in a quarry of Fontainebleau sand, using a Mala RAMAC system with antennae centered on 1600 MHz. We obtained saturated hydraulic conductivity, our retrieved saturated hydraulic conductivity from GPR data was compared to disk infiltrometer measurements.

Groundwater Recharge Modelling in the Nete Catchment (Belgium) with HYDRUS-1D–MODFLOW Coupling

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This study focuses on the characterization of groundwater recharge in the Nete catchment (1544 km²), in Northern Belgium. A calibrated catchment-scale MODFLOW groundwater model had been developed and reported previously (Gedeon and Wemaere, 2008) assuming constant (in space and time) recharge. To better approximate how groundwater recharge variations in space and time affect groundwater flow, we coupled a model of the vadose zone hydrology to the groundwater model. The HYDRUS package (Seo et al., 2007) for MODFLOW-2000 (Harbaugh et al., 2000) was chosen to perform the coupling. This paper describes the different steps and issues encountered for the practical implementation of this package in a real-world case study at the catchment scale.

The groundwater modelling domain for MODFLOW is discretized in cells of 400×400 m (9644 active cells in the top layer), grouped in a predefined number of zones for the coupling between HYDRUS and MODFLOW. The number of zones is a compromise: increasing the number of zones reduces the impact of averaging recharge fluxes and groundwater levels for each zone; while decreasing the number of zones diminishes CPU time. We based the clustering on three criteria: (i) groundwater depth estimated from the calibrated steady-state groundwater flow model, (ii) soil type, and (iii) land cover type. In the preliminary work presented here, only the first criterion was used to delineate 20 zones, while a unique soil type (podzol) and land cover (grass) were assumed over the entire area.

Despite the reduced complexity, several issues had to be overcome during the implementation of the coupling HYDRUS-MODFLOW. First, due to a shallow groundwater table (<1-2 m) in a significant part of the Nete catchment and due to topography averaging effects, groundwater level simulated by MODFLOW exceeded the ground level. The HYDRUS package could not properly handle this (non-convergence) and therefore the code was adapted to allow this water excess to be removed as a "seepage". Second, some numerical instability sometimes occurred (notably when the number of zones was too low or the number of coupling time steps insufficient in the early stress periods) and simulations showed highly oscillating fluxes and heads (even if tested with steady-state atmospheric input), and a non-convergence.

The coupled simulation was run for a 10 year time series (from 2000 to 2009) of daily precipitation (P) and potential evapotranspiration (ET_0). Average P and ET_0 over the 10 years are 941 mm y^{-1} and 562 mm y^{-1}, respectively. A warming-up period of 10 years with constant average P and ET_0 was included to achieve proper initial conditions preventing an artificial trend in the modelling results. The first month of the warming-up period needed to include from two to six MODFLOW time steps per day to prevent oscillations, followed by daily MODFLOW time steps for the rest of the warm-up and the simulation period.

For each zone, simulated groundwater depths were compared with data available from a network of piezometers in the study area showing generally good correspondence and identifying zones where further calibration of the groundwater flow model is necessary.

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Hg Modelling in Soil Systems Using HP1

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The main objective of this work was to develop a reactive transport model for simulating mercury fate and transport in the unsaturated zone, in order to gain insight in the fate and transport of Hg following soil contamination. The relative importance of different processes and parameters was assessed with a sensitivity analysis based on Morris (1991) method and evaluated for different initial speciation of Hg contamination and indicators for Hg fate.

The code HP1 (Jacques et al., 2006; 2008)) is based on two computer codes that have been extensively used and validated : HYDRUS-1D (Šimůnek et al., 2008) for water and solute transport and PHREEQC (Parkhurst and Appelo, 1999) for geochemical calculations. The database IM003_THERMODDEM (Blanc et al., 2012) was used for aqueous complexation, augmented with some Hg speciation data from Skyllberg (2012). However, complexation with organic compounds is not considered in IM003_THERMODDEM. Four organic compounds (three representing humic and fulvic acids, and one representing thiols) were therefore added. Interactions between Hg and these dissolved organic ligands were modelled as aqueous complexation reactions.

The main processes accounted for in the model are : Hg aqueous speciation (including complexation with dissolved organic matter (DOM) – humic and fulvic acids (HA and FA), and thiol groups), Hg sorption to solid organic matter (SOM) – also distinguishing humic and fulvic acids (HA and FA) and thiol groups, dissolution of solid phase Hg (e.g. cinnabar HgS(s)), dissolution of Hg non-aqueous liquid phase (NAPL), sunlight-driven HgII reduction to Hg^0, Hg^0 diffusion in the gas phase and volatilization, and DOM sorption to soil minerals. DOM production is not explicitly considered in the model but its effect is implemented by defining a DOM concentration in the rain water. Colloid facilitated transport is implicitly accounted for by solute transport of Hg-DOM complexes. Certain processes in contaminated sites may be very specific due to local circumstances and thus may not be consistent with predictions of thermodynamics. Therefore, some processes (e.g. Hg^{II} reduction to Hg^0) need to be modelled following kinetics rather than thermodynamic laws.

Using a 50 year time series of daily weather observations in Dessel (Belgium) and a 1-m deep sandy soil with deep groundwater (free drainage, oxic conditions), we implemented a sensitivity analysis using the elementary effects method (Morris, 1991). Processes and parameters identified as critical based on the sensitivity analysis differed from one scenario to the other depending on pollution type (cinnabar, NAPL or aqueous Hg), on the indicator assessed (leached Hg, Hg in soil horizon originally polluted…) and on time. However, in general concentration of DOM in soil and rainwater was the most critical parameter. Other important parameters were those related to Hg sorption on SOM (thiols, and humic and fulvic acids), and to Hg complexation with DOM. Initial Hg concentration was also often identified as a sensitive parameter. Interactions between factors and non linear effects as measured by the elementary effect method were generally important, but again dependent on the type of contamination and on time.

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Modeling Phytoextraction and Contaminant Transport Processes Using HYDRUS-1D

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Phytoextraction is an in situ remediation technique involving the uptake of contaminants by plant roots and their accumulation in plant tissues. Phytoextraction is dependent upon a complex set of interactive and generally nonlinear soil, plant, contaminant and atmospheric processes and parameters. The objective of this study was to use HYDRUS-1D to numerically estimate the effectiveness of the phytoextraction of Cd^{2+} , Pb^{2+} and Zn^{2+} from contaminated soil using Vetiver grass. Vitever is a perennial grass known for its tolerance to drought, resistance to diseases and fire, and ability to take up heavy metals.

In a previous study we calibrated HYDRUS-1D against observed greenhouse remediation experiments. Several scenarios were tested, including different planting densities and irrigation schemes. Results of our numerical analyses showed that the efficiency of phytoextraction increases significantly for more mobile contaminants, depending upon the advective contaminant transport rate in the soil root zone, the potential transpiration rate, and prevailing water stress conditions in the root zone. Our study provided useful insight into the design of more elaborate laboratory- and field-scale phytoremediation experiments that may be needed in the future.

Which Hydraulic Model to Use in Vertical Flow Constructed Wetlands?

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Modelling water flow in a Vertical Flow Constructed Wetland (VFWC) is a prerequisite to model wastewater treatment using process based filtering models. The material used in VFCW is very susceptible to generate preferential flow. If this occurs, water will bypass most of the soil porous matrix in a largely unpredictable way. Even if it is possible to simulate water content variations within a VFCW, we cannot correctly model outflow with the standard van Genuchten-Mualem function if preferential flow occurs. A number of various model approaches have been proposed to overcome this problem. These models mostly try to separately describe flow and transport in preferred flow paths and slow or stagnant pore regions. The objective of this study was to study and simulate the hydrodynamic behaviour and the solute transport through a simplified representation of a French VFCW by using both a classical equilibrium model and a non-equilibrium model (dual-porosity model: mobile-immobile water model, with water content mass transfer) included in the HYDRUS-1D software package. Modelling results were compared to a solute breakthrough curve obtained from a tracer experiment, carried out on an existing VFCW. Inlet concentrations were first corrected to take into account tracer loss and experimental uncertainties. Then, both the hydraulic parameters of the mobile and immobile regions ($\theta_{r\text{-}mo}/\theta_{s\text{-}mo}$ and $\theta_{r\text{-}imo}/\theta_{s\text{-}imo}$) and the transfer coefficient (ω) were optimized to fit the tracer experimental breakthrough curve. The comparison between measured and simulated tracer breakthrough curves indicates that the non-equilibrium approach seem to be the most appropriate for simulating preferential flow paths.

Keywords. Dual-porosity model, non-equilibrium, preferential flow path, vertical flow constructed wetland

Parameter Estimation of Soil Hydraulic Functions and Thermal Properties for Unsaturated Porous Media Using HYDRUS-2D Code

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Soil and water resources are of great importance to the mankind. The combined effects of different soil temperatures and water inputs on water redistribution under field conditions have not been fully studied. The objective of this study was to estimate the water flow parameter (the residual water content θ_r, the saturated water content θ_s, empirical shape parameters α and n, and the saturated hydraulic conductivity K_S) and heat transport parameter (coefficients b_1 and b_2 in the thermal conductivity functions). Real-time sensors built by authors were used to monitor soil temperatures at depths of 40, 80, 120, and 160 cm during 10 hours. Water temperature in a single infiltration ring was monitored simultaneously at the same location. The soil thermal conductivity is estimated from temperature measurements by solving a two-dimensional, inverse water flow and heat transport problem.

HYDRUS-2D, a two-dimensional software package for simulating movement of water and heat in variably-saturated porous media, was used to simulate water flow and heat transport under such conditions. The simulated soil temperatures during ring infiltration experiment compared favorably with their corresponding observed values. Soil hydraulics and heat transport parameters are optimized using the HYDRUS-2D code by solving the inverse problem.

Using HYDRUS Programs for Simulating Al and SO_4^{2-} Leaching from Forest Soils

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The aim of this study was to assess the impact of different vegetation on the distribution of rainfall (due to throughfall and stemflow), water regime, and Al and SO_4^{2-} leaching from forest soils. The study was performed at two elevation transects on the Paličník and Smědava Mountain in Jizera mountains. Podzols and Cambisols were prevailing soil units in this area. The impact of the precipitation redistribution under a beech tree on the water regime and Al transport within the one- and two-dimensional soil profiles was simulated using the HYDRUS-1D and HYDRUS 2D/3D simulation models (Nikodem et al., 2010). The water flow and Al and SO_4^{2-} transport under a grass cover, beech or spruce trees were modeled using HYDRUS-1D (Nikodem et al., 2013). The simulation results for the 1D and 2D scenarios (Nikodem et al., 2010) showed that the spatially redistributed precipitation under the beech tree caused funneled water flow and solute transport near the stem base, which resulted in the intensive simulated Al leakage around the tree stem. It was also shown (Nikodem et al., 2013) that the effect of the precipitation redistribution on water regime was considerable in the beech forest, while it was almost negligible in the spruce forest. Redistribution of precipitation under trees caused runoff (in one case), increased water discharge through the soil profile bottom, reduction of water storage in the soil, and thus reduction of root water uptake. Simulated Al leaching from the soil profile was determined mainly by the initial Al content in the soil profile bottom. Leaching of SO_4^{2-} was mainly determined by its initial content in the soil and to a lesser extent by redistributed precipitation and SO_4^{2-} deposition. The results suggest that spatially redistributed precipitation in beech forest should not be neglected when predicting potential leaching of toxic substances toward ground and surface water bodies.

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Agro-Ecological Application of Soil Hydrological Data: Two Local-Scale Modelling Examples

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Many soil and landscape (agro-ecosystem) processes are influenced by spatial and temporal changes of soil moisture. The content of soil water in root zone is crucial for crop development and crop production. The aim of paper is i) to present the ecological and geographical approach to the analyze and interpretation of the soil moisture in the context of crop production process and crop production, ii) to present examples and the results of WOFOST and DAISY models application at different spatial levels (soil profile, farm) with emphasis on those hydrological soil properties and processes which influence the crop production process intensity and the level of crop production. Weather data were obtained from weather stations (Slovak Hydrometeorological Institute), soil data (soil retention and soil hydraulic data) were prepared according to models requirements on the base of soil database of the Soil Science and Conservation Research Institute in Bratislava (data on soil samples) and/or on the base of detailed soil research at model area. Two models WOFOST and DAISY were applied to simulate crop development and crop production including the soil moisture conditions at day step within the vegetation season. Two models differ in the method of soil moisture content calculation. Model WOFOST model works with simple vertically homogenized soil profile and the soil water content in root zone is calculated on the base of soil water balance equation. Model DAISY is more detailed and requires the soil profile to be vertically differentiated into several horizons, which are described individually and Richards's equation is implemented to describe the soil water content and movement. Case study Hurbanovo weather station: Model DAISY was applied to simulate soil moisture conditions and several crop productions in the period 1961 – 2010. Crop rotations of five crops (spring barley, winter wheat, maize, sugar beet, potato) were set up. The water regime was simulated in 2 variants: rainfed and irrigated. Irrigation was applied automatically after decreasing of soil water content below 50% of available water capacity for each evaluated crop. Irrigation amount 30 mm was simulated. The soil water regime was evaluated using the ecological classification of soil water regime. The semiuvidic interval of the soil moisture is dominant. In winter period prevailed semiuvidic interval whereas in the summer period the semiarid interval. The most extreme drought occurred in the year 1990 when the duration of the arid and semiarid intervals in the topsoil was 292 days. Extreme drought occurred also in the years 1971, 1978 and 1982 when the duration of the arid and semiarid intervals in the topsoil was more than 200 days. Droughts negatively affect crop productivity. Decrease of water availability and consequently increase of days with water stress result in decrease of water productivity; irrigation positively affects the water productivity. Case study Selice farm: Model WOFOST was applied to simulate the grain maize production process including the soil moisture content in the root zone in the period 1961 - 2010; the number of days with water and oxygen stress and grain maize production were calculated in 1961 – 2010 and analyzed. As well, there was analyzed the spatial pattern of spatial variability related to grain maize production in two years (2000 and 2008) different from the rainfall and different soil moisture conditions in root zone points of view. The results of analyses confirmed the strong relations between rainfall, soil water content and grain production which are reflected by spatial variability related to simulated soil moisture and production indices. The geographical and ecological interpretations of analytical hydrological soil properties and processes especially in the context of crop development and crop production extend their applications in interdisciplinary research.

Slope Drainage by Logging Roads and its Contribution to the 2011 Flood Peak in the Píla Village. Simulation with HYDRUS-2D.

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One of the most discussed environmental problems in Slovakia has become the effect of wood logging on hydrological processes. Especially, the more frequent occurrence of floods in sub mountainous villages reported during the last two decades has been ascribed by various nongovernmental organizations to the devastative clear-cut forest management. The High Tatra Mt. wind-throw calamity in November 2004 provided a very good opportunity to study hydrological effects of large land cover changes in mountainous areas. 12,600 ha of the spruce forest were completely cut down and forest was subsequently replaced by other types of vegetation (grasses, herbs and shrubs). No significantly more positive effect of forests on storm floods was either predicted or observed when compared to other types of vegetation. However, mathematical simulations correctly predicted seasonal changes in the water balance towards enhanced soil water content and less evapotranspiration after deforestation. The qualitative effect of the clear-cut forest management on the water balance can be expected similar to that of the wind-throw.

There was a flood in the Píla village on June 7, 2011 after 104 mm rainfall during 3 hours. The usual "up-to-knee" deep base flow suddenly changed to a 3-m high wave, causing catastrophic damages in the village. The estimated total flood discharge was about 560,000 m^3. The area of the Gidra river catchment above the Píla village is 32 km^2. The catchment is forested by more than 90%. Visiting the place and investigating the state of the forest floor we found that there was an extremely high density of forest and logging roads, especially in the lower part of the catchment. The forest road density in the left part of the Gidra river catchment was up to 10 km/km^2. The average width of the roads is about 3-4 m and the roads are often deepened by harvesters and erosion by up to 2 m. Thus, the area of compacted surfaces (mostly roads) in the left part of the Gidra catchment was estimated to 0.7 km^2 (2.2% of the total area). The road density was not measured in the right part of the catchment. The direct forest-road discharge (i.e., water, which falls directly on their surface minus infiltration) was estimated to be about 56,700 m^3, which is about 10% of the estimated cumulative flood discharge.

The HYDRUS-2D simulations revealed that the drainage process, collecting water from up-slopes in deep logging roads (here estimated as 10% of all roads), transformed another 39,936 m^3 of subsurface flow to surface flow, which theoretically could contribute to the direct flood discharge. Then, the total contribution of logging roads to the flood discharge could be more than 17%. Although we do not know what was the real density of deep logging roads in the Gidra catchment it can be concluded that their contribution to the flood discharge in June 2011 was substantial. It was concludes that in forested catchments it is not the change of vegetation (natural or human-induced) but the presence of compacted surfaces (logging roads) that can significantly contribute to floods.

Seasonal Simulation of Water and Salinity Dynamics Under Different Irrigation Applications of Almond in Pulsed and Continuous mode

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The quantification of components of water balance is essential for designing strategies for improving irrigation efficiency and water productivity of crops under different irrigation systems and also needed for minimising the offsite movement of nutrients out of the rhizosphere. The HYDRUS-2D was used to simulate water balance and salinity distribution under full pulsed (FI_p), sustained deficit pulsed (SDI_p; 65% ET_C) and full continuous (FI_c) irrigation of surface drip irrigated almond over a season. The weekly measured and predicted values of moisture content at different distances from the dripper and at different soil depths matched well showing small variation in RMSE values. The sap flow underestimated the almond water uptake by 31% as compared to the modelled value. Water uptake efficiency under SDI_p (68%) was higher compared to full water application conditions under FI_p and FI_c (54-55%). The leaching fraction was estimated to be 0.14 under SDI_p and 0.25 in FI_p and FI_c treatments. The higher irrigation amounts under 100% ET_C treatments (FI_p and FI_c) largely contributed to non-productive water fluxes (deep drainage losses and evaporation). The seasonal water uptake by almonds under pulsed (FI_p) and slow discharge continuous irrigation (FI_c) remained almost on par, indicating that pulsing didn't provide any added advantage, although it is a viable alternative to slow discharge continuous irrigation. The average modelled soil solution salinity (EC_{sw}) of the profile also remained below the threshold for yield reduction during the growing season in all treatments. The irrigation water productivity (WP_I) increased substantially (37%), yield was reduced by 8% and about 35% of irrigation water was saved under sustained deficit irrigation (SDI_p) compared to full irrigation (FI_p). The SDI_p concluded to be a promising deficit irrigation strategy for almond cultivation. These outcomes can be utilized to improve irrigation efficiency and system design for drip irrigation of almonds.

HYDRUS-1D Modeling Applications to Waste Disposal Problems in Brazil

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In this study we used the HYDRUS-1D software package to investigate the performance of three types of waste disposal sites or repositories in Brazil: a conventional mining installation containing naturally occurring radioactive materials (NORMs), a municipal landfill and a radioactive waste repository.

The first application involved NORM waste disposed of in an industrial landfill on top of a base of earth materials to ensure integrity of the deposit over relatively long geologic times (thousands of years). HYDRUS-1D was used to predict long-term radionuclide transport vertically through both the landfill and the underlying unsaturated zone, and then laterally in groundwater. Calculations were carried out for both a best-case scenario assuming equilibrium transport in a fine-textured (clay) subsurface, and a worst-case scenario involving preferential flow through a more coarse-textured subsurface. Preferential flow and soil texture both were found to have a major effect on the results, depending upon the specific radionuclide involved.

The second study concerned water fluxes into and through a municipal solid waste (MSW) landfill in the city of Rio de Janeiro. Two cover systems were considered that would minimize infiltration into the landfill. One used a capillary barrier made from MSW compost, and another one a vegetation cover using grasses and native species from the area. Results for the capillary barrier system compared closely with observed leachate rates at the landfill.

The third application involved a near-surface repository containing Cs-137 wastes resulting from decontamination of Goiania city in Brazil after the 1987 accident with a CsCl teletherapy source. The study provided estimates of water fluxes through the soil cover into and through the repository and concrete liners towards underlying groundwater. This was done by first applying a detailed water balance to the soil cover accounting for local precipitation and evapotranspiration rates, including root water uptake by grass on the cover. Performance of the cover system and engineered barriers was followed for a 400-year period, which included accounting for the effects of concrete degradation on the hydraulic properties of concrete. HYDRUS-1D was used next to simulate Cs-137 transport from the repository through the concrete liner below the waste and the underlying vadose into the groundwater aquifer below the site. Simulations provided estimates of future radionuclide fluxes into groundwater, and hence possible exposure to the public.

Simulation of Groundwater Evapotranspiration with HYDRUS-1D in Desert Environments

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Groundwater evapotranspiration (ET_G) is an important part of the water balance for wetlands/riparian zones in desert environments; however, ET_G estimate in these regions still remains a challenge due to the difficulties involved in quantifying the atmospheric evaporative demand, the soil hydraulic properties, the vegetation parameters, and the changes in water tables. In this study we present a statistical approach toward reducing uncertainties in ET_G estimating from diurnal water table fluctuations. A one-dimensional saturated-unsaturated soil water flow model with HYDRUS-1D program (Šimůnek et al, 2008) was used to simulate daily and seasonal groundwater fluctuations in a desert area of northwest China for the period of 2009-2011. Simulations were conducted for four different soil profiles (sand, loam, silt, and sandy clay) and two typical vegetation covers (*Populus* and *Tamarix*) with temporal variability of precipitation, potential evaporation and transpiration input data, which was produced using special preprocessing code SurfBal 3.60 (Pozdniakov, 2012).

The results show that a strong linear relationship exists in all model settings between the ET_G values and the standard diversion of water table fluctuations. However, for low hydraulic conductivity aquifers (silt and sandy clay), root water uptake induces a considerably water table depression. In this case, the proposed method based on water-table fluctuation overestimates the prescribed ET_G. In contrast, for coarse aquifer type (sand and loam) the proposed method underestimates the ET_G rate because the decreasing storage can be readily recovered due to the high hydraulic conductivities. To correct the proposed method by using diurnal water table fluctuations, the "scaling factor (k)", which depends on the soil physical characteristics, were introduced in ET_G estimating.

Modeling Water and Nitrogen Fate in Plots with Sweet Sorghum Irrigated with Fresh and Blended Saline Waters Using HYDRUS-2D

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The Alentejo region in southern Portugal faces water scarcity and environmental problems as a result of high atmospheric evapotranspirative demand and irregular rainfall. The need to reduce irrigation water demand and non-point source pollution in the region has made sweet sorghum [*Sorghum bicolor* (L.) Moench] an interesting alternative crop to other traditional summer crops due to its lower water and nutrient requirements. This paper describes results from a long term simulation study where HYDRUS-2D was used to assess the fate of nitrogen in a plot planted with sweet sorghum, while considering drip irrigation scenarios with different levels of nitrogen and salty waters. HYDRUS-2D simulated water contents, EC_{sw}, and N-NH_4^+ and N-NO_3^- concentrations continuously between 2007 and 2010, while producing RMSE between simulated and measured data of 0.030 cm^3 cm^{-3}, 1.764 dS m^{-1}, 0.042 $mmol_c$ L^{-1}, and 3.078 $mmol_c$ L^{-1}, respectively. Transpiration varied between 360 and 457 mm depending upon the crop season and the irrigation treatment. Sweet sorghum showed to be tolerant to saline waters only during one crop season. After that, the continuous use of saline waters led to soil salinization, and to root water uptake reductions due to the increasing salinity stress. N-NO_3^- uptake was higher when fertigation events were more numerous and the amounts applied per event smaller. The yield function developed from the N-NO_3^- uptake and the dry biomass yield (R^2 = 0.71) estimated nitrogen needs between 130 and 180 kg/ha. The movement of N out of the root zone was dependent on the amount of water flowing through the root zone, the amount of N applied, the form of N in the fertilizer, and the timing and number of fertigation events. The effect of the osmotic stress on nitrogen leaching was only minimal. The simulations with HYDRUS-2D were thus useful to understand the best strategies toward increasing nutrient uptake and reducing nutrient leaching.

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Simulation of Peak Loads for Horizontal Flow Constructed Wetlands

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Constructed wetlands (CWs) are a wastewater treatment technology that exploits the physical, chemical, and biological processes developed in soil in order to improve the water quality. The low operation and maintenance costs allow for a widespread use of CWs, especially in treating wastewater from small communities (up to 2000 population). Despite the wide application of CWs, many aspect of CW behavior in real environment still needs to be investigated, including buffering capacity to sudden peak loads. Indeed, the stochastic behavior of real influent loads are generally neglected during the typical CW design procedure, and CW parameters should highly overestimated to face real load variability. Hence, further efforts are still need to improve the ability to properly design CWs. Here a process-based model approach is used to better understand the response of a horizontal flow (HF) CW subjected to peak loads. Laboratory experiments were conducted by Galvão and Matos [2012], where HW-CWs were subjected to sudden load of different intensities. Data from these laboratory experiments are used to calibrate a model of the HF-CW set-up using the HYDRUS wetland module [Langergraber and Šimůnek, 2012]. The calibrated model fits the data well and is further used to explore different loading scenarios. In this way, we are able to understand in which case the CW fails the maximum allowed effluent concentrations. In future, we will use the calibrated model to investigate the behavior of HF-CW to stochastic processes such as loading and temperature seasonal variations.

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Longitudinal Dispersivity Determination Using Conservative Tracer in the Field

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Solute transport parameters determination in the unsaturated zone is of great importance for groundwater pollution risk assessment. The subject of study was Fluvisol developed on the floodplain of Sava River. The goal of the study was estimation of longitudinal dispersivity which is one of the main solute transport parameters. Purpose of this paper is presentation of problems that occurred during experiment which led to doubtful results.

Field experiment using conservative tracer calcium chloride was carried out. Longitudinal dispersivity was estimated by modeling chloride concentration using HYDRUS-1D. Investigated site is situated about eight hundred meters from right bank of Sava River at Kosnica regional well field. The experimental site was equipped with two time domain reflectometry (TDR) probes, two electrical conductivity (EC) probes and four suction lysimeters. All vegetation was removed from the research area and the surface was levelled. The plot of 0.7 m^2 was irrigated with a 200 l tracer solution over two hours. During the experiment, soil moisture (using TDR probes) and electrical conductivity (using EC probes) were measured every twenty minutes. Percolating solution is sampled by suction lysimeter installed at 40 cm depth. Chloride concentrations in leachate were analyzed using ion chromatography (IC).

Due to collapse of pedological pit during application of tracer and sampling of percolating solution, field experiment was not completed. Therefore, estimation longitudinal dispersivity was performed on incomplete data set.

Keywords: Fluvisol, field experiment, solute transport parameters, HYDRUS-1D

Modelling Horizontal Flow Constructed Wetlands Treating Effluents of Wastewater Treatment Plants

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The HYDRUS Wetland Module has been used to estimate the efficiency of a constructed wetland (CW) system, designed for the treatment of effluents from wastewater treatment plants near the Tablas de Daimiel National Park (Spain). The purpose is to restore this natural wetland with the effluents of several plants in the surroundings, improving the water quality throughout CWs, so the quality requirements are higher than standards.

The main aim for the simulation was to verify the treatment system design of horizontal flow (HF) CWs consisting in several cells. The HF beds have a length of 23 m (including a 0.4 m inlet area), a width of 22 m and a depth of 0.6 m for the treatment of 96 m^3 d^{-1} each one, resulting in an hydraulic loading rate of 19 cm d^{-1}. The effluents characterization indicated that the system should be able to treat water with high concentrations of organic matter and ammonium. The influent concentrations have been considered 125 mg O_2 L^{-1} and 15 mg N L^{-1} for COD (mainly as slowly biodegradable particulate COD) and ammonium, respectively.

The implementation in HYDRUS used the CWM1 biokinetic model formulation simulating reactive transport in CWs, since it is considered more appropriate than CW2D for HF CWs (because CWM1 also models anaerobic processes). The influence of plants in wetlands has been considered in this implementation, with the typical values reported for common reed for transpiration rate and specific O_2 release: 7.4 mm d^{-1} and 5 g m^{-2} d^{-1}.

The first simulation results showed an excessive heterotrophic bacteria growth, especially near the inlet and the water table, with unrealistic values over 50000 mg kg^{-1} after 6 days simulation. Some kinetic and stoichiometric parameters have been then modified with respect to their original values in CWM1 to fix the heterotrophic bacteria development: maximum aerobic growth rate, rate constant for lysis, saturation/inhibition coefficient, fractions generated in biomass lysis and hydrolysis rate constant. After several simulations combining different values for these parameters, a steady state was found. A 30 days simulation based on this implementation shows better treatment efficiency than expected in the design: 66% of COD removal and 39% of NH_4 removal.

Key words: Constructed Wetlands, CWM1, HYDRUS wetland module, Tablas de Daimiel National Park.

Predicting the Impact of Treated Wastewater on Groundwater Recharge by Simulating Reactive Transport in the Unsaturated Zone

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According to the European Water Frame Directives, all EU member states shall protect, enhance and restore all bodies of groundwater, ensure a balance between abstraction and recharge of groundwater, with the aim of achieving a good chemical and ecological status until 2015. Since a significant part of groundwater recharge comes from wastewater, important steps in collecting and disposing it have been taken by the member states. The objective of this work is to use the soil natural treatment capacity to artificially recharge the groundwater system using treated wastewater effluent from small-scale treatment plants, thereby generating reserves for drinking water production and irrigation. For this purpose, the software tool PCSiWaPro® developed at the Technical University Dresden, Institute of Waste Management and Contaminated Site, and based on the SWMS2D model by SIMUNEK & VAN GENUCHTEN is further enhanced. PCSiWaPro® offers an application-oriented interface to the SWMS2D model for the simulation requirements of specific real-life applications, in this case for wastewater effluent prognosis. To account for the relevant biogeochemical reactions in unsaturated zone PCSiWaPro® is coupled to the geochemical software PHREEQC as well as to the groundwater model PCGEOFIM®. The impact of leaching of biologically treated wastewater can differ locally and depends on the hydrogeological and hydrological conditions. To forecast the physicochemical and microbiological processes and to detect the concentration of infiltrated treated wastewater into unsaturated zone, a series of scenarios are modeled with the help of the software PCSiWaPro®. To validate the enhanced simulation software, a series of column experiments were conducted. The results of the modeling and lab experiments have improved the understanding of the complex processes in unsaturated zone and its relationship with groundwater zone. It is now possible to efficiently design and operate small-scale wastewater treatment plants and also to predict groundwater recharge.

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Temporal Variations of Soil Hydraulic Properties and its Effect on Soil Water Simulations

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Simulating shallow soil water dynamics is challenging since this soil compartment is temporally highly dynamic as response to climate and crop growth. For accurate simulations the soil hydraulic properties have to be properly known. These properties may be subject to temporal changes as a response to both tillage and natural impact factors. The impact of different tillage techniques – conventional (CT), reduced (RT), and no-tillage (NT) – on the soil hydraulic properties and their temporal dynamics were observed by repeated experiments using tension infiltrometers. The experimental data was analyzed in terms of the near-saturated hydraulic conductivity, inversely estimated parameters of the van Genuchten/Mualem (VGM) model, and the water-conducting porosity. In a second step, the inversely estimated VGM parameters were incorporated into a soil water simulation. By using temporally variable versus constant sets of VGM parameters, the impact on soil water balance components was tested. Simulated water dynamics were compared to observed data in terms of the soil water content and water storage in the near-surface soil profile (0-30 cm). The results show that the near-saturated hydraulic conductivity was in the order CT > RT > NT, with larger treatment-induced differences where water flow is dominated by mesopores. The VGM model parameter α_{VG} was in the order CT < RT < NT, with high temporal variations under CT and RT, whereas the parameter *n* was hardly affected. The results give indirect evidence that NT leads to greater connectivity and smaller tortuosity of macropores, possibly due to a better established soil structure and biological activity. Simulations with temporally constant hydraulic parameters led to underestimations of soil water dynamics in winter and early spring and overestimations during late spring and summer. The use of temporally variable hydraulic parameters significantly improved simulation performance for all treatments, resulting in average relative errors below 13 %. Since simulation results agreed with observed water dynamics in two seasons, the applicability of inversely estimated hydraulic properties for soil water simulations was demonstrated. Our results also showed that simulations addressing applied questions in agricultural water management can be improved by time-variable hydraulic parameters. We currently work on the description of temporal changes of the hydraulic properties and its underlying pore-size distribution on a physically basis by accounting for swelling/shrinking cycles, crop root development and root-size distribution.

New Developments in the HPx Reactive Transport Code: Extensions to Two- and Three-Dimensional Flow and Transport Problems

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A large number of interacting physical, chemical, and biological processes determine the fate of major cations and anions, contaminants (e.g., heavy metals, pesticides), and colloids in soil systems. Also, modeling of soil CO_2 sequestration requires consideration of water flow, heat transport, gas diffusion, and microbiological soil respiration processes. The HP1 simulator (Jacques et al., 2008) is a state-of-the-art model that was specifically developed to evaluate these and similar processes in the unsaturated zone. HP1 couples the one-dimensional variably-saturated flow and transport model HYDRUS-1D (Šimůnek et al., 2008) with the generic geochemical model PHREEQC (Parkhurst and Appelo, 1999). Although HP1 is a versatile code for implementing different geochemical and transport conceptual models in variably-saturated porous media, one of its main limitations is that flow and transport is restricted to one dimension. Therefore, PHREEQC has recently been coupled also with HYDRUS (2D/3D) (Šimůnek et al., 2011) to handle flow and transport problems, which require a higher dimensionality (HP2/3). Typical examples are flow and transport in soil systems with tiled drains, or with drip and furrow irrigation, or in sloped layered or heterogeneous systems. A typical two-dimensional flow and transport problem illustrating the capability of the HP2 simulator will be presented. The HP2/3 code uses the graphical user interface of HYDRUS (2D/3D) for input and output processing, enabling definitions and finite element discretization of very complex flow domains.

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Hillslope Application of the HYDRUS-Wetland Wetland Module

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We applied HYDRUS-Wetland to the simulation of nitrate dynamics in a rural headwater catchment (Smethurst *et al*., 2013), i.e., production in soil and its delivery to a stream via surface and subsurface processes. A two-dimensional (hillslope) modeling approach was used. Total flow was mathematically separated into quick- and slow-flow components, and the latter was routed through the HYDRUS software with a nitrogen module designed for constructed wetlands. The model accurately accounted for nitrate turnover, leading to the hypotheses that denitrification was a minor flux (<3 kg N ha^{-1}) compared to uptake (98-127 kg N ha^{-1}), and that trees next to the stream would reduce denitrification if they lowered the water table. This research provides an example of the measurement and modeling of nitrate dynamics at a small-catchment scale with high spatial and temporal resolution. More information on the simulation results can be found in the publications (Smethurst *et al*., 2010, 2013) and will be presented in the poster. In this abstract we summarize our experiences regarding limitations that we faced when simulating a hillslope.

Several modeling limitations were identified that, if addressed, could improve the HYDRUS wetland module applications in this context:

1. *Overland flow* was simulated by pre- and post-HYDRUS processing. Temporal patterns of concentration in overland flow can be critical to accurately predicting solute export. Note that although an overland flow module for HYDRUS is now available, it does not consider overland solute transport yet.
2. *Preferential flow* was not possible while using the wetland module
3. *Runoff as saturation excess* is possible as a variable seepage zone, but rainfall was not continued on that portion of the slope. Hence, the water balance was altered.
4. Without a *variable seepage zone*, conditions that approach saturation near the surface dramatically slow or stop the model due to mathematical difficulties.
5. Only one *root type* was specified, wherever they are placed in the simulation domain. However, a two-root-type version of HYDRUS was being tested (Šimůnek pers. comm.).
6. *Nutrient uptake* is simulated only as the mass flow component. This might not be a serious issue for nitrate, for which uptake in many systems is predominantly via massflow. However, for nutrients that are taken up mainly via diffusive processes, e.g. ammonium, phosphorus and potassium, simulated uptake is likely to be greatly underestimated using HYDRUS. A version of HYDRUS is now available that includes active and passive compensated uptake (Šimůnek and Hopmans 2009).
7. For hillslope applications of HYDRUS, with or without the wetland module, it would be very useful to include outputs of pools and fluxes of both water and nitrate on a *per area* basis.
8. The wetland module was probably *over-specified* for our application, e.g. organic and microbial pools are not required for simpler, useful soil N dynamics models.

9. Over-specification contributed to *slow performance* (7 hours for an annual simulation using daily rainfall).
10. Denitrification doesn't split N gasses into N_2 and N_2O.
11. We were unable to parameterise O diffusion into the soil in a way that maintained a realistic O profile.
12. Nitrification sensitivity to soil water content needs further testing.

These simulations were also data-limited:

1. Data were not available for a full definition of the spatial and temporal heterogeneity of the initial and boundary conditions for soil water and nitrate, including preferential flow, saturated and unsaturated hydraulic conductivity, nitrogen turnover and root distribution and activity.
2. The solute dynamics of overland flow are highly complex, because they depend on poorly understood and poorly predicted interactions between overland flow and surface soil.
3. *In situ* rates of denitrification are extremely difficult to measure in a way that captures spatial and temporal variability.

Although these types of simulations can only be a gross simplification of reality, using a 2D hillslope modeling approach as demonstrated would probably be useful also for many other types of applications.

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CO_2 Fluxes to Aquifers Beneath Cropland: Merging Measurements and Modeling

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The global flux of CO_2 into the groundwater is <1 % of the diffusion flux of CO_2 from soils to the atmosphere. The potential for storage of dissolved inorganic carbon (DIC) in aquifers was investigated as a strategy to mitigate increasing atmospheric CO_2 concentrations. Data from unplanted and planted soil mesocosms were modeled using the HP1 software package with the objective to identify the main drivers in DIC transport to aquifers.

Soil was collected from the A and C horizon of cropped alluvial sand and packed into mesocosm columns above a bottom plate with an embedded suction disc. The hydraulic connection between the C horizon and the suction disc was optimized by means of a thin layer of quarts flour and a layer of quartz flour mixed with C horizon. For the modeling, these layers and the suction disc were regarded as one unit. Inverse modeling of the water flow was carried out by applying a coupling of the Monte Carlo algorithm and HYDRUS-1D to search for the global minima for the retention parameters of all three materials. The retention parameters were then inserted into HP1 for forward modeling of water contents. Equations for CO_2 production by microorganisms and roots from the SOILCO2 model (Simunek and Suarez 1993) were programmed into HP1 using only few modifications.

Preliminary results showed the model simulated water content throughout depth and time quite well, in particular in unplanted mesocosms. Due to a pressure drop across the suction disc and the lack of retention parameters for the quartz flour/C horizon layer, outflow was simulated less accurately than water content. The model provided a good fit to measured DIC efflux, CO_2 partial pressure (pCO_2) and alkalinity in both unplanted and planted mesocosms. However, the CO_2 efflux from the mesocosm top was significantly underestimated in unplanted mesocosms.

Data will be presented to show that DIC storage in aquifers is controlled by drainage volume, pH and pCO_2. If nutrient availability is not decreased, lime amendment could be a way to increase natural (plant-mediated) CO_2 storage in aquifers.

Fate and Transport of Nitrogen in Soils Based on a Coupled Nitrogen-Carbon Cycling Model Using the HP1 Code

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In order to predict fate and transport of nitrogen as a result of decomposition of organic matters in soils, we implemented a coupled carbon and nitrogen cycling model based on Johnsson (1987) and the LEACHM code (Hutson, 2005) using the PHREEQC program. Two types of principal organic matter were defined: a first cycling pool for litter and a slow cycling pool for stabilized humus. Separate litter pools were used for organic matters having a different decay rate and carbon-to-nitrogen (C/N) ratio such as plant residue and manure. Decay processes from the organic-C to biomass-C, humus-C, and carbon dioxide were described with a first-order kinetic. The biomass-C was recycled into the decomposable litter pool, forming the litter-decomposer complex. Decompositions from the organic-N to biomass-N and humus-N were related to the carbon cycle using the C/N rations of the organic matter, biomass and humus. Mineralization of ammonium from the organic matter and immobilization of ammonium to the organic matter were determined based on the available N in the litter pool and the N demand for the formation of biomass and humus. Nitrogen transformations were also described with first-order chain reactions for ammonification from uera, nitrification from ammonium, and denitrification from nitrate.

All the first-order kinetics equations for the carbon and nitrogen cycles described in PHREEQC were linked with water flow, root water uptake, solute transport, and passive root nutrient uptake in HYDRUS-1D using the HP1 code. Various nitrogen transport scenarios were demonstrated for the application of organic matters to a variable-saturated soil under a nonisothermal condition.

Simulation of Metal Transport in the Soil and into the Willows Using the HYDRUS Program

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The main aim of this study was to validate the HYDRUS program for the simulation of Cd, Cu, Pb and Zn transport within a soil column and for their willow uptake. A simulation of metal transport and accumulation into the willow was implemented using the HYDRUS-2D/3D code (version 1.11). Two scenarios of the column experiment were compared: filled by contaminated soil (C) and filled by contaminated soil with planted willow (V). Seeping water, soil water content and actual transpiration were measured over the period of time. Metal contents in soil water and willows were also analysed. The single-porosity model (applied for isotropic soil media) was sufficient for scenario C. The single-porosity (applied for anisotropic soil media) and dual-porosity models (characterizing non-equilibrium water flow) were explored in scenario V due to vertical roots modification of the soil structure. Simulated cumulative water and metal (Cd, Cu, Pb and Zn) outflow from the soil column in scenario C moderately approximated the measured data, when the isotropic single porosity system was used. On the other hand, for scenario V the best correspondence of modelled to the measured data was observed in case of dual-porosity model consideration. Additionally, measured cumulative Cd and Zn root uptake showed a 20- and 10-fold increased accumulation respectively in comparison with the model, due to the accumulation not only from the water soluble fraction (used for HYDRUS calculations). The modelled Pb uptake was modified by reducing the maximum value of the root uptake concentration c_{root} due to a very low accumulation and relatively high water soluble concentration. Measured and modelled Cu uptake was similar. No significant impact of anisotropy or dual-porosity soil media consideration has been revealed for this case. In summary, the HYDRUS-2D/3D code (version 1.11) was usable for modelling of Cd, Cu, Pb and Zn transport and their willow uptake. Additionally, consideration of dual porosity (also anisotropy) soil media was suitable for the experiment with roots presence in the soil.

Keywords: Soil column; HYDRUS-2D/3D code; Numerical optimization; Anisotropy and dual-porosity soil media; Metal transport; Root metal uptake

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Investigation of Recharge Fluxes under Different Land-Uses with Calibrated Models to Transient Deep Vadose Zone Data

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Recharge component plays a crucial role in determined groundwater quantity and quality assessments. Development of recharge estimation and prediction tool contributes to improving the management of groundwater resources. Vadose zone monitoring systems (VMS) were implemented under crop-field, grapefruit orchard and natural sand-dune. The VMSs have enabled the acquisition of continuous information on both the temporal variation of water content and the chemical composition of the sediments pore water at multiple depths in the deep vadose zones (~ 20 m). Vertical unsaturated flow models were calibrated to the transient data. Subsequently, the calibrated models provided an opportunity to investigate the temporal characteristics of groundwater recharge through long periods with variable rain patterns under the different sites. The models simulations resulted in low average recharge flux of 134 mm yr^{-1} under the orchard, 206 mm yr^{-1} under the crop-field and 341 mm yr^{-1} under the natural sand-dune which is 10%, 40% and 66% of the annual surface-water inputs, respectively. In addition, the calibrated models were implemented for examining the impacts on recharge quantity and quality due to climate change and land use change scenarios. A climate change scenario was performed with the calibrated model of the crop-field and revealed that reduction of 19% in total rain amount led to a drop of 46% in average recharge**.** Simulations of conversion of the natural sand dune to a commercial tomato greenhouse displayed a decrease in average recharge (from 341 to 150 mm yr^{-1}).

Microtopographic Enhancement of Soil-Based Wastewater Treatment

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Tertiary treatment of wastewater has become increasingly important. One option for tertiary treatment is the use of soil-based treatment systems. These may simply be vegetated plots irrigated with secondary treated wastewater. This enables the water quality regulating processes found within soils to be exploited.

There is evidence (Wolf et al., 2011) to suggest that enhancing the microtopography (MT) of a soil-based treatment system may influence nutrient cycling. For example, an increase in denitrification potential may occur within the depressions of a microtopographically-enhanced system as a result of: a lower redox potential; an accumulation of organic matter; and a larger population of denitrifying microorganisms. It may also be the case that vegetation species richness can be increased with enhanced MT (Moser et al., 2007).

In order to test the application of these theories to soil-based treatment of wastewater and evaluate the potential benefits and drawbacks, a field trial has been established at a treatment works in Hampshire, UK. The trial consists of several grass plots, each irrigated with secondary treated wastewater from the adjacent wastewater works. Excluding the control plots, the surface MT of each plot has been enhanced by the introduction of ridge-and-furrows. The MT of each plot has been characterised using various indices; subsurface soil water is monitored for NH_4, NO_3, PO_4, total nitrogen and total phosphorus concentrations; soil moisture and redox potentials are monitored over the course of irrigation cycles; and soil samples are periodically analysed for total and extractable nitrogen and phosphorus, total carbon, organic matter, pH, electrical conductivity and sodium adsorption ratio (SAR).

To extrapolate the findings of this study beyond the limitations of a field trial, the HYDRUS-2D program with the Wetland Module will be employed. The hydraulic and biogeochemical processes within the soils of the trial plots will be modeled. Once validated, parameters within the model will be changed to allow hypothetical modeling of soil-based treatment systems for a number of soil types, over a range of microtopographic values and irrigation loading rates. The results of this modeling may then be used to: optimise microtopographic design of soil-based treatment systems; estimate removal rates; and inform risk assessments for their use.

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Using HYDRUS and HP1 Codes to Study Possible Impacts of Irrigation with Non-Conventional Water Under Two Different Vadose Zone Monitoring Strategies

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South-east of Spain is a region characterized by low annual rainfall (200-300mm) and high potential evapotranspiration rates (~1200 mm/year). Joint with that situation, an endemic scarcity of water resources is presented, and the potential development of the region is hindered by this lack of water. In the last years, desalination of both brackish groundwater and seawater has become a new and important water source; firstly to satisfy urban demands and lately for agricultural purposes too. The effects of non-conventional water use on the vadose zone might produce impacts in porous media which could lead to changes in soil hydraulic properties, among others. In this context, monitoring vadose zone water dynamics is a key aspect to study those possible impacts and to manage the scarce water resources. According to the available literature, different monitoring systems have been carried out independently, however less attention has received comparative studies between different techniques.

A 9x5 m^2 experimental plot was set with automatic and non-automatic sensors to control θ and h up to 1.5m depth. The automatic system composed of five 5TE sensors (Decagon Devices®) installed at 20, 40, 60, 90 and 120 cm for θ measurements and one MPS1 sensor (Decagon Devices®) at 60 cm depth for h. Installation took place laterally in a 40-50 cm length hole bored in a side of a trench that was excavated. All automatic sensors hourly recorded and stored in a data-logger. The non-automatic system consisted of ten Jet Fill tensiometers at 30, 45, 60, 90 and 120 cm (Soil Moisture®) and a polycarbonate access tube of 44 mm (i.d) for soil moisture measurements with a TRIME FM TDR portable probe (IMKO®). Vertical installation was carefully performed; measurements with this system were manual, twice a week for θ and three times per week for h. Boundary conditions were controlled with a volume-meter and with a meteorological station. ET was modelled with Penman-Monteith equation. A complete soil characterization was carried out in laboratory to determine grain size distribution, bulk density, gravimetric water content and water retention curves. Unsaturated soil hydraulic parameters were model-fitted through SWRC-fit code and ROSETTA based on soil textural fractions when laboratory data were no available.

Simulation of water flow using automatic and non-automatic date was carried out by HYDRUS-1D. A good agreement from collected automatic and non-automatic data and modelled results can be recognized. General trend was captured, except for the outlier values as expected. Slightly differences were found between hydraulic properties obtained from laboratory determinations, and from inverse modelling from the two approaches. Differences up to 14% of flux through the lower boundary were detected between the two strategies. According to results, automatic sensors were more accurate and so more appropriated to detect subtle changes of soil hydraulic properties. Nevertheless, if the aim of the research is to control the general trend of water dynamics, no significant differences were observed between the two systems. Finally geochemical processes simulation is being carried out with HYDRUS and PHREEQC (HP1).

Simulation of Heavy Metal Transport in Unsaturated Soil: Use of Scale Factors to Quantify Variable Sorption Isotherms

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Heavy metals are toxic soil pollutants. They are stored in soils by sorption processes. At a small scale (soil sample) the sorption process can be observed and quantified by sorption isotherms. However, environmental issues have to be treated at large scales (e.g., a field scale). At the field scale heavy metal sorption isotherms are mostly highly variable in space. This variability makes representative quantification of the sorption process (e.g., for soil protection and management of soil functions) and its consideration in reactive transport modeling (e.g., for groundwater protection) hard. Many transport simulation studies therefore treat the soil as homogeneous to avoid complex datasets and calculations. In the present study we use a recently developed method - calculation of scale factors - to quantify the spatial variability of heavy metal sorption in soils at the field scale. This method reduces the wide spread of the sorption isotherms into a single average relation, while at the same time preserving their variation through the use of the scale factors. We investigated the spatial variability of heavy metal sorption isotherms for an agricultural field on a Luvisol developed in loess material near Hannover, Germany. 50 samples were taken from each A and B horizons along a 250 m transect. Sorption isotherms for heavy metals and soil properties as pH, CEC, and texture were measured, and scale factors were calculated. The heavy metal transport is simulated with HYDRUS with a unique reference sorption isotherm (derived from the scale procedure or from the mixed soil sample, respectively). Spatial variability of sorption at every sampling point is represented using a scale factor, which was directly calculated (scaling procedure), or indirectly estimated (transferred) by regression models from another heavy metal or from soil properties, respectively.

In our contribution we will present results on (1) a numerical simulation of the heavy metal transport in unsaturated soil, considering the sorption variability by directly calculated and indirectly estimated scale factors, and (2) a comparison with the transport behavior simulated with the sorption isotherms measured at each sampling point.

Comparison of Ion (Salt) Movement in the Soil Profile Subject to Leaching with the HYDRUS-1D Simulations

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There is an increasing trend to require more efficient use of water resources, both in urban and rural environments. Drainage water can be beneficially reused for agricultural irrigation before being discarded after its use. The quality of the discarded water depends on many factors, including the irrigation water quality and irrigation management, i.e., the salt content and the quantity of irrigation water to be applied during the vegetation period.

A variety of analytical and numerical models have been developed during the past several decades to predict water and solute transfer processes between the soil surface and groundwater table. The HYDRUS-1D software package is one of such models simulating water movement and solute transport in the soil. In this study, we use HYDRUS-1D to analyze water flow and solute transport in soil columns 115 cm long and with a diameter of 40 cm, irrigated with waters of different quality at different leaching rates. Three different irrigation water salinities (0.25, 1.5, and 3.0 dS/m) and four leaching fractions (10, 20, 35, and 50% more water than required) were used in a fully randomized factorial design experiment. Each experiment was run in three replicates, resulting in the total of 36 lysimeters. Following every irrigation, the drainage waters were collected using the plastic pods situated under each lysimeter. Water fluxes, concentrations of individual ions (Na^+, K^+, Ca^{2+}, Mg^{2+}, Cl^-, SO_4^{2-}, CO_3^{2-}, and HCO_3^-), EC of the soil solution, and SAR were monitored at five depths (20, 40, 60, 80, and 100 cm) in all soil columns. The soil used for the experiments was SCL. In all leaching experiments, the salts accumulated in the profile due to irrigation with salty water could be leached out from the soil. More soluble salts, such as Cl^-, leached more easily than the less soluble salts, such as CO_3^{-2} and HCO_3^-.

The results showed that HYDRUS-1D was able to successfully simulate soil water salinity and movement of salts (ions) in the soil profile. The RMSE values for all treatments and for different soil depths varied for EC (dS/m) between 2.50-5.21 and 1.36-4.38 and for SAR between 1.26-3.18 and 1.45-1.88 during the first (2010) and second (2011) experimental year, respectively. The RMSE values for ions Ca^{2+}, Mg^{2+}, Na^+, K^+, SO_4^{2-}, and Cl^- were between 0.50-24.14 in 2010, and 0.28-14.25 in 2011. HYDRUS-1D proved to be a powerful tool for analyzing solute concentrations related to overall soil salinity.

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