5th International Conference

HYDRUS Software Applications to Subsurface Flow and Contaminant Transport Problems

March 30-31 2017

Prague, Czech Republic
Preliminary Program

Thursday, March 30, Morning session:

**Variably-Saturated Water Flow and Transport of Contaminants**

<table>
<thead>
<tr>
<th>Time</th>
<th>Authors and Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>8:20-8:50</td>
<td>Arrival, registration</td>
</tr>
<tr>
<td>8:50-9:00</td>
<td>Radka Kodešová and Rien van Genuchten (presiding): Opening remarks</td>
</tr>
</tbody>
</table>
| 9:00-9:30| **Keynote Presentation: Jirka Šimůnek**  
| 9:30-9:50| Batalha, M. S., E. M. Pontedeiro, and M. Th. van Genuchten, Groundwater recharge calculations as affected by temporal averaging of meteorological data. (Brazil) |
| 10:10-10:30| Liang, J., S. A. Bradford, J. Šimůnek, and A. Hartmann, Modeling non-equilibrium overland flow and transport processes using HYDRUS-1D. (USA) |
| 11:00-11:30| **Keynote Presentation: Giuseppe Brunetti**  
Brunetti, G., and J. Šimůnek, Selected Applications of HYDRUS Models for Engineering Problems. (Italy and USA) |
| 11:50-12:10| Berger, K., Comparison and validation of SWMS_2D and HYDRUS (2D/3D) for capillary barriers using data of a 10-m tipping through. (Germany) |
| 12:10-12:30| Suskin, V. V., I. V. Kapyrin, and A. V. Rastorguev, Modeling unsaturated groundwater flow and transport in the vadose zone using GeRa code. (Russia) |

Coffee Break

<table>
<thead>
<tr>
<th>Time</th>
<th>Authors and Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>12:30-13:00</td>
<td>Lunch</td>
</tr>
</tbody>
</table>
### Thursday, March 30, Afternoon Session:

#### Irrigation Applications, Roots, and Miscellaneous Topics

<table>
<thead>
<tr>
<th>Time</th>
<th>Authors and Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>2:00-2:30</td>
<td><strong>Keynote Presentation: Naftali Lazarovitch</strong></td>
</tr>
<tr>
<td></td>
<td>Raij, I., G. Bel, and Naftali Lazarovitch, Unveiling multi-dimensional water flow and solute transport using HYDRUS codes. (Israel)</td>
</tr>
<tr>
<td>2:30-2:50</td>
<td>Hartmann, A., J. Šimůnek, M. K. Aidoo, S. J. Seidel, and N. Lazarovitch, A new HYDRUS add-on module to model the interactions between plant roots, soil properties, and water flow conditions in soils. (Germany, USA, and Israel)</td>
</tr>
<tr>
<td>2:50-3:10</td>
<td>Diamantopoulos, E., M. Walkinshaw, T. O’Geen, and T. Harter, Assessing nitrate leaching potential in California’s agricultural soils through Hydrus-1D simulations. (USA)</td>
</tr>
<tr>
<td>3:10-3:30</td>
<td>Glass, J., T. Fichtner, and C. Stefan, Stepwise calibration of hydraulic conductivity changes in a laboratory tank simulating managed aquifer recharge operation. (Germany)</td>
</tr>
<tr>
<td>3:30-3:50</td>
<td>Fér, M., R. Kodešová, A. Nikodem, and A. Klement, Using HYDRUS-1D for estimating soil hydraulic parameters from capillary rise and evaporation rates measured using a clay tank and soil respiration chamber, respectively, and their correlation with a net CO₂ exchange rate. (Czechia)</td>
</tr>
</tbody>
</table>

**Coffee Break**

<table>
<thead>
<tr>
<th>Time</th>
<th>Authors and Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>4:10-4:40</td>
<td><strong>Lightning Session</strong></td>
</tr>
<tr>
<td></td>
<td>(3 min presentations of the posters)</td>
</tr>
<tr>
<td>4:40-6:00</td>
<td><strong>Poster Session</strong></td>
</tr>
<tr>
<td>6:00 - ....</td>
<td><strong>Mixer, Beer Session</strong></td>
</tr>
</tbody>
</table>
**Friday, March 31 Morning session:**

### Biogeochemical Transport and Reactions

<table>
<thead>
<tr>
<th>Time</th>
<th>Authors and Title</th>
</tr>
</thead>
</table>
| 9:00-9:30  | **Keynote Presentation: Günter Langergraber**  
Langergraber, G., Process-based models for subsurface flow treatment wetlands: Recent developments and challenges. (Austria)                                                                                                         |
| 9:30-9:50  | Hochfeldt, V., B. Pucher, and G. Langergraber, Simulating a full-scale two-stage vertical flow wetland system using the HYDRUS Wetland Module. (Austria)                                                                                                                                                                                                                                                                                                                                                                         |
| 9:50-10:10 | Pucher, B., and G. Langergraber, Simulation results using the HYDRUS Wetland Module for different sized filter medias in vertical flow treatment wetlands. (Austria)                                                                                                                                                                                                                                                                                                                                                      |
| 10:10-10:30| Llorens, C., B. Pucher, and G. Langergraber, Determination of parameters describing the hydraulic behavior of filter materials for stormwater filters using HYDRUS. (Austria)                                                                                                                                                                                                                                                                                                                                 |
|            | **Coffee Break**                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
| 11:00-11:30| **Keynote Presentation: Diederik Jacques**  
| 11:30-11:50| Filipović, V., Y. Coquet, V. Pot, P. Cambier, L. Filipović, S. Houot, and P. Benoit, Modeling the effect of tillage and urban waste compost addition on water flow and contaminant (Isoproturon, Cu, Cd) transport in agricultural field using HYDRUS-2D. (Croatia and France)                                                                                                                                                                                                                                                                 |
| 12:10-12:30| Arye, G., and J. Šimůnek, Surface-active root exudates induced flow phenomena in the rhizosphere: A numerical study. (Israel and USA)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
|            | **Lunch**                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
### Friday, March 31: Afternoon Session:

**Inverse Problems, Nonequilibrium Flow**

<table>
<thead>
<tr>
<th>Time</th>
<th>Authors and Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>2:00-2:20</td>
<td><strong>Keynote Presentation:</strong> Rien van Genuchten</td>
</tr>
<tr>
<td></td>
<td>Bezerra Coelho, C. R., L. Zhuang, and M. Th. van Genuchten, Hydrus-1D tests of the Hyprop evaporation method for estimating the unsaturated soil hydraulic functions. (Brazil)</td>
</tr>
<tr>
<td>2:20-2:40</td>
<td>Sittig, S. Coupling DREAM Suite and PEARL for parameter inference in a Bayesian framework. (Germany)</td>
</tr>
<tr>
<td>2:40-3:00</td>
<td>Khaddam, I., S. Werisch, and N. Schuetze, A modeling-based optimization framework for reclamation leaching practices. (Germany)</td>
</tr>
<tr>
<td>3:00-3:20</td>
<td>Iden, S. C., E. Diamantopoulos, and W. Durner, Capillary, film and vapour flow during transient evaporation: Inverse simulation of lab experiments using pressure head and humidity data. (Germany)</td>
</tr>
<tr>
<td></td>
<td><strong>Coffee Break</strong></td>
</tr>
<tr>
<td>4:00</td>
<td><strong>Closing Remarks and Departure</strong></td>
</tr>
</tbody>
</table>
List of Abstracts

Invited Keynote Presentations:

1. Brunetti, G., and J. Šimůnek, Selected Applications of HYDRUS Models for Engineering Problems. 16
4. Langergraber G., Process-based models for subsurface flow treatment wetlands: Recent developments and challenges. 32
5. Raji, I., G. Bel, and Naftali Lazarovitch, Unveiling multi-dimensional water flow and solute transport using HYDRUS codes. 40
6. Šimůnek, J., M. Th. van Genuchten, D. Jacques, and M. Šejna, Recent developments and applications of the HYDRUS software packages. 41

Oral Presentations:

1. Arye, G., and J. Šimůnek, Surface-active root exudates induced flow phenomena in the rhizosphere: A numerical study. 11
2. Batalha, M. S., E. M. Pontedeiro, and M. Th. van Genuchten, Groundwater recharge calculations as affected by temporal averaging of meteorological data. 12
3. Berger, K., Comparison and validation of SWMS_2D and HYDRUS (2D/3D) for capillary barriers using data of a 10-m tipping through. 13
4. Diamantopoulos, E., M. Walkinshaw, T. O’Geen, and T. Harter, Assessing nitrate leaching potential in California’s agricultural soils through Hydrus-1D simulations. 18
5. Fér, M., R. Kodešová, A. Nikodem, and A. Klement, Using HYDRUS-1D for estimating soil hydraulic parameters from capillary rise and evaporation rates measured using a clay tank and soil respiration chamber, respectively, and their correlation with a net CO₂ exchange rate. 19
6. Filipović, V., Y. Coquet, V. Pot, P. Cambier, L. Filipović, S. Houot, and P. Benoit, Modeling the effect of tillage and urban waste compost addition on water flow and contaminant (Isoproturon, Cu, Cd) transport in agricultural field using HYDRUS-2D. 21
7. Glass, J., T. Fichtner, and C. Stefan, Stepwise calibration of hydraulic conductivity changes in a laboratory tank simulating managed aquifer recharge operation. 22


13. Liang, J., S. A. Bradford, J. Šimůnek, and A. Hartmann, Modeling nonequilibrium overland flow and transport processes using HYDRUS-1D.


17. Sittig, S. Coupling DREAM Suite and PEARL for parameter inference in a Bayesian framework.

18. Suskin, V. V., I. V. Kapyrin, and A. V. Rastorguev, Modeling unsaturated groundwater flow and transport in the vadose zone using GeRa code.


**Poster Presentations:**


4. Goddard, M., C. Mendoza, and M. Hassanizadeh, The movement of groundwater and dissolved salts through an oil-sand tailings storage facility using Hydrus-2D.


Surface-Active Root Exudates Induced Flow Phenomena in the Rhizosphere: A Numerical Study

Gilboa Arye1 and Jirka Šimůnek2

1French Associates Institute for Agriculture and Biotechnology of Drylands, J. Blaustein Institutes for Desert Research, Ben-Gurion University of the Negev.
2Department of Environmental Sciences, University of California, Riverside, California, USA.

Plants can extract or alternatively exude water and solutes at their root surface. Therefore, concentration gradients are expected from the root surface toward the rhizosphere and vice versa. Among root exudates, the mucilage exhibits surface-activity, expressed in considerable reduction in the surface tension (ST) at the water-air interface. According to the Laplace equation, for a given water content and a contact angle, a reduction in ST is associated with a proportional reduction in the capillary pressure. Consequently, the hydraulic characteristics of the rhizosphere will differ significantly from those of the bulk soil. Furthermore, the spatial and/or temporal concentration gradient of surface-active root exudates will be expressed in ST and/or contact angle gradients and, thus, capillary pressure gradients – a moving force for unsaturated water flow - can be induced. The small flow domain of the rhizosphere posed a practical difficulty in experimental studies. Therefore, our modeling effort with HYDRUS will provide us with a tool to explore the role and a function of surface-active root exudates on unsaturated water flow between the rhizosphere and the bulk soil.
Simulations of water flow rates into and through the near-surface vadose zone can provide useful estimates of deep drainage and groundwater recharge. Past studies have shown that results can be very sensitive to the temporal resolution of meteorological data used in the simulations. In this study we used HYDRUS-1D to quantify the effects of using weather-related data of different resolutions (hourly, daily, weekly, monthly and yearly averaged precipitation and potential evaporation rates) on predictions of groundwater recharge at three sites in Brazil having different climatological conditions: a tropical savanna (the Cerrado), a humid subtropical area (the temperate south of Brazil), and a very wet tropical area (Amazonia). Our current analysis was limited to evaporation processes and hence did not consider any land use effects by ignoring root water uptake. Temporal averaging was found to lead to very different predictions of recharge, with the yearly averaged data always producing by far the lowest recharge rates. Results were especially sensitive to averaging when applied to the Cerrado site for which the daily averaged weather data produced up to 9 times the recharge rates obtained with yearly averaged data. The effects at the Cerrado site are due to the very uneven rainfall distribution over the year involving distinct wet and dry seasons. Long-term averaging can lead to especially poor recharge estimates for coarse-textured soils since averaging limits deep penetration of moisture in response to precipitation events. Infiltrated water will then remain in the upper part of the vadose zone and become subject to possible upward flow and evaporation. Accounting for short-term high-frequency precipitation events is also important when estimating surface runoff.
Comparison and Validation of SWMS_2D and HYDRUS (2D/3D) for Capillary Barriers Using Data of a 10-m Tipping Through

Klaus Berger

University of Hamburg, Institute of Soil Science, Allende-Platz 2, 20146 Hamburg, Germany

Capillary barriers, i.e. a fine-grained/porous capillary layer on a coarse-grained/porous capillary block (e.g. made of sand and gravel, resp.) with a sharp, sloped boundary, are a curious soil hydrological phenomenon and an interesting alternative component for cover systems of landfills and contaminated sites. However, little is known on how to dimension capillary barriers and on the effect of their design parameters like soil-hydrologic parameters, slope and slope length, or inflow into the capillary layer. Empirical investigations using large lysimeters or tipping troughs are close to reality, but limited to few parameter values, time-consuming and expensive. Soil hydrologic models could be fast and powerful tools for dimensioning provided they are sufficiently validated for capillary barriers, especially by output comparisons of model results with measured data.

Water flow and effectiveness of capillary barriers were empirically investigated at the Institute of Soil Science of the University of Hamburg in a 50 m x 10 m large test field (lysimeter) at the landfill Hamburg-Georgswerder and in a 10 m long tipping trough (tilt gutter). Measured data of the tipping trough for one material combination and two slopes (20 % and 4 %, resp.) from periods with stationary flow were compared to simulation results of SWMS_2D (Vs. 1.1) in 1996 and recently to results of HYDRUS 2D/3D (Vs. 2.05). The measured data show a typical pattern with no outflow or very small outflow rates of the capillary block at smaller inflow rates. Beyond a specific inflow rate (that indicates the maximum efficiency of the capillary barrier), the water is breaking through the boundary between capillary layer and capillary block, and most to all of the additional inflow occurs as outflow in the capillary block.

This measured flow pattern could not be reproduced with SWMS_2D. Four simulation series were run with different parametrizations, three of them with calibrations considering the heterogeneity of the parameters ks and van-Genuchten α and n. SWMS_2D always showed a smooth increase of the outflow rates of the capillary layer and the capillary block with increasing inflow rates. Thus, the validation attempt failed. This failure may be caused by different reasons: measurement errors, errors of the model including incompleteness and inappropriateness, or inappropriate application of the model. One reason might be the assumption that the materials are homogeneous in the simulation, what they actually were not (although they were well sorted). Due to the spatial heterogeneity, the breakthrough of the capillary barrier may hypothetically occur in fingers. HYDRUS 2D/3D includes the feature ‘stochastic distribution of scaling factors’ that can be used to consider spatial heterogeneity in simulation. Therefore, the validation has been retried with HYDRUS 2D/3D with a 2D general geometry.

In a first simulation series to determine the impact of the FE mesh on the results of a particular steady state (inflow rate), very different outflow rates occurred dependent on the FE mesh (FE size, stretching, refinements). A second series was performed for all steady state periods using that FE mesh from the first series with the best match of measured and simulated outflow rates; scaling was not applied. As SWMS_2D, HYDRUS 2D/3D results show a smooth flow pattern that visually looks closer to the measured values. However, a statistical deviation measure leads to higher values than for the SWMS_2D results. A third simulation series was performed using stochastic distribution of scaling factors with Miller-Miller similitude. The match of simulated and measured outflow rates, however, is even worse than without scaling. First simulation results using stochastic distribution of independent scaling factors indicate a similar result. Thus, currently the validation attempt for HYDRUS 2D/3D seems to fail too. Reasons for the mismatch of measured and simulated outflow rates as categorized above will be discussed.

C. R. Bezerra Coelho¹, L. Zhuang², and M. Th. van Genuchten²,³

¹Department of Civil Engineering, Federal University of Rio de Janeiro, UFRJ,
Rio de Janeiro, Brazil
²Department of Earth Sciences, Utrecht University, Utrecht, Netherlands
³NIDES Interdisciplinary Center for Social Development, Federal University of Rio de Janeiro,
UFRJ, Rio de Janeiro, Brazil

Many subsurface water flow and solute transport applications require information about the unsaturated soil hydraulic functions. The evaporation method has long been used to estimate the drying branches of the hydraulic functions. An increasingly popular version of the evaporation method is the semi-automated Hyprop measurement system (HMS) commercialized by Decagon Devices (Pullman, WA, USA) and UMS AG (München, Germany). We used Hydrus-1D to test the HMS methodology by generating synthetic evaporation (sample weight loss) and soil tensiometric measurements assuming applicability of the traditional van-Genuchten-Mualem (VG) soil hydraulic functions. HMS analyses of the synthetic data agreed closely with the original functions for a broad range of soil textures. Accurate estimates were especially obtained for the water retention curve over the range of available retention input data. We also successfully tested a dual-porosity soil, as well as a medium with a relatively high VG n parameter value. The latter test gave excellent results for water retention, but failed for the unsaturated hydraulic conductivity. Our results confirm that independent estimates of the saturated hydraulic conductivity should be obtained for very coarse-textured soils. Overall, the HMS methodology was found to be a very useful addition to current methods for measuring the unsaturated soil hydraulic properties.
Episodic Groundwater Recharge in the Arid Interior of Australia:
Multi-Model Transfer Function Approach

Theresa Boas¹, Dirk Mallants², and Jirka Šimůnek³

¹Steinmann-Institut für Geologie, Mineralogie und Paläologie, Rheinische Friedrich-Wilhelms-
Universität Bonn, Germany
²CSIRO, Adelaide, South Australia, Australia, dirk.mallants@csiro.au
³University of California Riverside, Riverside, California, USA

Recharge in arid and semiarid regions is hypothesized to be highly intermittent and related to extreme precipitation and associated flooding events. Previous tracer-based studies have indicated that precipitation events of at least 150 – 200 mm are required to generate significant recharge throughout the arid environments of Central Australia. In this study, the vadose zone simulator HYDRUS-1D was used to estimate groundwater recharge in the Northern Territory Ti-Tree Basin based on a 130-year time series of daily meteorological data. Hydraulic properties for deep unsaturated regolith were generated from a set of 10 pedotransfer functions (PTFs) that used grain size and bulk density data collected from an 11-m long core. Multiple PTFs were used to account for conceptual model uncertainty in generating regolith hydraulic properties. The multi-model transfer function approach consisted of running HYDRUS-1D multiple times with different sets of hydraulic properties, assuming each PTF has an equal likelihood. To test the effect of vegetation on recharge, simulations were performed for both bare soil and for a savanna-type vegetation. In the current study, root water uptake for the predominant Mulga (Acacia aneura) savanna vegetation was incorporated in the recharge estimation. The analysis of the 130-year precipitation records revealed extreme events (linked to monsoonal thunderstorms during the summer months) have an average return period of 3 years for a 100-mm rainfall event and 7 years for a 150-mm event. A total of eight major recharge events were recorded at the bottom of an 11-m deep regolith over the whole time series (1889-2015). The analysis of simulated recharge for bare soil indicated that most of the extreme rainfall events yielded recharge events of 9 mm averaged across PTFs and extreme events (ranging from 5 to 14 mm). Mean annual recharge events ranged from 0.18 mm to 27 mm, averaging at 5.49 mm. Long-term average recharge for Mulga vegetation ranged from 4.5 mm to 8.5 mm based on ten water balance models, each using a different pedotransfer function to generate regolith hydraulic properties.
The HYDRUS models have been used extensively to address several scientific and engineering problems. The ability to simulate coupled water, vapor and energy transport in both the subsurface and at the soil-atmosphere interface guarantees a high modeling flexibility and a broad range of applicability. Moreover, the combination of HYDRUS with new numerical techniques is increasingly commonly used, opening up new application fields. In this view, recent studies have investigated the use of HYDRUS models for the numerical evaluation of the hydrological behavior of Low Impact Development techniques, such as permeable pavements, green roofs, and stormwater filters, which were because of their complexity traditionally analyzed using empirical or conceptual models. One of the most widespread criticism against mechanistic models, namely the computational cost, is challenged by the use of new numerical methods. A recent HYDRUS application evaluated the use of Gaussian Process Emulators, which mimic the original model while being computationally inexpensive, for the inverse estimation and the global sensitivity analysis of soil hydraulic properties. In this perspective, applications are not restricted to hydrological problems. The Lower-Fidelity Physically-Based Surrogate models have been applied in both agricultural and geothermal engineering problems. A pseudo-3D model, which couples HYDRUS-2D and a surface flow model, has been used to simulate furrow irrigation. A similar approach has been adopted to interpret and describe a thermal response test, used to investigate the thermal properties of the ground. In this case, HYDRUS-2D has been coupled with a one-dimensional advection equation to simulate the heat transfer between a carrier fluid in a pipe and the surrounding soil. All these applications demonstrate the versatility of HYDRUS, and how the contribution of modern numerical techniques could increase its potential in a variety of scientific and engineering problems.
A Computationally Efficient Pseudo-2D Model for the Numerical Analysis of Permeable Pavements

Giuseppe Brunetti¹, Jirka Šimůnek², Thomas Wöhling³, Michele Turco¹, and Patrizia Piro¹

¹Department of Civil Engineering, University of Calabria, Rende, CS 87036, Italy
²Department of Environmental Sciences, University of California, Riverside, CA 92521, USA
³Department of Hydrology, Technische Universität Dresden, Dresden, Germany

Mechanistic models have proven to be accurate and reliable tools for simulating the hydraulic behavior of permeable pavements. However, their widespread adoption is limited by their complexity and computational cost. Recent studies have tried to address this issue by investigating the application of new techniques, such as surrogate-based modeling. One of such approaches includes the development of Lower-Fidelity Physically-Based Surrogates (LFS). LFSs focus on reducing the computational complexity of a numerical problem by computing an approximation of the original model. While this technique has been extensively used in water-related problems, no studies have evaluated its use in LIDs modeling. Thus, the main aim of this study is the development of the LFS model for the numerical analysis of the hydraulic behavior of permeable pavements. The proposed model decouples the subsurface water dynamics of a permeable pavement into a) a one-dimensional (1D) vertical infiltration process and b) one-dimensional saturated lateral flow along the impervious base. The pavement is horizontally discretized in N elements. HYDRUS-1D is used to simulate the infiltration process. Simulated outflow from the vertical domain is used as a recharge term for saturated lateral flow, which is described using the kinematic wave approximation of the Boussinesq equation. The proposed model has been compared with HYDRUS-2D, which numerically solves the Richards equation for the entire two-dimensional domain. Results confirmed the accuracy of the LFS model, which was able to reproduce both subsurface outflow and the moisture distribution in the permeable pavement, while significantly reducing the computational cost.
Assessing Nitrate Leaching Potential in California’s Agricultural Soils Through Hydrus-1D Simulations

Efstathios Diamantopoulos1*, Mike Walkinshaw1, Toby O’Geen1, and Thomas Harter1

1Department of Land, Air and Water Resources, University of California, Davis
*corresponding author: ediamant@ucdavis.edu

Nitrate is considered one of California’s most widespread groundwater contaminants. It is a secondary product of nitrogen fertilization applied for agricultural purposes, mainly from non-point sources. The fate of nitrate in the soils and the risk of reaching groundwater is a function of complex physical, chemical and biological processes which occur at different time and spatial scales. The objective of this study is the simulation of nitrate dynamics across the wide diversity of agricultural soils in California. The parameterization of the Hydrus-based assessment was based on the SoilWeb Database, taking into account the vertical heterogeneity of soil hydraulic properties in individual soil series. We conducted over 200-thousand Hydrus simulations across different combinations of about 6000 different soil types, 7 climates and 58 crops. Water flow was simulated using the Richards equation and nitrate transport simulated using the advection-dispersion equation assuming that nitrate behaves as a conservative tracer.

Based on the spatial distribution of the soil types as described in SoilWeb database, we present California-wide maps, helping identify agricultural regions in California that may need improved irrigation and/or fertilization management. Moreover, this analysis allows us to estimate deep percolation rate under the root zone, annual nitrate mass leached under the root zone and finally, the concentration of nitrate in the leaching water. All these parameters are very important for assessing the risk of groundwater contamination. Finally, the results of the simulations were validated against independent estimates of nitrate in harvest for 58 different crops.
Using HYDRUS-1D for Estimating Soil Hydraulic Parameters from Capillary Rise and Evaporation Rates Measured Using a Clay Tank and Soil Respiration Chamber, Respectively, and Their Correlation with a net CO₂ Exchange Rate

Miroslav Féř, Radka Kodešová, Antonín Nikodem, and Aleš Klement

Czech University of Life Sciences Prague, Kamýcká 129, 16500 Prague 6 - Suchdol, Czech Republic, mfer@af.czu.cz

Study was performed on the soil samples from the morphologically diverse study site in loess region of the Southern Moravia, Czech Republic. The original soil type within this area is a Haplic Chernozem (remaining on top parts), which was due to erosion changed into a Regosol (steep parts) and colluvial soils (base slope and the tributary valley). Sampling locations were selected to characterize diverse soil conditions within the area, i.e. soil samples were collected in July 2014 after wheat harvest from topsoil at 5 points (summit, shoulder, backslope, footslope and toeslope) of the elevation transect and also from the parent material (loess). Grab soil samples were used to measure basic soil properties and colony forming units (CFU). Soil hydraulic properties (drying curves) were measured on 100-cm³ undisturbed soil samples using the multistep outflow experiment and numerical inversion with HYDRUS-1D. Larger soil samples (diameter of 11 cm and height of 7.5 cm) were taken to measure a net CO₂ exchange rate and net H₂O exchange rate under increasing soil water content under greenhouse conditions. Initially air-dried soil samples were placed at the top of a kaolin tank and samples were wetted by a capillary rise up to almost full saturation. Soil respiration properties were measured using the LCi-SD portable photosynthesis system with Soil Respiration Chamber. During the experiment potential evaporation from water surface was recorded. Numerical inversion of the measured cumulative capillary rise and potential evaporation data using the HYDRUS-1D program were again applied to simulate water regime in the columns and to estimate some of the soil hydraulic parameters (wetting curves). In all cases, the net CO₂ exchange rate rapidly increased in the beginning of wetting. Next the net CO₂ exchange rate decreased with increasing soil water content (samples collected at summit, shoulder, backslope and in the parent material) or remained relatively stable (footslope and toeslope). Rapid decrees in soil respiration rate associated with initial fast wetting rate (i.e. with parameters of hydraulic conductivity curve), which was the most evident for soil substrate, followed by samples from summit, shoulder and backslope. Maximal values of the net CO₂ exchange rate were related to the organic carbon content \( R=0.87 \) and less closely to CFU \( R=0.78 \). No relationship was found between the net CO₂ exchange rate and parameters obtained from the multistep outflow experiment. On the other hand, close correlation was obtained between the net CO₂ exchange rate and \( \alpha \) \( R=0.86 \), \( n \) \( R=0.88 \) or slope at the inflection point \( R=-0.90 \) of the retention curve resulted from numerical inversion of cumulative capillary rise and potential evaporation data.
Modeling the Effect of Tillage and Urban Waste Compost Addition on Water Flow and Contaminant (Isoproturon, Cu, Cd) Transport in Agricultural Field Using HYDRUS-2D

Vilim Filipović¹, Yves Coquet², Valérie Pot³, Philippe Cambier³, Lana Filipović¹, Sabine Houot¹, and Pierre Benoit³

¹Department of Soil Amelioration, Faculty of Agriculture, University of Zagreb, Svetošimunska 25, 10000 Zagreb, Croatia; ²UMR 7327 ISTO Univ. d’Orléans, CNRS-INSU, BRGM, 45071 Orléans, France; ³UMR ECOSYS, INRA, AgroParisTech, Univ. Paris-Saclay, 78850 Thiverval-Grignon, France;

Tillage practices and compost amendments modify soil structure and can create heterogeneity at the local scale within agricultural fields. Urban waste compost may contain certain contaminants e.g. trace metals, and also affect sorption and degradation processes of other contaminants (e.g. pesticides). Modeling was performed to evaluate how the presence of heterogeneity due to soil tillage and repeated compost application affects water flow, pesticide dynamics and trace metal mobility in soil in the long-term QualiAgro¹ field experiment. Two experimental plots amended with a co-compost of sewage sludge and green wastes (SGW) or with a municipal solid waste compost (MSW) were compared with a control plot (CONT). In each plot, wick lysimeters, TDR probes and tensiometers were installed to monitor water and solute dynamics. In the ploughed layer, four zones differing in their structure were identified: compacted clods, non-compacted soil, interfurrows and the plow pan which were precisely reproduced in the HYDRUS-2D. Metals (Cu and Cd) soil mobility was modeled using sorption estimation based on equilibrium between CaCl₂ and EDTA extractable metal concentrations or using equations based on pedotransfer functions. From 2004 to 2010, the unamended control (CONT) plot had the largest cumulative water outflow (1388 mm) compared to the MSW plot (962 mm) and SGW plot (979 mm). Continuous compost addition seems to limit downward water flow by preventing preferential flow. HYDRUS was able to describe cumulative water outflow with a model efficiency value of 0.99 for all three plots. The model was able to simulate isoproturon leaching patterns except for the large preferential flow events which were observed in the MSW and CONT plots immediately after pesticide application. Modeling results indicate that spatial and temporal variations in pesticide degradation rate due to tillage and compost application play a major role in isoproturon dynamics. Trace metal mobility simulation showed very limited metal mobility in the tilled layer even at high trace metal inputs rates due to high sorption to organic matter originating from compost addition.

References:

¹ QualiAgro is a field experiment conducted within a INRA-Veolia collaboration.
Simulating Subsurface Lateral Flow in Eroded Soils with Contrasting Horizon Properties Using HYDRUS-2D

Vilim Filipović¹, Horst H. Gerke², Lana Filipović¹, and Michael Sommer²,³

¹Department of Soil Amelioration, Faculty of Agriculture, University of Zagreb, Svetosimunska 25, 10000 Zagreb, Croatia
²Institute of Soil Landscape Research, Leibniz-Centre for Agricultural Landscape Research (ZALF), Müncheberg, Germany
³Institute of Earth and Environmental Science, University of Potsdam (UP), Potsdam, Germany

Subsurface lateral flow can be important pathway for water flow and consequently transport of solutes (e.g., nutrients, pesticides, trace metals, antibiotics) in soil. This type of preferential flow is generally initiated when water percolates vertically through an unsaturated soil profile, meets an impeding layer of soil on hillslope, and is diverted laterally downslope when approaching saturated conditions. Such conditions can be found in the hummocky arable soil landscape where tillage and water erosion has shaped the surface topography and modified the soil horizons above a relatively dense glacial till. Objective of this work was to explore subsurface lateral flow occurrence using explicit soil profile information in combination with 2D modeling performed using HYDRUS software. The field data was collected from CarboZALF-D experimental trial. The soil profile was equipped with FDR probes and tensiometers at different depth (i.e., 10, 20, 40, 80, 130 and 200 cm) and additional climatic data collected daily at the site. Modeling was performed for a period from October 2009 till August 2014 for a 500 cm x 200 cm vertical cross-section using field morphological and profile layering descriptions with crop rotation included. First forward simulations using laboratory measured hydraulic parameters derived from 300 cm³ soil cores did not satisfactorily describe the observed field water dynamics. Inverse modeling and optimization was then performed on shorter periods to improve the model performance. With the improved parameter sets from the fitting, two daily rainfall events with same large intensity (74.6 mm/day) were evaluated for reproducing lateral subsurface flow more closely. These events led to saturated conditions in the profile above the C horizon, which had a sloping upper boundary and relatively low hydraulic conductivity. Pressure head and velocity vectors distribution in the soil profile efficiently captured the extent of subsurface lateral flow. After isolating these events with lateral flow occurrence, bromide tracer was inserted into the model just above the C horizon. This modeling exercise showed effects of subsurface lateral flow on solute flow pathways, which was evidently shifted in the sloping direction and distribution of tracer in the whole soil profile. Although the sloping landscape was qualitatively known for the lateral subsurface flow, the simulations still revealed relatively little tendency towards lateral flow during the long simulation period. This indicates that processes such as non-equilibrium type of preferential flow and the small scale layering with potential anisotropy of the hydraulic conductivity should be explored more precisely.
Stepwise Calibration of Hydraulic Conductivity Changes in a Laboratory Tank Simulating Managed Aquifer Recharge Operation

Jana Glass¹, Thomas Fichtner¹, and Catalin Stefan¹

¹Department of Hydrosciences, Technische Universität Dresden, Dresden, Germany
jana.glass@tu-dresden.de

Clogging represents one key issue during the operation of managed aquifer recharge (MAR) schemes, especially relevant when recharging an aquifer with treated wastewater or surface water. The accumulation of suspended solids and biomass in the soil pore space leads to a decrease in the soil hydraulic parameters and hence a performance reduction of infiltration systems. Thus, restoration measures need to be applied to recover the infiltration capacity. Minimizing clogging can therefore increase the overall performance and bring down the operative costs of MAR facilities.

Four MAR operational scenarios with different combinations of hydraulic loading cycles (6h:18h, 24h:72h) and loading rates (146 m/a, 300 m/a) were simulated in a laboratory tank. The set-up consists of a 3D, rectangular-shaped stainless steel lysimeter (1.5 x 1.0 x 1.0 m) with an infiltration basin (0.45 x 0.3 x 0.06 m) installed in the center of its surface. River water with an average 25 mg/l dissolved organic carbon and 15 mg/l total suspended solids was infiltrated in the basin. The spatial and temporal distribution of soil moisture was measured by an array of tensiometers and TDR probes in two different depths at 0.28 m and 0.68 m below surface. Each of the scenarios resulted in clogging of the soil material at varying time and extent. The clogging rate was estimated taking into account tensiometer data and soil water content measurements. Furthermore, tracer tests using KBr were conducted to quantify the reduction of travel time and relate it to hydraulic conductivity changes.

The specific objective of this paper was to setup a numerical variable-saturated flow model of the cross section of the laboratory tank using HYDRUS-2D and calibrate it at different times during the infiltration period with the help of measured tensiometer and water content data to represent clogging. The simulation time was chosen to be in accordance with the tracer test dates to be able to compare the results and covered 3 - 4 days each. The model domain was divided into three principal layers consistent with the laboratory setup including the main loamy soil (from the surface down to 78 cm underneath infiltration basin), a 2-cm sand layer followed by 12.5 cm of coarse gravel as filter layer. Different approaches to calibrate the HYDRUS-2D model at the different time steps were followed: 1) only the saturated hydraulic conductivity was inversely optimized and 2) in addition to saturated hydraulic conductivity also the van Genuchten parameters α and n were optimized. The saturated hydraulic conductivity changes received by the stepwise HYDRUS-2D simulations were compared to those measured by tracer tests.
The Movement of Groundwater and Dissolved Salts Through an Oil-Sand Tailings Storage Facility Using Hydrus-2D

Marie Goddard¹, Carl Mendoza², and Majid Hassanizadeh¹

¹Department of Earth Sciences, Utrecht University, Utrecht, 3508 TA, Netherlands (goddard.marie@gmail.com)
²Department of Earth and Atmospheric Sciences, University of Alberta, Edmonton, AB, T6G 2E3, Canada (Carl.Mendoza@UAlberta.ca)

We used Hydrus-2D to simulate groundwater flow and dissolved salt transport through a very large, partially covered, sand tailings dam. The project goal was to predict future discharge rates and salt concentrations to aid in understanding the potential impacts on a vegetative cover and salt loadings to the surrounding environment. Transects of piezometers and other instruments have been established across the dam, resulting in high frequency data sets for climate, groundwater levels and groundwater quality. These data sets make it possible to calibrate our 2D model with transient (seasonal) boundary conditions. The unique characteristics of this project were: the extreme climate; the large size of the modeled area; the man-made stratigraphy; and the material properties of the tailings.

The dam is located in northern Canada (56° north) and is subject to five months of sub-zero temperatures (winter), followed by a rapid spring melt (~95 mm of snow water equivalent), followed by sparse summer rainfall (~280 mm). The spring melt results in a lengthening of the seepage faces over this brief period, which necessitates a compromise to the boundary conditions (i.e., seepage vs. flux) at the toes of the slopes. Ideally, a temporal dual-boundary condition would permit for a better calibration. Additionally, Hydrus-2D cannot simulate frozen soils and groundwater. Consequently, simulated heads and discharge rates during the winter months were not fully representative of site conditions.

Our 2D model was unusually large for a Hydrus simulation, with a cross-sectional area of 56,000 m² with about 90 % of the section being fully saturated. The cross-section was subdivided into man-made “depositional” cells representing either the dam (active earthworks) or the beach (passive settlement).

The dam and storage facility are composed of oil-sand tailings (predominantly quartz sand with minor silt, clay and bitumen) which are unique and therefore not described by the standard soil databases, specifically residual saturation, alpha and n. Our final material properties were chosen using a combination of previously reported results and by trial-and-error calibration. Compared to values predicted by the UNSODA and Rosetta databases, the resulting parameter sets are characterized by residual saturation values higher by a factor of three; alpha values lower by a factor of three; and similar n values. The characterization of these oilsands tailings aid not only the specific goals of this study, but the more general objective to understand the flushing behavior of this unique material.
A New HYDRUS Add-On Module to Model the Interactions Between Plant Roots, Soil Properties, and Water Flow Conditions in Soils

Anne Hartmann1, Jiří Šimůnek2, Moses Kwame Aidoo3, Sabine J. Seidel4, Naftali Lazarovitch5

1UGT Environmental Measurement Devices GmbH, Research & Development, Germany
2Department of Environmental Sciences, University of California Riverside, CA, USA
3Wyler Department for Dryland Agriculture, The French Associates Institute for Agriculture and Biotechnology of Drylands, Jacob Blaustein Institutes for Desert Research, Ben-Gurion University of the Negev, Sede Boqer Campus, Israel
4Institute of Crop Science and Resource Conservation, University of Bonn, Germany

The standard versions of the HYDRUS software do not consider the feedback between the root growth and conditions in the soil and the root growth is fully defined using input parameters. A new root growth module was developed as an add-on for the HYDRUS software package (both HYDRUS-1D and HYDRUS (2D/3D)) to model the root growth as a function of different environmental stresses. In this module, the root growth and the roots spatial distribution is dynamically affected by various environmental factors such as soil water content or soil temperature. The root growth model is based on the approach developed by Jones et al. (1991). The model assumes that various environmental factors, including soil hydraulic properties (determining the availability of water and oxygen for plants) and various other physical, chemical, and biological variables, can influence the root development under suboptimal conditions. The environmental conditions are characterized by various growth stress factors.

To incorporate the modeling approach into the HYDRUS software the model of Jones et al. (1991) was slightly modified. A time-dependent growth function is used to evaluate the potential rooting depth that is reached when the root development is assumed to be independent of environmental conditions. The actual rooting depth is derived based on the potential rooting depth by taking into account sub-optimal environmental conditions. The calculation of the actual root length density distribution is based on the use of shape functions. Such functions represent the potential root length density distribution under optimal conditions. Due to sub-optimal environmental conditions, the potential root distribution is altered to an actual root distribution.

The modified root-growth stress-factor approach is only a first approximation of the effects of environmental factors on root growth and thus still needs to be verified against experimental data. The temperature stress factor was the first part of the newly developed HYDRUS add-on module to be validated by comparing modeling results with measured rooting depths of bell peppers in an aeroponic experimental system, provided by the Jacob Blaustein Institutes for Desert Research of the Ben-Gurion University of the Negev in Israel. The experiment was conducted at three different root zone temperatures of 7, 17, and 27°C. Inverse optimization was used to estimate a single set of parameters of the newly developed root growth module that was found to well reproduce measured time series of rooting depths for all temperature treatments. It was also found that it is reasonable to approximate parameters representing biological factors such as the maximum rooting depth and cardinal temperatures with values from the literature to reduce the number of calibration parameters.
The Effects of Rock Fragment Shapes and Positions on Modeled Hydraulic Conductivities of Stony Soils

Hana Hlaváčiková¹, Viliam Novák¹, Jirka Šimůnek², Ladislav Holko¹, Zdeněk Kostka¹, and Michal Danko¹

¹Institute of Hydrology, Slovak Academy of Sciences, Bratislava, Slovakia (hlavactkova@uh.savba.sk)
²Dept. of Environmental Sciences, Univ. of California Riverside, Riverside, CA 92521, USA

Mountain or forest soils usually contain a large number of rock fragments (RF). The amount of rock fragments, their size, shape, position, and spatial distribution in the soil influence hydraulic properties of stony soils as well as various processes such as water infiltration, water movement, or the occurrence of runoff. We present measured hydrophysical properties of stony soils from a small mountain catchment, the methodology of evaluation of stony soil properties, and a numerical assessment of the influence of rock fragments (stoniness), their shape, positions, and distributions in a soil matrix on the saturated hydraulic conductivity of a stony soil. Properties of stony soils were measured in the Jalovecký creek catchment, the Western Tatra Mts., Slovakia. Hydrological research conducted in the catchment since the late 1980s proved that subsurface flow often dominates in catchment runoff, the catchment response to rainfall is very fast, and that the fast response may be enhanced by the high stoniness of the soils (up to 40 – 70 %).

Despite a lot of field and laboratory data, it is still difficult to assess the influence of rock fragment properties on water flow in stony soils. Therefore, we used a numerical model to evaluate the effects of particular properties of stony soils on the saturated hydraulic conductivity. The assessment was based on a numerical version of the Darcy's classic experiment that involved steady-state flow through a porous material under a unit hydraulic gradient using the HYDRUS model. Three different shapes of hypothetical rock fragments were used: a sphere, an ellipsoid with two different positions, and a pyramid. We tried to find out how the shape, orientation, and distribution (regular and irregular) of RFs affect the effective saturated hydraulic conductivity of the soil. Differences in the effective saturated hydraulic conductivities of stony soils simulated by the model were also compared with those calculated using existing empirical equations. The usefulness of the numerical model to assess the influence of soil matrix texture on the effective saturated hydraulic conductivity of stony soils was also evaluated. Finally, we have attempted to derive relationships between stoniness and the effective saturated hydraulic conductivity for different rock fragments properties. The modeling also provided the spatial distributions of pressure heads, volumetric water contents, and water fluxes in heterogeneous stony soil profiles which may be nearly impossible to measure in practice.
Simulating a Full-Scale Two-Stage Vertical Flow Wetland System Using the HYDRUS Wetland Module

Vincent Hochfeldt, Bernhard Pucher, and Guenter Langergraber*

Institute for Sanitary Engineering and Water Pollution Control, University of Natural Resources and Life Sciences, Vienna (BOKU University), Austria, *guenter.langergraber@boku.ac.at

Treatment wetlands are natural treatment technologies that efficiently treat many different types of polluted water. Treatment wetlands are engineered systems designed to optimize processes found in natural environments and are therefore considered environmentally friendly and sustainable options for wastewater treatment. In Austria, treatment wetlands with a single-stage vertical flow (VF) bed that is intermittently loaded are state-of-the-art because this configuration can guarantee the legal requirements regarding effluent concentrations. Currently, about 5'700 of this treatment systems are in operation. A two-stage VF wetland system was developed to optimize the treatment performance of VF wetlands. In 2010, the first two-stage VF wetland system was implemented in full-scale.

In this study, the full-scale two-stage VF wetland system is simulated using the HYDRUS Wetland Module whereby the CW2D biokinetic model was used (Langergraber and Šimůnek, 2012). The results of the study can be summarized as follows:

- The matrix flow model (Richard's equation) used provides a good description of the water flow in both stages of the two-stage VF wetland.
- When simulating the tracer experiment the results vary between the coarser sand filter media used in the first stage and the finer sand media in the second stage parameters.
- Parameter adjustments of the CW2D biokinetic model were needed to fit measured and simulated effluent concentrations in the first stage. For the second stage, the best fit was achieved when using the standard parameter set. This can be explained by the assumed matrix flow model and its limits in describing water flow in coarse media such as used in the 1st stage.
- The implementation of the dual-porosity model within the HYDRUS Wetland Module, also described by Morvannou et al. (2013) would most likely provide better fit.

References
Evaporation from bare soil is an important component of the water cycle and the surface energy balance in arid and semi-arid regions. Actual evaporation from dry soil cannot be predicted without detailed knowledge of the complex interplay between liquid, vapor and heat flow. Soil hydraulic properties exert a strong influence on evaporation rates during stage-two evaporation. Recently, significant progress has been made in the experimental characterization of the soil water retention curve in dry soils and the inclusion of vapor flow into flow models has become more widespread. However, the determination of unsaturated hydraulic conductivity in medium to dry soils remains a challenge and most model applications still predict the hydraulic conductivity curve from the water retention curve by capillary bundle models and thus ignore the effect of water flowing in incompletely-filled pores, i.e. film and corner flow, on the hydraulic conductivity function. The objective of this study was to identify soil hydraulic properties by inverse modeling, with a particular focus on the medium to dry moisture range. We conducted evaporation experiments on large, packed soil columns under laboratory conditions and used an extended instrumentation, consisting of minitensiometers and relative humidity sensors, to measure the pressure head over a wide range from saturation to -100 MPa. Evaporation rates and column-averaged water content were measured gravimetrically. The resulting data were evaluated by inverse modeling using the isothermal Richards equation as process model and the Hydrus-1D code as numerical solver for the direct problem. Our results clearly demonstrate that classic models of soil hydraulic conductivity which are based on the assumption that water flows exclusively in water-filled capillaries cannot describe the observed time series of pressure head and relative humidity. Although the additional inclusion of isothermal vapor flow improved the agreement between model and data, an adequate description of the data was only possible by accounting for an additional flow of liquid water. The physical cause of the latter could be film and corner flow as proposed before based on a theoretical analysis of water flow in angular porous media.
Colloid and Colloid-Facilitated Transport Modeling using HPx

Diederik Jacques¹, D. Zhou², J. Makselon³, I. Engelhardt², and S. Thiele-Bruh⁴

¹Engineered and Geosystems Analysis, Institute for Environment, Health and Safety, Belgian Nuclear Research Centre (SCK-CEN), Mol, Belgium, djacques@sckcen.be
²Institute for Applied Geosciences, Hydrogeology Department, TU Berlin, Berlin, Germany
³Agrosphere (IBG-3), Institute of Bio- and Geosciences, Forschungszentrum Jülich GmbH, Jülich, Germany
⁴Department of Soil Science, University of Trier, Trier, Germany

HPx is a reactive coupled transport model using HYDRUS-1D or HYDRUS (2D/3D) as the transport solver (water flow, solute transport and heat transport) and PHREEQC-3 as the geochemical solver. Coupling these two codes resulted in a flexible and extendible coupled model as a powerful tool to simulate complex processes in variably-saturated porous media. Recently, two studies (Zhou et al., 2016; Makselon et al., 2017) used the model to calculate transport of colloids and contaminated attached to colloids through the subsurface.

The first study (Zhou et al., 2016) simulated the transport of sulfonamides in the absence or presence of manure colloids from different origin. The model consists of the transport of dissolved organic matter including interaction of DOM with the solid phase (attachment and detachment, decay and straining), transport of sulfonamides and their interaction with the solid phase and the colloids. The model was successfully calibrated to experimental data. Model results show that mobile colloids act as carriers for sulfomoxole, while immobile colloids block sulfomoxole from sorbent on the soil. On the other hand, the high affinity of sulfadiazine and sulfamethoxypyridazine for sorbing on immobile colloids retarded their transport.

The second study (Makselon et al., 2016) investigated the effect of flow interruption and ionic strength on the transport of surfactant-stabilized silver nanoparticles (AgNP). The model combined the DLVO theory with an extended colloid filtration theory and a colloid release model. The numerical model reproduced the measured AgNP and indicated that attachment to the air-water interface occurring during flow interruption was the process for AgNP retention.

These two studies illustrate the versatility of the HPx code to study complex processes such as colloid and colloid-facilitated transport in subsurface systems.

References:
A Modeling-Based Optimization Framework for Reclamation Leaching Practices

Issam Khaddam, Stefan Werisch, and Niels Schuetze

Institute of Hydrology and Meteorology, Technische Universität Dresden, Dresden, Germany

The aggravating worldwide water scarcity problems induce all users, especially agriculture, to optimize their irrigation and leaching water usage. Leaching is considered the most efficient measure for managing soil salinity and thereby improving the yield productivity. Traditional approaches estimate the leaching fraction in dependence of the salinity of the applied water and the target salinity in the soil and only some additionally consider evapotranspiration. However, these approaches ignore the two-dimensional distribution of salts in the soil profile, and the time required to apply the evaluated LF. Therefore, more attention should be paid to the 2D soil salinity distribution in the root zone under leaching practices in order to improve the salinity management. For this purpose, a 2D simulation-based optimizing framework for leaching was developed. The framework employs the Hydrus 2D model and focuses on reclamation practices under virtual field conditions. Subsequently, the leaching performance of three different irrigation techniques, namely: (i) sprinkler irrigation, (ii) surface drip irrigation and (iii) subsurface drip irrigation, was investigated. The framework investigates the leaching sensitivity to the typical management parameters of the irrigation systems, such as the operation time, sprinkler intensity, drip line positioning and discharge rate. At the end, numerous number of leaching scenarios that combine the individual techniques and their management parameters were simulated in two soil types, which are loam and silt. Thereafter, the simulation results were evaluated in a multi-objective optimization framework to identify the most effective combinations and the optimal trade-offs between the applied water and remaining salt mass in the soil. Moreover, the framework allows a segment-based analysis by dividing the soil profile to many sub-regions. This division is used in the evaluation stage for targeting (aggregation) a specific part of the soil profile such as the dense root zone. The proposed framework is flexible to be modified or expanded to cover different soil types, water application techniques and initial conditions. It can serve as a valuable tool for planning reclamation or seasonal leaching measures.
Using HYDRUS-1D and 2D for Assessing the Impact of Different Root Distributions on Simulated Root Water Uptake

Aleš Klement, Miroslav Fér, Šárka Novotná, Antonín Nikodem, and Radka Kodešová

Czech University of Life Sciences Prague, Kamýcká 129, 16500 Prague 6 - Suchdol, Czech Republic, klement@af.czu.cz

Knowledge of the distribution of plant roots in a soil profile (i.e. root density) is needed when simulating root water uptake from soils using the HYDRUS programs. Barley and wheat were planted in a flat laboratory box under greenhouse conditions. Roots were excavated at the end of the experiment and root densities were assessed using root zone image processing and by weighing. For this purpose, the entire area (width of 40 and height of 50 cm) of each scenario was divided into 80 segments (area of 5x5 cm). Root density in each segment was expressed as a root percentage of the entire root cluster. Vertical root distributions (i.e. root density with respect to depth) were also calculated as a sum of root densities in each 5 cm layer. Resulting root densities, measured evaporation from the water table (used as the potential root water uptake), and the Feddes stress response function model were used for simulating substrate water regime and actual root water uptake for all scenarios using HYDRUS-1D and HYDRUS-2D. The application of two root detecting techniques resulted in noticeably different root density distributions. Differences were mainly attributed to the fact that fine roots of high density (located mostly at the deeper part of the box) had lower weights in comparison to the weight of few large roots (at the box top). Thus, at the deeper part, higher root density (with respect to the entire root zone) was obtained using the image analysis in comparison to that from the gravimetric analysis. Conversely, lower root density was obtained using the image analysis at the upper part in comparison to that from the gravimetric analysis. On the other hand, fine roots overlapped each other and therefore were not visible in the image, which resulted in lower root density values from image analysis. Root water uptakes simulated with HYDRUS-1D using diverse root densities obtained for each cereal declined differently from the potential root water uptake values depending on water scarcity at depths of higher root density. Usually, an earlier downtrend associated with gradual root water uptake decreases and vice versa. Similar root water uptakes were simulated for the presented scenario using the HYDRUS-1D and HYDRUS-2D models. The impact of the horizontal root density distribution on root water uptake was, in this case, less important than the impact of the vertical root distribution resulting from different techniques and sowing scenarios. For more details see Klement et al. (2016).

Reference:
Klement, R., M. Fér, Š. Novotná, A. Nikodem, R. Kodešová, Root distributions in a laboratory box evaluated using two different techniques (gravimetric and image processing) and their impact on root water uptake simulated with HYDRUS, Journal of Hydrology and Hydromechanics, 64(2), 196-208, 2016.
Using HYDRUS-1D for Simulating Water Flow and Heat Transport under Various Surface Covers

Radka Kodešová¹, Miroslav Fér¹, Aleš Klement¹, Antonín Nikodem¹, Daniela Teplá¹, Pavel Neuberger¹, and Petr Bureš²

¹Czech University of Life Sciences Prague, Kamýcká 129, 16500 Prague 6 - Suchdol, Czech Republic, kodesova@af.czu.cz
²VESKOM, Ltd, Dolnoměcholupská 522/12a, 102 00 Prague 10, Czech Republic

Different soil covers influence water and thermal regimes in soils within urban areas. Knowledge of these regimes is needed, particularly when assessing effectiveness of energy gathering from soils using horizontal ground heat exchangers. The goal of this study was to calibrate the model HYDRUS-1D for simulating coupled water and thermal regime in Technosol type soils with grass cover, and to use this model for predicting water and thermal regimes under different materials covering the soil surface. For this purpose, soil water contents were measured at depths of 10, 20, 30, 40, 60 and 100 cm at 4 locations and temperatures were measured at depths of 20, 40, 80, 120, 150 and 180 cm at three locations (all covered by grass) from June 2011 to December 2012. In addition, sensors for simultaneous measuring soil water contents and temperatures were installed under different soil covers (grass, bark chips, sand, basalt gravel and concrete paving) at a depth of 7. The parameters of soil hydraulic properties were obtained on the 100-cm³ undisturbed soil samples using the multi-step outflow experiment and numerical inversion of the measured transient flow data using HYDRUS-1D. HYDRUS-1D was then used to simulated the water regime within the soil profile under the grass cover using climatic data from June 2011 to December 2012 and some of the soil hydraulic parameters were additionally numerically optimized using soil water contents measured at all depths. Water flow and heat transport were then simulated using these parameters, measured thermal properties and temperatures measured close to the surface applied as a top boundary condition. Simulated temperatures at all depths successfully approximated the measured data.

Next, water and thermal regimes under another 4 different surface covers were simulated. Soil hydraulic properties of different materials were partly measured and partly optimized when simulating soil water regime from June 2011 to December 2012 using the soil water contents measured at the depth of 7 cm (sand, bark chips, and concrete paving) or set (basalt gravel). The greatest soil water content variability was obtained (measured at the depth of 7 cm and simulated at different depths) for grass and gradually decreased for sand, basalt gravel, bark chips and concrete paving. However, in the case of concrete paving the measured soil water contents at the depth of 7 cm could not be successfully approximated using HYDRUS-1D due to the fact that measured soil water contents reflected 3D character of water flow below the paving. The largest temperature oscillations during each day at the depth of 7 cm were measured for concrete paving (due to this large daily data oscillation measured values could not be influence by surrounding area) and decreased as follows: basalt gravel, sand, grass and bark chips. As a result, also temperature oscillations simulated at different depths using measured temperatures as top boundary conditions followed the same trends. The highest temperatures at different depths during the warm periods were simulated for concrete paving and decreased as daily temperature oscillations. The highest temperatures during the cold period were simulated for basalt gravel and decreased for grass, bark chips, sand and concrete paving. Thus, the basalt gravel scenario appeared to be the most efficient for increasing heating systems effectiveness. For more details see Kodešová et al. (2014).

Reference:
To date, only few process-based models for subsurface flow treatment wetlands have been developed. For modeling a treatment wetland, these models have to comprise a number of sub-models to describe water flow, pollutant transport, pollutant transformation and degradation, effects of wetland plants, and transport and deposition of suspended particulate matter. The two most advanced models are the HYDRUS Wetland Module and BIO-PORE. These two models are briefly described. This paper shows typical simulation results for vertical flow wetlands and discusses experiences and challenges using process-based wetland models in relation to the sub-models describing the most important wetland processes. Experiences with applying the HYDRUS Wetland Module and other existing simulation tools can be summarised as follows:

• Process-based models are a powerful tool for understanding the processes in treatment wetlands in more detail.
• All sub-models required to describe the different processes in treatment wetlands are important.
  – Good calibration of the water flow model is a pre-requisite for achieving a good match between measured and simulated pollutant concentrations. Due to the intermittent loading, more data are required for VF wetlands compared to HF wetlands. If the water flow model is calibrated, good results can be obtained in most applications when using the standard parameter sets of the biokinetic models.
  – A good description of solute transport including adsorption and desorption is of equal importance for good simulation results for pollutant degradation and removal.
  – Influent fractionation (i.e., fractionation of influent COD and the N and P contents of different COD fractions) has a high impact on simulation results and thus is an essential part of calibrating reactive transport models.
  – Simulating the influence of wetland plants is possible by considering uptake and release via the plant roots linked to evapotranspiration.
  – Models describing clogging are important to describe the long-term behaviour of treatment wetlands. Up to now, clogging models are the least established and tested among the sub-models mentioned.

Reference:
The HYDRUS-1D code is a popular numerical model for solving the Richards equation for variably-saturated water flow and solute transport in porous media. This code was adapted to solve rather than the Richards equation for subsurface flow the diffusion wave equation for overland flow at the soil surface. The numerical results obtained by the new model produced an excellent agreement with the analytical solution of the kinematic wave equation. Model tests demonstrated its applicability to simulate the transport and fate of many different solutes, such as non-adsorbing tracers, nutrients, pesticides, and microbes. However, the diffusion wave or kinematic wave equations describe surface runoff as sheet flow with a uniform depth and velocity across the slope. In reality, overland water flow and transport processes are rarely uniform. Local soil topography, vegetation, and spatial soil heterogeneity control directions and magnitudes of water fluxes, and strongly influence runoff characteristics. There is increasing evidence that variations in soil surface characteristics influence the distribution of overland flow and transport of pollutants. These spatially varying surface characteristics are likely to generate non-equilibrium flow and transport processes. HYDRUS-1D includes a hierarchical series of models of increasing complexity to account for both physical equilibrium and non-equilibrium flow and transport in the subsurface, e.g., dual-porosity and dual-permeability models, up to a dual-permeability model with immobile water. The same conceptualization as used for the subsurface was implemented to simulate non-equilibrium overland flow and transport at the soil surface. The developed model improves our ability to describe non-equilibrium overland flow and transport processes, and improves our understanding of factors that cause this behavior.

Recently, the HYDRUS overland flow and transport model was extended to simulate soil erosion. HYDRUS-1D soil erosion model has been validated by comparing its predictions with other soil erosion models (e.g., Kineros). The model performed well when the soil particle size is relatively large. The performance of the soil erosion model will be further evaluated by comparing its predictions with selected examples from the literature and experimental datasets.
Determination of Parameters Describing the Hydraulic Behavior of Filter Materials for Stormwater Filters Using HYDRUS

Carlos Mir Llorens, Bernhard Pucher*, and Guenter Langergraber

Institute for Sanitary Engineering and Water Pollution Control, University of Natural Resources and Life Sciences, Vienna (BOKU University), Austria, *bernhard.pucher@boku.ac.at

With the increase of extreme events leading to floods, droughts, heat islands and also water shortage, the demand for interdisciplinary solutions within the urban space is needed. The city of Vienna is characterized for having several green zones within its city limits including a wide variety of vegetation. Those green zones shall be used for the retention and treatment of street runoff but also be able to provide a good environment for the vegetation such as trees. To cope with this demand a variety of filter materials are under investigation (Beinlich, 2016).

With the ability of the HYDRUS software package (Simůnek et al., 2011) to simulate water flow and solute transport, adsorption behavior as well as biokinetic reactions as included in the HYDRUS Wetland Module (Langergraber and Šimůnek, 2012) the interest and need of modeling is constantly rising. The most important step to take advantage of this tools is to determine the needed data for setting up a proper model while the main experiments are carried out.

In this study the soil hydraulic parameters for the van Genuchten-Mualem soil hydraulic model are determined of the filter materials under investigation including the following steps:

- Column experiments determining the water flow behavior of each filter material by applying three different rainfall events.
- Determining the saturated hydraulic conductivity (by carrying out a constant head test according to ÖNORM B2506-3, 2016) and the porosity for each filter material.
- Set up a water flow model using HYDRUS based on the measured data.
- Using the in HYDRUS implemented inverse solution, the unknown soil hydraulic parameters, namely the residual water content and the form parameters $\alpha$ and $n$ are determined, while the tortuosity parameter in the conductivity function is set to 0.5 (Mualem, 1976).

References:
ÖNORM B2506-3, Test criteria for technical filter materials, 2016.
Coal seam gas (CSG) production in Australia generates large volumes of produced water. Such water may contain elevated concentrations of naturally occurring inorganic and organic compounds, and generally has a high salinity. Chemicals unintentionally released from storage ponds may potentially enter soil, shallow groundwater, as well as receiving surface waters. We here demonstrate how the reactive transport simulator for variably-saturated porous media HP1 (coupled HYDRUS-1D - PHREEQC) was used to assess risks to soil and shallow groundwater associated with leaching of CSG produced water. We evaluate the fate of naturally occurring inorganic chemicals, cadmium, lead and uranium, in soil as a result of unintentional release from storage ponds. Our work reviews exposure pathways and relevant hydrogeochemical processes, and collates physico-chemical properties of inorganic contaminants as input to a set of generic simulations of transport and attenuation in variably saturated soil profiles. In addition to modeling the coupled processes of variably-saturated flow and transport of multiple contaminants and major ions in soil, sensitivity analysis are undertaken to test the robustness of chemical migration and attenuation with regards to hydraulic and chemical parameters and boundary conditions. The focus of the assessment is on the trace metals cadmium, lead, and uranium. Chemical attenuation processes in soil include adsorption of metals through cation exchange and surface complexation. The assessment is based on an analysis, in space and time, of adsorbed and aqueous phase metal concentrations and relative abundance of dissolved metal species. Results show that the main process responsible for metal migration in soil is complexation of naturally present metals with inorganic ligands such as (bi)carbonate, chloride, and hydroxyl ions. These ligands enter the soil upon infiltration with alkaline produced water. Metals naturally present in soil on the adsorption sites, albeit at low levels, will desorb due to formation of mobile metal-ligand compounds. These metal-ligand compounds travel relatively unretarded through soil.
Defining Safe Water Quality Requirements for Sustainable Irrigation with Coal Seam Gas Produced Water

Dirk Mallants¹ and Jirka Šimůnek²

¹CSIRO, Adelaide, South Australia, Australia, dirk.mallants@csiro.au
²University of California Riverside, Riverside, California, USA, jiri.simunek@ucr.edu

Coal seam gas produced water is generally high in total dissolved solids and has a high salinity which may affect soil and plant health if used untreated for irrigation. Use of irrigation waters with a high sodium absorption ratio (SAR) will result in salt accumulation in the soil profile, potentially impacting crop yield. Use of irrigation water with high SAR values may further result in dispersion of soil clay minerals resulting in loss of soil structure, increasing erodibility, restricting water entry and reducing infiltration capacity. This study considers coupled processes of variably-saturated water flow, plant water uptake and coupled transport of multiple major ions in soils irrigated with produced water featuring different water qualities. By coupling major ion soil chemistry to unsaturated flow and plant water uptake, and by explicitly incorporating effects of salt concentrations on soil hydraulic properties and on root water uptake (the so-called salinity stress), critical soil processes required for salinity risk assessment associated with coal seam gas produced water are included in the analysis. Simulations with different irrigation water qualities provided detailed results regarding chemical indicators of soil and plant health, i.e., SAR, EC, and sodium concentrations. By comparing such indicators in the soil profile with permissible ANZECC values, an assessment was made of the risk to soil and plant health. We also evaluated the effect of high salt concentrations in the soil profile on plant salinity stress, a condition which reduces the capacity for plants to uptake water causing yield reduction. Finally, the simulations also allowed to test if soil hydraulic properties, in particular the hydraulic conductivity, are negatively impacted by high salt concentrations, especially by the accumulation of the monovalent cations sodium and potassium.
Coal seam gas produced water contains compounds originating from the use of hydraulic fracturing fluids together with naturally occurring organic chemicals (geogenics). If leakage of produced water from storage ponds occurs as a result of flooding or containment failure, contamination of surface waters and shallow groundwater may happen. This study was conducted to evaluate the fate of such chemicals in soil as a result of unintentional releases. We simulated coupled processes of flow, transport and first-order transformation of hydraulic fracturing chemicals (a biocide, a surfactant and a solvent) and geogenics (phenol, 2-methylphenol and naphthalene) in a clay soil. A literature review of transformation pathways for chemical additives found hydrolysis as the only degradation mechanism for bronopol (a biocide, half-life $T_{1/2} = 1.5$ years); limonene (a solvent, $T_{1/2} = 2.3$-18 days) was found to degrade under aerobic conditions, while both aerobic and anaerobic biodegradation had been considered for 2-butoxyethanol (a surfactant, $T_{1/2} = 7$ – 112 days). Hydrolysis was found the only transformation pathway for phenol ($T_{1/2} = 0.11$-23 days), while aerobic and anaerobic biodegradation had been reported for 2-methylphenol ($T_{1/2} = 1.6$-7 days) and naphthalene ($T_{1/2} = 80$ days). Literature values for the organic carbon partition coefficient $K_{OC}$ were shown to be medium (up to ~10 L/kg) for 2-butoxyethanol, large (up to ~ $10^3$ L/kg) for 2-methylphenol, bronopol and phenol, to very large (up to ~$10^4$ L/kg) for naphthalene and limonene. All of the chemical transformation products were found to have either $T_{1/2}$ or $K_{OC}$ values supportive of natural attenuation. Simulation with the variably saturated HYDRUS code showed that the combined effect of generally strong sorption and fast degradation resulted in nearly complete removal of all chemicals in the top 5 to 10 cm of the soil profile.
Using HYDRUS Codes and Scaling Factors Characterizing Spatial and Temporal Variability of Soil Hydraulic Properties for Assessing the Impact of Soil Erosion on Soil Water Hydrology

Antonín Nikodem, Radka Kodešová, Miroslav Fér, and Aleš Klement

Czech University of Life Sciences Prague, Kamýcká 129, 16500 Prague 6 - Suchdol, Czech Republic, nikodem@af.czu.cz

Study was performed on soil samples from the morphologically diverse study site in loess region of the Southern Moravia, Czech Republic. The original soil type within this area is a Haplic Chernozem (remaining on top parts), which was due to erosion changed into a Regosol (steep parts) and colluvial soils (base slope and the tributary valley). One representative transect, with the most diverse terrain attributes (i.e. elevation, slope, curvature, exposition etc.), which caused the most variable soil properties of surface horizon, was delineated. Five sampling points were selected assuming that soil at different points should be modified by different stages of erosion-accumulation processes: summit, shoulder, backslope, footslope, and toeslope. Grab soil samples were used to measure basic soil properties. Soil hydraulic properties, $\theta(h)$ a $K(h)$, were measured on 100-cm3 undisturbed soil samples (taken before and after the vegetation period) using the multistep outflow experiment and numerical inversion with HYDRUS-1D. Next the reference soil hydraulic properties, $\theta^*(h^*)$ a $K^*(h^*)$, and scaling factors ($\alpha_h$, $\alpha_K$ a $\alpha_\theta$) were evaluated to describe spatial and temporal variability of the soil hydraulic properties. In general, larger values of $\alpha_h$ factor and lower values of $\alpha_K$ a $\alpha_\theta$ factors were obtained before vegetation period in comparison to those obtained after the vegetation period. While no trends in scaling factors along the elevation transect were observed before vegetation season, the evident trends were observed after the harvest. Finally, HYDRUS-1D and 2D programs were used to evaluate variable conditions on a soil water regime.
Simulation Results Using the HYDRUS Wetland Module for Different Sized Filter Medias in Vertical Flow Treatment Wetlands

Bernhard Pucher* and Guenter Langergraber

Institute for Sanitary Engineering and Water Pollution Control, University of Natural Resources and Life Sciences, Vienna (BOKU University), Austria, *bernhard.pucher@boku.ac.at

The field of treatment wetland (TW) simulation is constantly growing over the last decades and has evolved from looking at such systems as a black box to describing the simultaneous occurring physio-chemical and biological processes responsible for the degradation of pollutants (Meyer et al., 2015). Named processes are described within the two biokinetic model formulations implemented in the HYDRUS Wetland Module, namely CW2D (Langergraber and Šimůnek, 2005) and CWM1 (Langergraber et al., 2009).

In this study, three vertical flow TW systems (Table 1) with different filter media and grain size are used in order to compare the simulation results of the HYDRUS Wetland Module using the CW2D biokinetic model and its standard parameter set.

<table>
<thead>
<tr>
<th>System</th>
<th>Type</th>
<th>Wastewater</th>
<th>Main filter media</th>
<th>Depth</th>
<th>Grain size</th>
<th>Area</th>
<th>Drainage</th>
</tr>
</thead>
<tbody>
<tr>
<td>System 1</td>
<td>Austrian system</td>
<td>pre-treated</td>
<td>Sand</td>
<td>50cm</td>
<td>0.063-4 mm</td>
<td>1 m²</td>
<td>free</td>
</tr>
<tr>
<td>System 2</td>
<td>Austrian system</td>
<td>pre-treated</td>
<td>Sand</td>
<td>50cm</td>
<td>1-4 mm</td>
<td>1 m²</td>
<td>impounded</td>
</tr>
<tr>
<td>System 3</td>
<td>French system</td>
<td>raw</td>
<td>Pea gravel</td>
<td>40cm</td>
<td>2-4 mm</td>
<td>2.3 m²</td>
<td>free</td>
</tr>
</tbody>
</table>

The simulation of each system is carried out using the following steps:

- Simulation of the water flow using the van Genuchten-Mualem soil hydraulic model with measured and literature values depending on the availability.
- Fitting the hydraulic model using the inverse solution provided in HYDRUS.
- Solute transport and degradation of the wastewater constituents, namely COD, NH₄-N, NO₂-N, NO₃-N and P using the Wetland module with the CW2D model.

For all three systems a good fit of the flow model can be achieved and hence should lead to a good fit of the biokinetic model. The results will show that this true for fine filter materials as used in System 1 while for coarse materials represented by Systems 2 and 3 the simulated results give better treatment performances than measured. For those system a good fit can only be achieved when adjusting several parameters of the CW2D model.

References:


Unveiling Multi-Dimensional Water Flow and Solute Transport Using HYDRUS Codes

Iael Raij, Golan Bel, and Naftali Lazarovitch

Jacob Blaustein Institutes for Desert Research, Ben-Gurion University of the Negev, Israel

Numerical models are used as a research tool to understand, quantify and predict phenomena and processes in the soil-plant-atmosphere continuum of the agricultural field. Despite the inherent complexity, their use is growing thanks to a better understanding of processes related to water flow and solute transport in porous media, the development and improvement of mathematical methods for solving equations and the rapid development of computers that are able to calculate different processes at finer time and space intervals.

Even though irrigation and fertigation in agriculture are usually addressed unidimensionally (e.g., irrigation depth in mm), plant growth, water and solute distribution are, in fact, multidimensional. The use of one-dimensional models to represent three-dimensional patterns may lead to erroneous conclusions.

While models are cost-effective tools for optimizing input regimes, as well as for estimating and preventing environmental damage by agricultural activities, their value is highly dependent on the accuracy of their parameterization, often determined by calibration. However, currently with new personal computers, long computational times are required for multicomponent multidimensional modeling.

Using numerical results from four different studies, we will present possibilities for facilitating the optimal use of computational resources. These examples include: A. encapsulating water flow from surface drip irrigation using an artificial neural network; B. describing infiltration from surface sources by adding an edge effect into 1D simulations; C. inferring soil and irrigation heterogeneity effects on drainage amount and concentration in lysimeters using sequential simulations; and D. determining first-order degradation in heterogeneous soil using ParSWMS.

As of today, large domains, long simulation times and high heterogeneity exhaust both the computer and the user. Regrettably, optimization procedures such as inverse modeling remain impractical for 3D simulations with the current average user’s computational resources.
Recent Developments and Applications of the HYDRUS Software Packages

Jiří Šimůnek¹, Martinus Th. van Genuchten²,³, Diederik Jacques⁴, and Miroslav Šejna⁵

¹Department of Environmental Sciences, University of California, Riverside, CA 92521, USA
²Department of Mechanical Engineering, Federal University of Rio de Janeiro, UFRJ, Brazil
³Department of Earth Sciences, Utrecht University, Netherlands
⁴Institute for Environment, Health, and Safety, Belgian Nuclear Research Centre (SCK•CEN), Mol, Belgium
⁵PC-Progress, Ltd., Prague, Czech Republic

The HYDRUS-1D and HYDRUS (2D/3D) software packages are widely used finite element models for simulating the one-, and two- or three-dimensional movement of water, heat, and multiple solutes in variably saturated media, respectively. In 2013, at the previous Hydrus conference (also in Šimůnek et al., 2008), we described the entire history of the development of the various HYDRUS programs and related models and tools, such as STANMOD, RETC, ROSETTA, UNSODA, UNSATCHEM, HP1, and others. The objective of this presentation (and also of Šimůnek et al., 2016) is to review selected capabilities of HYDRUS that have been implemented since then. Our review is not limited to listing additional processes that were implemented in the standard computational modules, but also describes many new standard and non-standard specialized add-on modules that significantly expanded the capabilities of the two software packages. We also review additional capabilities that have been incorporated into the graphical user interface that supports the use of HYDRUS (2D/3D). Another objective of this manuscript is to review selected applications of the HYDRUS models, such as evaluation of various irrigation schemes, evaluation of the effects of plant water uptake on groundwater recharge, and/or assessing the transport of particle-like substances in the subsurface.

Reference:
Current Developments in the HYDRUS Software Packages

Jiří Šimůnek¹, Martinus Th. van Genuchten²,³, and Miroslav Šejna⁴

¹Department of Environmental Sciences, University of California, Riverside, CA 92521, USA
²Department of Mechanical Engineering, Federal University of Rio de Janeiro, UFRJ, Brazil
³Department of Earth Sciences, Utrecht University, Netherlands
⁴PC-Progress, Ltd., Prague, Czech Republic

In this presentation, we will review current developments of the latest versions of the HYDRUS software packages. There developments include updates to both the graphical user interface (GUI) as well as the computational modules. The following improvements are made to GUI:

1. Overall review of the code and its update for a new MS Visual Studio, resulting in better performance, parallelization of graphical operations, availability of more memory (32-bit/64-bit versions), Unicode, etc.
2. Improved 3D graphics: transparency, smoothing, clipping, slicing, 3D raster for vector fields, numbering of isolines, etc.
3. 3D particles (for transient flow) and 2D/3D streamlines (for steady flow), animation of particle movement.
4. Export of results to ParaView, which offers new visualization options including custom post-processing based on scripting or plugin modules.
5. Resizable dialogs with tables and charts, new components for tables and charts.
6. Displaying results for multiple time layers in cross-section and boundary line charts.
7. About 100 other minor improvements in GUI.
8. Updated documentation (CHM help, online help, User’s manual).

The following new options are being implemented into the computational modules:

1. CO₂ transport and production module.
3. Reservoir boundary condition.
4. Coupled water, vapor, and energy transport and the mass and energy balance at the surface interface. Considering of the effects of slope inclination and azimuth, and plant shading

With respect to the last option, mass and energy fluxes in the subsurface are closely coupled and cannot be evaluated without considering their mutual interactions. While hydrological and thermal processes in the subsurface are commonly implemented in existing models, which often consider both isothermally and thermally induced water and vapor flow, the interactions at the soil-atmosphere interface are often simplified, and the effects of slope inclination, slope azimuth, variable surface albedo and plant shading on incoming radiation and spatially variable surface mass and energy balance, and consequently on soil moisture and temperature distributions, are rarely considered. In this presentation, we discuss these missing elements and our attempts to implement them into the HYDRUS model. We demonstrate implications of some of these interactions and their impact on the spatial distributions of soil temperature and water content, and their effect on soil evaporation.
Environmental fate risk assessment for plant protection products (PPP) is conducted partly with numerical models. The required input parameters are usually derived from direct measurements in laboratory or field studies or otherwise inferred with inverse modeling techniques.

In this study, the application of the DiffeRential Evolution Adaptive Metropolis algorithm (DREAM; Vrugt, 2016) to inversely estimate parameters on the basis of results from a forward simulation using the PEARL model (van den Berg, 2016) is demonstrated. To this end, DREAM Suite v1.02 was used to derive joint posterior parameter distributions of four parameters describing the fate of an example PPP in the environment (FOCUS standard substance C, incl. its metabolite): DegT50 (degradation half-life) for both substances, the formation fraction of the metabolite and the initially applied mass. A plug-in was developed to enable the coupling of DREAM Suite and PEARL. The FOCUS Hamburg scenario (FOCUS, 2014a) was applied, using a standard application of 1 kg ha\(^{-1}\), shortly before the emergence of summer cereals. Total mass dynamics in the uppermost 30 cm of a soil profile of parent substance and its primary metabolite were produced in a forward simulation. After the measurements’ corruption with a 5-% random error, the parameters were inferred. Convergence was controlled with the Gelman-Rubin criterion, and the multivariate joint posterior distribution functions were analyzed. Generally, this procedure allows for the representation of all processes contributing to the dissipation of the species, i.e. microbial degradation, plant uptake, leaching below the layer under investigation etc. We show a comparison with the standard procedure following FOCUS kinetics (FOCUS 2006, 2014b), regarding the dissipation only (dissipation half-lives, DT50), after normalization of the time-steps to standard conditions (20°C and field capacity).

We observed an excellent recovery of the parameters used for the production of the synthetic measurements. The comparison of the standard procedure and the inverse modeling procedure using a numerical model leads to similar values describing the dissipation (DegT50 or DT50, respectively) with a considerably reduced formation fraction in the standard approach. The procedure presented herein can be used to derive true DegT50 values from legacy field studies, especially for leaching compounds or compounds which were presumed to be uptaken by plants.

References:
FOCUS, Generic guidance for Estimating Persistence and Degradation Kinetics from Environmental Fate Studies on Pesticides in EU Registration, 2014b.
Modeling Unsaturated Groundwater Flow and Transport in the Vadose Zone Using GeRa Code

Viktor V. Suskin, I. V. Kapyrin, and A. V. Rastorguev

*Nuclear Safety Institute of Russian Academy of Sciences, Russia, viksus@ibrae.ac.ru*

In the present study we demonstrate the ability of unsaturated groundwater flow and transport in the vadose zone modeling using GeRa code, which is jointly developed by Nuclear Safety Institute and Institute of Numerical Mathematics. Also a comparative analysis of unsaturated unconfined groundwater flow models is done. The code is designed for the safety assessment of radioactive waste repositories and problems of groundwater protection from chemical pollution. GeRa is a three-dimensional integral computational code, focused on providing a full sequence of hydrogeological modeling, starting from the generation of the geological model and meshing, and ending with the calculation of individual radiation doses, which can occur with the transfer of radionuclide contamination. The features of the code are the availability of geological modeling tools, the use of adaptive unstructured grids and the ability of parallel calculations. The basic modeled processes are the following:

3. Radioactive decay chains.
4. Density-driven flow.
5. Heat transport and thermal convection.

This report presents the results of verification and cross-verification of unsaturated groundwater flow models implemented in the GeRa code with codes FEFLOW, VS2DT and HYDRUS on three test problems. The first is the capillary barrier problem, the second is a two-dimensional problem of unsaturated flow and transport in heterogeneous vadose zone with radioactive decay, and the third is an experimental problem of groundwater flow and mass transport in the drained tray.

Unconfined model, implemented using pseudounsaturated approach, was cross-verified with the unconfined MODFLOW model on a two-dimensional problem. The fourth test demonstrates the fundamental difference between these two models and shows the capillary effect on the groundwater flow processes in the vadose zone.
Development and Evaluation of the Hydrus Package for Modflow

Adam Szymkiewicz¹, Jirka Šimůnek², Anna Gumuła-Kawęcka¹, Sahila Beegum², Bertrand Leterme³, Beata Jaworska-Szulc¹, Małgorzata Pruszkowska Caceres¹, Wioletta Gorczewska-Langner¹, Rafael Angulo-Jaramillo⁴, and Diederik Jacques³

¹Gdańsk University of Technology, Faculty of Civil and Environmental Engineering, Gdańsk, Poland, ²Department of Environmental Sciences, University of California, Riverside, CA, USA ³Institute for Environment, Health and Safety, Belgian Nuclear Research Centre, Mol, Belgium ⁴Laboratoire d’Ecologie des Hydrosystèmes Naturels et Anthropisés (LEHNA) UMR 5023, France

The Hydrus package for Modflow (based on the Hydrus-1D code) allows to include vertical water flow in the vadose zone, described by the Richards equation, in the modeling framework of the Modflow family of computer codes. Simulations of vadose zone flow are used to predict the rate of recharge or capillary uptake occurring at the groundwater table, as a function of the soil hydraulic properties, vegetative cover, and atmospheric conditions. A sequential coupling scheme is used, in which vadose zone flow is solved in a number of soil profiles and resulting values of the exchange flux are incorporated into the discretized equation describing saturated groundwater flow in Modflow. The original package, developed by Seo et al. (2007) and Twarakavi et al. (2008), has been updated to be compatible with the Modflow-2005 standard. Multiple new features are currently being implemented, including alternative models of soil hydraulic functions and different methods for the evaluation of internodal permeabilities. In this presentation we focus on: (i) the implementation of the coupling condition between 1D variably saturated flow in the soil profiles and 3D saturated groundwater flow, (ii) the investigation of the influence of time resolution of the weather data on calculated values of the recharge. Preliminary evaluation results will be presented for the case of a 2D strip aquifer, bounded by surface water bodies and recharged by infiltration.

Reference:

Acknowledgements
This work has been partly supported by National Science Centre, Poland, in the framework of the project 2015/17/B/ST10/03233 "Groundwater recharge on outwash plain".
Water Flow Modeling in the Highly Permeable Pavement Using Hydrus-2D

Michele Turco¹, Giuseppe Brunetti¹, Antonín Nikodem², Miroslav Fér², Radka Kodešová², and Patrizia Piro¹

¹Department of Civil Engineering, University of Calabria, Rende, CS 87036, Italy
²Faculty of Agrobiology, Food and Natural Resources, Dept. of Soil Science and Soil Protection, Czech University of Life Sciences, Kamycká 129, CZ-16521 Prague 6, Czech Republic

The increase of urbanization in the last decades has caused, among others, the increase of impervious surfaces in spite of those permeable. This is one of the major aspects of the increasing frequency of flooding events in urban catchments that highlighted all the critical issues of the traditional urban drainage systems and oriented science and technical towards new stormwater management approaches such as Low Impact Development techniques (LID). LID systems consist of a series of facilities whose purpose is to intercept stormwater runoff. Among the most common LID, permeable pavement (PP) is a facility constructed in layers that represent a good solution to solve stormwater management problems.

Despite the benefits that it would adopt by using PP, these techniques are not yet widespread probably because modeling tools often used simplified methodologies, based on empirical and conceptual equations, that do not take into account hydrological processes in a physical way.

The aim of this work is to assess the suitability of the HYDRUS-2D model correctly describe the hydraulic behavior of a lab-scale permeable pavement system. The hydraulic properties of two (porous concrete blocks and fine gravel used for bedding layers) of the three layers that composed the system were measured using two experimental procedures (clay tank and the multistep outflow experiment, respectively). Soil water retention and hydraulic conductivity curves were described by the van Genuchten functions. In addition some of the parameters were optimized with the HYDRUS-2D model from observed water fluxes in the lab-scale porous pavement system and soil water contents measured in bedding layer. The inverse solution optimization, which implements a Marquardt-Levenberg type parameter estimation technique for the estimation of the soil hydraulic parameters, was carried out to calibrate the model. Measured and modeled hydrographs were compared using the Nash-Sutcliffe efficiency (NSE) index, while the coefficient of determination $R^2$ was used to assess the measured water content versus modeled ones in the bedding layer. Obtained results have confirmed the suitability of HYDRUS-2D to correctly interpret the hydraulic behavior of the lab-scale permeable pavement system.
Agricultural crop yields depend largely on soil moisture conditions in the root zone. Climate change leads to more prolonged drought periods that alternate with more intensive rainfall events. With unaltered water management practices, reduced crop yield due to drought stress will increase. Therefore, both farmers and water management authorities search for opportunities to manage risks of decreasing crop yields. Available groundwater sources for irrigation purposes are increasingly under pressure due to the regional coexistence of land use functions that are critical to groundwater levels or compete for available water. At the same time, treated wastewater from industries and domestic wastewater treatment plants (wwtp) are discharged to surface waters. Re-use and exploitation of these freshwater sources may be an effective strategy to balance regional water supply and agricultural water demand. We present results from a pilot field study in a drought sensitive sandy region in the eastern Netherlands. In this field pilot, agricultural water supply through reuse of domestic treated wastewater is delivered to the plant root zone through sub-irrigation by controlled drainage systems. This sub-irrigation method can be more efficient than classical, aboveground irrigation methods using sprinkler installations.

Domestic wastewater treatment plants in the Netherlands produce annually 40 to 50 mm freshwater. A pilot project has been setup in the eastern part of the Netherlands, in which treated wastewater is applied to a corn field by sub-irrigation during the growing seasons of 2015 and 2016, using a climate adaptive drainage system. The chemical composition of treated domestic wastewater is different from rainfall excess water and agricultural drainage water. In the pilot project, specific chemicals in the treated wastewater are used as a tracer to describe water and solute transport in the soil system. Focus of this pilot study is on quantifying potential contamination of both the root zone and the deeper groundwater with pharmaceutical residues. We have installed a field monitoring network at several locations on the vadose zone and the local groundwater system, which enables us to measure vertical solute profiles in the soil water by taking samples. Based on field data obtained during the experiments, combined with SWAP (1D) and Hydrus (2D) model simulations, flow and transport of the sub-irrigated treated wastewater are quantified.
Model of Near-Surface Flow in Drying Sandstone

Tomáš Weiss¹, Martin Slavík¹, and Jiří Bruthans¹

¹Faculty of Science, Charles University, Albertov 6, 128 43 Prague 2, Czechia, tomas.weiss@natur.cuni.cz

Porous coarse materials, after reaching a certain low value of water content, form a dry subsurface layer. Through this layer, water migrates only as vapor, and its flux is governed by diffusion from subsurface evaporation front to the surface. The goal of this study was to develop a 1D model that would describe both the near-saturated and the virtually dry evaporation from sandstone using the Richards equation with van Genuchten – Mualem hydraulic functions. The model was calibrated to measured evaporation rate from 4 cm deep initially fully saturated sandstone samples placed in a climate chamber with constant relative humidity (50 %) and temperature. For the numerical modeling, we used the HYDRUS-1D software with inverse solution to fit the alpha, n, and l parameters with predefined ranges in functions for retention curves and unsaturated hydraulic conductivity. The study showed that it is possible to use Richards equation for very low water content values in near surface with partially altered hydraulic functions and it suggests to use this approach in combination with coupled Richards-diffusion equations when solving problems of evaporation from nearly-dry coarse materials. The study was supported by Czech Science Foundation (GA CR no. 16-19459S).