



Modeling Water Flow and Contaminant Transport in Soils and Groundwater Using the HYDRUS Software Packages

Jirka Šimůnek¹

Rien van Genuchten², Miroslav Šejna², and Diederik Jacques⁴

¹Department of Environmental Sciences, University of California, Riverside, CA

²Department of Mechanical Engineering, Federal University of Rio de Janeiro, Brazil

³PC-Progress, Ltd., Prague, Czech Republic

⁴Belgian Nuclear Research Centre (SCK•CEN), Mol, Belgium

Jirka Šimůnek

A Professor of Hydrology with the Department of Environmental Sciences of the University of California Riverside. Received M.Sc. in Civil Engineering from the Czech Technical University, Prague, Czech Republic, and Ph.D. in Water Management from the Czech Academy of Sciences, Prague, Czech Republic.



Expertise in Numerical Modeling of subsurface water flow and solute transport processes, equilibrium and nonequilibrium chemical transport, multicomponent major ion chemistry, field-scale spatial variability, and inverse procedures for estimating soil hydraulic and solute transport parameters.

Dr. Šimůnek has authored and coauthored over 200 peer-reviewed journal publications, over 20 book chapters, and 2 books. His numerical HYDRUS models are used by virtually all scientists, students, and practitioners modeling water flow, chemical movement, and heat transport through variably saturated soils. Dr. Šimůnek is a recipient of the Soil Science Society of America's (SSSA) Don and Betty Kirkham Soil Physics Award, the past chair of the Soil Physics (S1) and Fellow of SSSA, and Fellow of American Geophysical Union.

An Associate Editor of Journal of Hydrology and Hydromechanics, and a past AE of Water Resources Research, Vadose Zone Journal, and Journal of Hydrological Sciences.

Rien van Genuchten

A soil physicist originally with the US Salinity Laboratory, USDA, ARS, Riverside, CA. Received B.Sc. and M.Sc. in irrigation and drainage from Wageningen University in The Netherlands, and Ph.D. in soil physics from New Mexico State University.



Rien van Genuchten

Dr. van Genuchten is a recipient of the Soil Science Society of America's Don and Betty Kirkham Soil Physics Award, of the EGU Dalton Medal, and Fellow of the Soil Science Society of America, American Society of Agronomy, American Geophysical Union and American Association for the Advancement of Sciences. Founding Editor of the Vadose Zone Journal. Currently with the University of Rio de Janeiro, Brazil.

Research on variably-saturated water flow and contaminant transport, analytical and numerical modeling, nonequilibrium transport, preferential flow, characterization and measurement of the unsaturated soil hydraulic functions, salinity management, and root-water uptake. The most often referenced researcher in the field of Soil Physics. Dr. van Genuchten is probably best known for the theoretical equations he developed for the nonlinear constitutive relationships between capillary pressure, water content and the hydraulic conductivity of unsaturated media.

Miroslav Šejna

A Director and Development Lead of PC Progress, Software company located in Prague, Czech Republic. Received B.Sc. and M.Sc. from the Charles University of Prague, Faculty of Mathematics and Physics, Prague, Czech Republic, and PhD. from the Czech Academy of Sciences, Prague, Czech Republic.

Expertise in Numerical Modeling of Transonic Flow with homogeneous and heterogeneous condensation and chemicals in steam through Turbine Cascade (Euler and Navier-Stokes equations).

Recently specializes in the development of GUI (Graphical User Interfaces) for FEM/CFD software packages for Windows. He has more than twenty years of experience in developing programs for numerical modeling in Fluid Mechanics and Structural Engineering. His software helps thousands of scientists and engineers from around the world.

Selected Software Projects:

- RFEM, RSTAB Structural Engineering Software packages, 1995-2009, Ing.-Software Dlubal, GmbH, Germany
- HYDRUS-1D, HYDRUS 2D/3D Software package for simulating water, heat, and solute transport in variably saturated porous media.
- MESHGEN Plus FE-mesh generator and open modeling environment for Finite-Element and Finite-Volume applications.
- COCHEM Flow Software package simulating 2D water steam flow with homogeneous and heterogeneous Condensation.



Mirek Sejna

Diederik Jacques

Diederik Jacques is a head if the Performance Assessment Unit, Institute of Environment, Health and Safety of the Belgian Nuclear Research Centre (SCK•CEN) in Mol, Belgium.



He received B.Sc. and M.Sc. in Bio-Engineering Land and Forest Management, M.Sc. in Statistic, and Ph.D. in Soil Physics; all at the Catholique University of Leuven, Belgium.

His expertise is in modeling water flow and solute transport in unsaturated porous media including characterizing spatial variability and estimating parameters. He has some experience with experiments at the field scale. He is working on different aspects of coupling unsaturated water flow, solute transport and geochemical reaction including the development and testing of the coupled code HP1, application to (long-term) solute transport in soils and interaction between different systems (clay–concrete, or soil–concrete). He is involved in safety and performance analysis of surface and deep geological waste disposal sites, including supporting calculations using reactive transport models.

Czech Republic (Czechoslovakia)



Known for: 1.Beer (Pilsner Urquel) 2.Ice Hockey (Jágr, Hašek) 3.Vaclav Havel (former president) 4.Beauty of its capital (Prague) 5.Dumplings (meal) 6.HYDRUS



Central Europe

Area part of Central Europe Area sometimes included as part of Central Europe

Holland (Netherlands) + Belgium



Known for: 1.Beer (Grolsch, Heineken) 2.Soccer (Robben, Sneijder) 3.Beatrix (Queen) 4.Beauty of its towns (A'dam, Utrecht) 5.Herrings and Cheese 6.HYDRUS



HYDRUS-1D



Software for Simulating Water Flow and Solute Transport in One-Dimensional Variably-Saturated Soils Using Numerical Solutions



Software for Simulating Water Flow and Solute Transport in Two/Three-Dimensional Variably-Saturated Soils Using Numerical Solutions HYDRUS

Software for simulating water, heat, and solute transport in variably saturated porous media.



HYDRUS - History of Development



HYDRUS-1D - History of Development



Agricultural Applications

- Precipitation
- Irrigation
- Runoff
- Evaporation
- Transpiration
- Root Water Uptake
- Capillary Rise
- Deep Drainage
- Fertigation
- Pesticides
- Fumigants
- Colloids
- Pathogens
- Nanoparticles



Industrial Applications

- Industrial Pollution
- Municipal Pollution
- Landfill Covers
- Waste Repositories
- Radioactive Waste Disposal Sites
- Remediation
- Brine Releases
- Contaminant Plumes
- Seepage of Wastewater from Land Treatment Systems



Environmental Applications

- Ecological Apps
- Carbon Storage and Fluxes
- Heat Exchange and Fluxes
- Nutrient Transport
- Soil Respiration
- Microbiological Processes
- Effects of Climate Change
- Riparian Systems
- Stream-Aquifer Interactions



Governing Equations

Variably-Saturated Water Flow (Richards Equation)

$$\frac{\partial \theta(h)}{\partial t} = \frac{\partial}{\partial z} \left[\frac{K(h)}{\partial z} - 1 \right] - \frac{S(h)}{\partial z}$$

Solute Transport (Convection-Dispersion Equation) $\frac{\partial(\rho s)}{\partial t} + \frac{\partial(\theta c)}{\partial t} = \frac{\partial}{\partial z} \left(\theta D \frac{\partial c}{\partial z} - qc \right) - \phi$

Heat Movement

$$\frac{\partial C_p(\theta)T}{\partial t} = \frac{\partial}{\partial z} \left[\lambda(\theta) \frac{\partial T}{\partial z} \right] - C_w \frac{\partial qT}{\partial z} - C_w ST$$

HYDRUS – Main Processes

Water Flow:

- Richards equation for variably-saturated water flow
- Various models of soil hydraulic properties
- Hysteresis
- Sink term, accounting for water uptake by plant roots (uncompensated and compensated; reduced due to osmotic and pressure stress)
- Preferential flow
- Isothermal and thermal liquid and vapor flow

Solute Transport:

- Convective-dispersive transport in the liquid phase
- Diffusion in the gaseous phase
- Linear and nonlinear reactions between the solid and liquid phases
- Linear equilibrium reactions between the liquid and gaseous phases
- Zero-order production, First-order degradation
- Physical and chemical nonequilibrium solute transport
- Sink term, accounting for nutrient uptake by plant roots (active and passive)

Heat Transport:

Conduction and convection with flowing water (transport of latent heat)

PTFs by Carsel and Parrish (1988)

Average values of selected soil water retention parameters for 12 major soil textural groups

Texture	θ _r	θ,	α 1/cm	n	<i>K</i> , cm/d	
Sand	0.045	0.43	0.145	2.68	712.8	
Loamy Sand	0.057	0.41	0.124	2.28	350.2	
Sandy Loam	0.065	0.41	0.075	1.89	106.1	
Loam	0.078	0.43	0.036	1.56	24.96	GLAY
Silt	0.034	0.46	0.016	1.37	6.00	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
Silt Loam	0.067	0.45	0.020	1.41	10.80	AM 80
Sandy Clay Loam	0.100	0.39	0.059	1.48	31.44	the root is a start of the star
Clay Loam	0.095	0.41	0.019	1.31	6.24	
Silty Clay Loam	0.089	0.43	0.010	1.23	1.68	
Sandy Clay	0.100	0.38	0.027	1.23	2.88	
Silty Clay	0.070	0.36	0.005	1.09	0.48	10 territy men from Strong St
Clay	0.068	0.38	0.008	1.09	4.80	SAND 3 8 8 5 8 8 5 8 8 5 8 5 5 5

USDA Soil Textural Triangle

Percent by weight sand

ROSETTA

Software for predicting the Soil Hydraulic Parameters (van Genuchten, 1980) from Soil Textural Properties (Schaap et al., 2001).

2001).	Rosetta Lite v. 1.1 (June 2003)				
Hierarchical Models	Select Model				
Input Data	Input Output Textural Class Unknown Sand [%] 30 Sint [%] 30 Silt [%] 20 Clay [%] 50 BD [gr/cm3] 1.3				
Predicted Parameters	TH33 [cm2/cm3] Help! Predict Accept Cancel				

Schaap, M. G., Leij, F. J., and van Genuchten, M. Th., Rosetta: a computer program for estimating soil hydraulic parameters with hierarchical pedotransfer functions, *Journal of Hydrology*, 251, 163-176, 2001.

HYDRUS – Solute Transport

- Transport of Single Ions or Particles (colloids, viruses, bacteria)
- Transport of Multiple Ions (sequential first-order decay)
 - **Radionuclides:** ${}^{238}Pu {}^{234}U {}^{230}Th {}^{226}Ra$
 - Nitrogen: $(NH_2)_2CO \rightarrow NH_4^+ \rightarrow NO_2^- \rightarrow NO_3^-$
 - Pesticides:
 aldicarb (oxime) -> sulfone (sulfone oxime) -> sulfoxide (sulfoxide oxime)
 - Chlorinated Hydrocarbons: PCE -> TCE -> c-DCE -> VC -> ethylene
 - Pharmaceuticals, Hormones: Estrogen (17bEstradiol -> Estrone -> Estriol), Testosterone
 - **Explosives:** TNT (-> 4HADNT -> 4ADNT -> TAT), RDX, HMX
 - Transport of Major Ions (the UNSATCHEM module)
 - General BioGeoChemical Reactions (the HP1 module)
 - Processes in Wetlands (the CW2D and CWM1 modules)
 - Colloid-Facilitated Solute Transport (the C-Hitch module)







Subsurface Drip Irrigation System Soil water content simulated as: A. a Three-Dimensional system with two point sources B. a Two-Dimensional system with a line source **C. An Axisymmetrical** two-dimensional system with a point source

Kandelous, M. M., J. Šimůnek, M. Th. van Genuchten, and K. Malek, Soil water content distributions between two emitters of a subsurface drip irrigation system, *Soil Science Society of America Journal*, 75(2), 488-497, 2011.



Leak (2 mm diameter) at the bottom of the Palmdale Reservoir.



Finite element mesh and material distribution. Two-dimensional transect 411 m wide and 61 m deep with a freeway in the middle.



Velocity vectors

Two-dimensional transect 411 m wide and 61 m deep with a freeway in the middle



Three-Dimensional Transport Domain

HYDRUS (2D/3D) Projects



🕼 Gaometry 📶 FE Mach | 🚱 Domain Properties | 🖾 Initial Conditions | 🙆 Boundary Conditions | 🗰 Results |

HYDRUS - Transport Domains

- A. 2D Simple **B.** 2D – General C. 3D – Simple **D.** 3D – Layered E. 3D – General **HYDRUS Levels: 2D – Lite** (A) **2D – Standard (A+B)** 3D - Lite (A+C)
- 3D Standard (A+B+C+D)
- **3D Professional (All)**















HYDRUS (2D/3D) - Geometries

3D-General Geometries:

Geometry defined using Planar Surfaces:

Geometry defined using Curved Surfaces:



The tunnel (the red object) is defined using a surface that intersects all other three surfaces

General 3D Geometries

Import of complex Geometries (e.g., **DXF**, **TIN**, **STL**)



b-bin of the @ Seture _______ dison. ______ Heads ______ Seture _____ Seture _____ Seture _____ Seture ______ Seture ______ Seture ______ Seture ______ Seture ______ Seture ______ Seture _____ Seture ______ Seture _____ Seture ______ Seture _____ Seture ______ Seture _____ Seture _

HYDRUS: 3D-Professional

Discontinuous 3D Layers



HYDRUS: 3D-Professional

Complex Drainage Systems



HYDRUS: 3D-Professional

Infiltration Basin



ParSWMS – Parallelized Version of HYDRUS

- ParSWMS (Hardelauf et al., 2007) Parallelized version of SWMS_3D (Šimůnek et al., 1995).
- **Developed by** *Forschungszentrum Jülich, Germany.*
- **SWMS_3D** earlier and simpler version of Hydrus-3D
- MPI (Message-Passing Interface) a library specification for message-passing between the different processors. MPI is free software for LINUX or UNIX operating systems.

♦ Test

- Water flow and solute transport problem 492264 finite element nodes
- Supercomputer with 41 SMP nodes with 32 processors each (total 1312 processors Power4+ 1.7 GHz)

ParSWMS – Parallelized Version of HYDRUS

2D Water flow and solute transport (Hardelauf et al., 2007) 492,264 finite element nodes





3D Water flow problem 275,706 finite element nodes (Herbst et al., 2008)
ParSWMS – Parallelized Version of HYDRUS



Time gain as compared to the one processor run (in log2) as a function of the number of processors n_p (in log2) for solute transport scenario with 492,264 nodes (open circles) and water flow with atmospheric upper boundary conditions (diamonds).

HYDRUS Codes and its Modules

HYDRUS + PHREEQC = HP1 (hydrological + biogeochemical processes) ♦ HYDRUS + UNSATCHEM (hydrological + CO₂ + geochemical processes) HYDRUS + Wetland (W2D/CWM1) (processes in constructed wetlands) HYDRUS + C-Hitch (colloid-facilitated solute transport) HYDRUS + MODFLOW (hydrological processes at the large scale)

HP1 (HYDRUS+PHREEQC)

Simulating water flow, transport and biogeochemical reactions in environmental soil quality problems



A Coupled Numerical Code for Variably Saturated Water Flow, Solute Transport and BioGeoChemistry in Soil Systems



HP1 (HYDRUS+PHREEQC)

HYDRUS-1D:

- Variably Saturated Water Flow
- Solute Transport
- Heat transport
- Root water uptake

PHREEQC [Parkhurst and Appelo, 1999]:

Available chemical reactions:

- Aqueous complexation
- Redox reactions
- Ion exchange (Gains-Thomas)
- Surface complexation diffuse double-layer model and nonelectrostatic surface complexation model
- Precipitation/dissolution
- Chemical kinetics
- Biological reactions



HYDRUS-1D GUI for HP1



Jacques, D., and J. Šimůnek, Notes on the HP1 software – a coupled code for variably-saturated water flow, heat transport, solute transport and biogeochemistry in porous media, HP1 Version 2.2, *SCK*•*CEN*-*BLG-1068*, Waste and Disposal, SCK•CEN, Mol, Belgium, 114 pp., 2010.

HP1 - Transport and Cation Exchange

Involving major ions (Ca, Na, Al, Cl) and Heavy Metals (Zn, Pb, Cd)



8-cm column is initially contaminated with heavy metals (in equilibrium with the cation exchanger). The column is then flushed with a solution without heavy metals.

HP1 Examples

- Transport of Heavy Metals (Zn²⁺, Pb²⁺, and Cd²⁺) subject to multiple cation exchange
- ◆ Transport and mineral dissolution of amorphous SiO₂ and gibbsite
- Heavy metal transport in a medium with a pH-dependent cation exchange
- Infiltration of a Hyperalkaline Solution in a clay sample (kinetic precipitation-dissolution of kaolinite, illite, quartz, calcite, dolomite, gypsum, hydrotalcite, and sepiolite)
- Kinetic biodegradation of NTA (biomass, cobalt)
- Long-term Uranium transport following mineral phosphorus fertilization (pH-dependent surface complexation and cation exchange)
- Transport of Explosives, such as TNT and RDX
- Property Changes (porosity/conductivity) due to precipitation/ dissolution

HYDRUS + UNSATCHEM

HYDRUS and HYDRUS (2D/3D)

- variably saturated water flow
- heat transport
- root water uptake
- solute transport

• UNSATCHEM (Šimůnek et al., 1996)

- Carbon Dioxide Transport
- Major Ion Chemistry
 - cation exchange
 - precipitation-dissolution (instantaneous and kinetic)
 - complexation

UNSATCHEM Module

1	Aqueous components	7	Ca ²⁺ , Mg ²⁺ , Na ⁺ , K ⁺ , SO ₄ ²⁻ , CI ⁻ , NO ₃ ⁻
2	Complexed species	10	$CaCO_3^{\circ}$, $CaHCO_3^+$, $CaSO_4^{\circ}$, $MgCO_3^{\circ}$, MgHCO_3^+, MgSO_4^{\circ}, NaCO_3^-, NaHCO_3^{\circ}, NaSO_4^-, KSO_4^-
3	Precipitated species	6	$\begin{array}{l} CaCO_{3}, CaSO_{4} \cdot 2H_{2}O, MgCO_{3} \cdot 3H_{2}O, \\ Mg_{5}(CO_{3})_{4}(OH)_{2} \cdot 4H_{2}O, \\ Mg_{2}Si_{3}O_{7.5}(OH) \cdot 3H_{2}O, CaMg(CO_{3})_{2} \end{array}$
4	Sorbed species (exchangeable)	4	Ca, Mg, Na, K
5	CO ₂ -H ₂ O species	7	P_{CO2} , $H_2CO_3^*$, CO_3^{2-} , HCO_3^- , H^+ , OH^- , H_2O
6	Silica species	3	H_4SiO_4 , H_3SiO_4 , $H_2SiO_4^2$.

Kinetic reactions: calcite precipitation/dissolution, dolomite dissolution Activity coefficients: extended Debye-Hückel equations, Pitzer expressions

UNSATCHEM - Lysimeter Study



Gonçalves, M. C., J. Šimůnek, T. B. Ramos, J. C. Martins, M. J. Neves, and F. P. Pires, Multicomponent solute transport in soil lysimeters irrigated with waters of different quality, *Water Resources Research*, *42*, 17 pp., 2006.

UNSATCHEM-2D Module



Šimůnek, J., and D. L. Suarez, Two-dimensional transport model for variably saturated porous media with major ion chemistry, *Water Resources Research*, *30*(4), 1115-1133, 1994.

Wetland Module

Constructed Wetlands (CWs) or wetland treatment systems

- designed to improve water quality
- use the same processes that occur in natural wetlands but have the flexibility of being constructed
- effective in treating organic matter, nitrogen, phosphorus, and additionally for decreasing the concentrations of heavy metals, organic chemicals, and pathogens
- **CW2D :** aerobic and anoxic processes for organic matter, nitrogen and phosphorus
- **CWM1:** aerobic, anoxic and anaerobic processes for organic matter, nitrogen and sulphur

Subsurface Vertical (CW2D) and Horizontal (CWM1) flow constructed





Wetland Modules: Components

CW2D : aerobic and anoxic processes for organic matter, nitrogen and phosphorus CWM1: aerobic, anoxic and anaerobic processes for organic matter, nitrogen and sulphur Components:

CW2D (Langergraper and Simunek 2005)	CWMI (Langergraher et al. 2009b)	Water Cantent	
CWED (Langergrader and Sumanck, 2003)	C Whit (Langergrader et al., 20050)		
Organic matter, nitrogen, phosphorus	Organic matter, nitrogen, sulphur		
CW2D components	Soluble components		
 SO: Dissolved oxygen, O2. CR: Readily biodegradable soluble COD. CS: Slowly biodegradable soluble COD. CI: Inert soluble COD. XH: Heterotrophic bacteria XANs: Autotrophic ammonia oxidizing bacteria (Nitrosomonas spp.) XANb: Autotrophic nitrite oxidizing bacteria (Nitrobacter spp.) NH4N: Ammonium and ammonia nitrogen. NO2N: Nitrite nitrogen. NO3N; Nitrate nitrogen. N2: Elemental nitrogen. PO4P: Phosphate phosphorus 	 SO: Dissolved oxygen, O2. SF: Fermentable, readily biodegradable soluble COD. SA: Fermentation products as acetate. SI: Inert soluble COD. SNH: Ammonium and ammonia nitrogen. SNO: Nitrate and nitrite nitrogen. SNO: Nitrate and nitrite nitrogen. SSO4: Sulphate sulphur. SH2S: Dihydrogensulphide sulphur. Particulate components XS: Slowly biodegradable particulate COD. XI: Inert particulate COD. XI: Inert particulate COD. XI: Heterotrophic bacteria. XA: Autotrophic nitrifying bacteria. XFB: Fermenting bacteria. 	 I.1 - Dissolved Oxygen I.2 - Fermentable Biodegr. COD I.3 - Fermentation Products I.4 - Inert Soluble COD I.5 - Ammonia NH4-N I.6 - Nitrate and Nitrite (NO2+NO3) I.7 - Sulphate Sulphur (SO4) I.8 - Dihydrogensulphide Sulphur (H2S) I.9 - Slowly Biodegr. COD I.10 - Inert Particulate COD I.17 - Tracer I.17 - S2 - Fermentable Biodegr. COD I.17 - S - Fermentable Biodegr. COD I.17 - S - Fermentable Biodegr. COD I.17 - S2 - Fermentable Biodegr. COD III - S2 - Fermentable Sidegr. COD III - S2 - S10000 - S2 - S1	
Organic nitrogen and organic phosphorus are modeled as part of the COD. Nitrification is modeled as a two-step process. Bacteria are assumed to be immobile. It is generally assumed that all components except bacteria are soluble.	 XAMB: Acetotrophic methanogenic bacteria. XASRB: Acetotrophic sulphate reducing bacteria. XSOB: Sulphide oxidizing bacteria. Organic nitrogen and organic phosphorus are modeled as part of the COD. 	 \$10 - Inert Particulate COD \$11 - Heterotrophic Bacteria \$12 - Autotrophic Bacteria \$13 - Fermenting Bacteria \$14 - Acet. Methan. Bact. \$15 - Acet. Sulphate Red. Bact. \$16 - Sulphide Oxidising Bacteria 	

Langergraber, G., and J. Šimůnek, The Multi-component Reactive Transport Module CW2D for Constructed Wetlands for the HYDRUS Software Package, Manual – Version 1.0, *HYDRUS Software Series 2*, Department of Environmental Sciences, University of California Riverside, Riverside, CA, 72 pp., 2006.

Langergraber, G., D. Rousseau, J. Garcia, and J. Mean, CWM1 - A general model to describe biokinetic processes in subsurface flow constructed wetlands, *Water Science Technology*, 59(9), 1687-1697, 2009.

Wetland Modules: Processes

Processes: CW2D (Langergraber and Šimůnek, 2005) Heterotrophic bacteria:

- 1. Hydrolysis: conversion of CS into CR.
- Aerobic growth of XH on CR (mineralization of organic matter).
- Anoxic growth of XH on CR (denitrification on NO2N).
- Anoxic growth of XH on CR (denitrification on NO3N).
- 5. Lysis of XH.

Autotrophic bacteria: 6. Aerobic growth of XANs on SNH (ammonium oxidation).

- Lysis of XANs.
 Aerobic growth of XANb on SNH (nitrite oxidation).
- 9. Lysis of XANb.

1. Hydrolysis: conversion of XS into SF. 2. Aerobic growth of XH on SF (mineralization of organic matter). 3. Aerobic growth of XH on S.A (mineralization of organic matter). 4. Anoxic growth of XH on SF (denitrification). 5. Anoxic growth of XH on SA (denitrification). 6. Lysis of XH. Autotrophic bacteria: 7. Aerobic growth of XA on SNH (nitrification). 8. Lysis of XA. Fermenting bacteria: 9. Growth of XFB (fermentation). 10. Lysis of XFB. Acetotrophic methanogenic bacteria: 11. Growth of XAMB: Anaerobic growth of acetotrophic, methanogenic bacteria XAMB on acetate SA. 12. Lysis of XAMB. Acetotrophic sulphate reducing bacteria: 13. Growth of XASRB: Anaerobic growth of acetotrophic, sulphate reducing bacteria. 14. Lysis of XASRB. Sulphide oxidizing bacteria: 15. Aerobic growth of XSOB on SH2S: The opposite process to process 13, the oxidation of SH2S to SSO4. 16. Anoxic growth of XSOB on SH2S: Similar to process 15 but under anoxic conditions.

CWMI (Langergraber et al., 2009b)

Heterotrophic bacteria:

17. Lysis of XSOB.





0.0 0.5 1.0 1.5 2.0 2.5 3.0 3.5 4.0

6

5

(1/bm) NH4N 2

10

8

2

Π

(I/gm) NEON

0 cm

30 cm

0 cm

5 cm

30 cm

15 cm

5 cm

15 cm

Heterotrophic Organisms XH



HYDRUS + C-Hitch

HYDRUS and HYDRUS (2D/3D)

- variably saturated water flow
- heat transport
- root water uptake
- solute transport
- ♦ C-Hitch (Šimůnek et al., 2006)
 - Particle Transport
 - colloids, bacteria, viruses, nanoparticles
 - attachment/detachment, straining, blocking
 - Colloid-Facilitated Solute Transport
 - transport of solutes attached to particles

Colloid, Virus, and Bacteria Transport



Colloid-Facilitated Solute Transport



Colloid-Facilitated Solute Transport



Breakthrough curves for colloids (black line), solute sorbed to colloids (blue line), and solute (red line) when:

Left: solute and colloids are applied independently or

Right: solute is attached initially to colloids

The retardation factor for colloids is equal to 1 and for solute to 4 Unit input concentrations.

The DualPerm Module

Water flow and Solute Transport in Dual-Permeability Variably-Saturated Porous Media



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

HYDRUS Package for Modflow

The HYDRUS Package for Modflow-2000

Hyeyoung Sophia Seo, Navin Twarakavi, Jirka Šimůnek, and Eileen P. Poeter

- Seo, H. S., J. Šimůnek, and E. P. Poeter, Documentation of the HYDRUS Package for MODFLOW-2000, the U.S. Geological Survey Modular Ground-Water Model, *GWMI 2007-01*, International Ground Water Modeling Center, Colorado School of Mines, Golden, Colorado, 96 pp., 2007.
- Twarakavi, N. K. C., J. Šimůnek, and H. S. Seo, Evaluating interactions between groundwater and vadose zone using HYDRUS-based flow package for MODFLOW, *Vadose Zone Journal*, doi:10.2136/VZJ2007.0082, Special Issue "Vadose Zone Modeling", 7(2), 757-768, 2008.

HYDRUS Package for MODFLOW



HYDRUS Package: Zoning

MODFLOW model domain is divided into zones based on similarities in soil hydraulic characteristics, hydrogeology and meteorology. A HYDRUS vertical profile is assigned to each of the zones, in which the 1D Richards equation is solved.



Zone 1



HYDRUS - MODFLOW - Case Study

Hypothetical regionalscale ground water flow problem:

- a) Land surface elevation
- b) depth to bedrock
- c) water table depth at the beginning of the simulation

(a) Land surface elevation (m)



(c) Initial water table depth (m)



(b) Aquifer thickness (m)







HYDRUS - MODFLOW - Case Study

Hypothetical regional-scale ground water flow problem:

MODFLOW zones used to define **HYDRUS soil** profiles





Zones

1

2

3

4 5

6 7

8

9



HYDRUS - MODFLOW - Case Study

Hypothetical regionalscale ground water flow problem:

Ground water table fluxes (recharge vs discharge) as predicted by the HYDRUS package at the end of stress periods (a) 3, (b) 6 and (c) 12.









HYDRUS - Existing Applications

Agricultural:

- Irrigation management (Bristow et al., 2002; Dabach et al., 2011)
- **Drip irrigation design** (Bristow et al., 2002; Kandelous et al., 2010, 2011)
- Sprinkler irrigation design (Hansen et al., 2007, 2008)
- Tile drainage design and performance (Mohanty et al., 1998, do Vos et al., 2000)
- Studies of root and crop growth (Vrugt et al., 2001, 2002; Šimůnek and Hopmans, 2010)
- Salinization and reclamation processes (Šimůnek and Suarez, 1998; Goncalves et al., 2006; Ramos et al., 2011)
- Nitrogen dynamics and leaching (Ventrella et al., 2001; Jacques et al., 2002)
- **Transport of pesticides and degradation products** (Wang et al., 1998; Pot et al., 2005; Köhne et al., 2010)
- Non-point source pollution
- Seasonal simulation of water flow and plant response
- ••

HYDRUS - Existing Applications

Non-Agricultural:

- Leaching from radioactive waste sites at the Nevada test Site (DRI, DOE)
- Flow around nuclear subsidence craters at the Nevada test site (Pohll et al., 1996; Wilson et al., 2000)
- Capillary barrier at Texas low-level radioactive waste disposal site (Scanlon, 1998)
- Evaluation of approximate analytical analysis of capillary barriers (Morris and Stormont, 1997; Kampf and Montenegro, 1997; Heiberger, 1998)
- Landfill covers with and without vegetation (Abbaspour et al, 1997; Albright, 1997; Gee et al., 1999, Scanlon et al., 2002)
- Risk analysis of contaminant plumes from landfills
- Seepage of wastewater from land treatment systems
- Tunnel design flow around buried objects (Knight, 1999)
- Highway design road construction seepage (de Haan, 2002; Hanssen et al., 2005)
- Stochastic analyses of solute transport in heterogeneous media (Tseng and Jury, 1993; Roth, 1995; Roth and Hammel, 1996; Kasteel et al. 1999; Hammel et al., 1999; Roth et al., 1999; Vanderborght et al., 1998, 1999)
- Lake basin recharge analysis (Lee, 2000)

HYDRUS - Existing Applications

Non-Agricultural:

- ♦ Stream-aquifer interactions
- Environmental impact of the drawdown of shallow water tables
- Analysis of cone permeameter and tension infiltrometer experiments (Gribb et al., 1996; Kodešová et al., 1998, 1999; Šimůnek et al., 1997, 1998, 1999)
- Virus and bacteria transport (Shijven and Šimůnek, 2002; Bradford et al., 2002a,b; Yates et al., 2000; Gargiulo et al., 2007, 2008)
- Hill-slope analyses (Hopps et al., 2010)
- Transport of TCE and its degradation products (Scharlaekens et al., 2000; Casey and Šimůnek, 2002)
- Multicomponent geochemical transport (Jacques and Šimůnek, 2002, 2008, 2011)
- Analyses of riparian systems (Whitaker, 2000)
- Fluid flow and chemical migration within the capillary fringe (Silliman et al., 2002)
- Flow in historical monuments (Ishizaki et al., 2001)
- Flow and transport around land mines (Das et al., 2001; Šimůnek et al., 2001)
- Analyses of Chloride profiles in deep vadose zones to evaluate historical fluxes (Scanlon et al., 2003)



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HYDRUS 2D/3D - software package for simulating water, heat, and solute transport in variably saturated porous media.

MESHGEN Plus - open modeling environment for Finite-Element and Finite-Volume applications. Includes 2D/3D geometry modeller, FE-mesh generator and customizable modules for pre- and post-processing.

Hydrus-1D - one-dimensional publicdomain version of HYDRUS. This program has been developed and maintained in cooperation with University of California, Riverside, USA.

Services

HYDRUS Services

Extended support of the standard version of HYDRUS and/or modifications of the graphical user interface or computational modules based on clients' specification.

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Rapid development of FEM applications based on the MESHGEN Plus software package.







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HYDRUS Tutorials

Two-Dimensional Examples



2.01 - 2D Domain composed of three irregular regions Video (1.2 MB) - Play - Download

This demo demonstrates how to use multiple surfaces to define a single transport domain, and how these multiple surfaces can be used to assign various domain properties (e.g., materials).













Domain Design and FE-Mesh generation



2.02 - 2D Domain with holes and integrated subregion Video (1.2 MB) - Play - Download

This demo demonstrates how to design a complex two-dimensional transport domain that includes two holes and an internal surface. The transport domain is then discretized using a refined FE-Mesh inside of the internal surface.

2.03 - 3D Domain, Solid 1 - three video tutorials Open tutorial

This series of three demos shows how users can create a transport domain shown on the picture. The demonstration is divided into three parts. First, the main transport domain is defined, then a vertical hole is created in the domain, after which the heights are adjusted.





2.04 - 3D Domain. Solid 2 - three video tutorials Open tutorial

This series of three demos shows users how to create a transport domain shown on the picture and to discretize it into finite elements. We first create the transport domain, then add lines at the surface that will help us to discretize the transport domain into finite elements in the next step, after which we implement the finite element discretization.

2.05 - 3D Domain, Solid 3 - three video tutorials Open tutorial

This series of three demos shows users how to create a transport domain in the picture, to discretize the domain into finite elements, to create sections, and to specify initial and boundary conditions.

2.06 - 3D Domain, Solid 4 - splitting a Solid into Sub-Layers and Columns Video (5.3 MB) - Play - Download

This demo shows how to design a complex three-dimensional transport domain (which includes horizontal pipes). The transport domain is divided into four sub-layers (one with variable thickness). Additional FE-Mesh sections are generated as intersections of sub-layers and vertical columns. The use













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See also HYDRUS-1D selected references

Outside reviews of the HYDRUS software packages

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- Diodato, D. M. 2000. "Software Spotlight (Review of HYDRUS-2D)". Ground Water, 38(1), 10-11.

Customer Projects

Dear HYDRUS users, we would like to encourage you to publish here your projects.



Virtual Experiments to Explore Non-Linear Soil Moisture-Hydrology Interactions at the Hillslope Scale L. Hopp and J.J. McDonnell Department of Forest Engineering, Oregon State University, Corvallis, USA

Abstract <u>Hopp_AGU07_abstract.pdf</u> (19 kB), Read more about the project: <u>Hoop_AGU07.pdf</u> (4.4 MB)

Dynamics of Water Flow in Putting Greens via Computer Simulation McCoy, Ed. and Kevin McCoy, USGA Turfgrass and Environmental Research Online 5(17):1-15, 2006. Read more about the project <u>TurfGrass-2006.pdf</u> (636 kB)

Have we missed your work? Please, let us know. HYDRUS team.

HYDRUS Workshops Proceedings

- Proceedings of the First HYDRUS Workshop, October 19, 2005, S. Torkzaban and S. M. Hassanizadeh (eds.), Department of Earth Sciences, Utrecht University, The Netherlands, ISBN 90-39341125, PDF document, size 4MB.
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Over one thousand applications of HYDRUS-1D and HYDRUS (2D/3D) published in peer-reviewed journal articles, and many more unpublished.

Public Library of HYDRUS-1D Projects

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HYDRUS Projects - Drip

- Project Group: Drip
- Description: Examples involving subsurface drip irrigation; described in Hanson et al. (2006, 2008), Skaggs et al (2004), and Siyal et al. (2009).
- Availability: Download HYDRUS projects now (11.1 MB)

Project	Description
Sub2f1a	Subsurface drip irrigation for the B fertigation strategy (fertigation near beginning of irrigation). Solutes considered: urea-ammonium-nitrate, potassium, phosphorus (Hanson et al., 2006).
Sub2f1c	Subsurface drip irrigation for the E fertigation strategy (fertigation near the end of irrigation). Solutes considered: urea-ammonium-nitrate, potassium, phosphorus (Hanson et al., 2006).
Sub2f3	Subsurface drip irrigation for the M50 fertigation strategy (fertigation during the middle 50% of the irrigation event). Solutes considered: urea-ammonium-nitrate, potassium, phosphorus (Hanson et al., 2006).
Sub1112	Subsurface drip irrigation, water table depth of 0.5 m, 0.3 dS/m, irrigation efficiency=0.9, 7 per week (Hanson et al., 2008).
Sub1212	Subsurface drip irrigation, water table depth of 0.5 m, 1.0 dS/m, irrigation efficiency =0.9, 7 per week (Hanson et al., 2008).
Sub2111	Subsurface drip irrigation, water table depth of 1.0 m, 0.3 dS/m, irrigation efficiency =0.9, 2 per week (Hanson et al., 2008).

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Short Courses

HYDRUS shortcourse: November 18 - 20, 2009, San Luis Potosi, Mexico

"Modeling Water Flow and Contaminant Transport in Soils and Groundwater Using the Hydrus Computer Software Packages"

"(Modelado del Flujo de Aqua y Transporte de Contaminantes en Suelos y Aqua Subterránea Usando los Paquetes de Cómputo Hydrus)"

Shortcourse instructor:

Jirka Šimunek, Dept. of Environmental Sciences, University of California, Riverside (CA)

HYDRUS and HP1 shortcourse: September 28 - October 2, 2009, Gent, Belgium

"Simulating soil water movement and transport using the biogeochemical transport model HP1"

Belgium Nuclear Research Center, SCK.CEN, Mol. Belgium

Shortcourse instructors:

linka Simulaek Dent of Environmental Sciences University of California Diverside (CA)

HYDRUS shortcourse: July 12-14, 2009, Sede Boger Campus of the Ben-Gurion University, Israel

"Modeling water flow and contaminant transport in soils and groundwater using the HYDRUS software packages"

Albert Katz International School of Desert Studies at the Sede Boger Campus of the Ben-Gurion University in Israel

The shortcourse instructors:

Dr. Jirka Simunek, Dept. of Environmental Sciences, University of California, Riverside (CA) Dr. Naftali Lazarovitch, French Associates Institute for Agriculture and Biotechnology of Drylands, The Ben-Gurion University of the Negev, Sede Boger Campus, Israel

The course begins with a detailed conceptual and mathematical description of water flow and solute transport processes in the vadose zone, followed by an brief overview of the use of finite element techniques for solving the governing flow and transport equations. Special attention is given to the highly nonlinear nature of the governing flow equation. Alternative methods for describing and modeling the hydraulic functions of unsaturated porous media are also described. "Hands-on" computer sessions will provide participants an opportunity to become familiar with the Windowsbased HYDRUS-1D and HYDRUS (2D/3D) software packages. Emphasis will be on the preparation of

input data for a variety of applications, including flow an flow through a dam, flow and transport to a tile drain, a landfill through the unsaturated zone into groun demonstrated by means of a one-dimensional inverse

HYDRUS shortcourse: March 17-19, 2009, Prague, Czech Republic

"Advanced modeling of water flow and contaminant transport in porous media using the HYDRUS software packages"

Czech University of Life Sciences, Faculty of Agrobiology, Food and Natural Resources, Prague, Czech Republic PC Progress, Ltd, Prague, Czech Republic

The shortcourse instructors:

Dr. Jirka Šimunek, Dept. of Environmental Sciences, University of California, Riverside (CA) Dr. Radka Kodešová, Department of Soil Science and Geology of the University of Life Sciences, Prague, Czech Republic

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