Tutorial 4

I. Water Flow and Solute Transport in a Layered Soil Profile

Diederik Jacques, Jirka Šimůnek, and Rien van Genuchten

In this tutorial with HYDRUS-1D we consider water flow and the transport of tracers and adsorbing chemicals through a Podzol soil profile. The tutorial is divided into two parts. In the first part (II) only water flow is simulated, while in the second part (I) solute transport is additionally considered. Examples in the first part of this tutorial involve both steady-state and transient variably saturated flow in a 1-m deep multi-layered soil profile. Transient flow is induced by atmospheric boundary conditions. No root water uptake is considered, thus restricting the atmospheric boundary conditions to daily values of precipitation and evaporation. The example is divided into two parts:

A. Initial conditions for transient water flow example
B. Transient water flow (atmospheric conditions) example

Soil hydraulic and physical parameters (Table 1) of the dry Spodosol located at the "Kattenbos" site near Lommel, Belgium were taken from Seuntjens (2000, Tables 3.1 and 7.1).

***Table 1** Soil hydraulic and other properties of six soil horizons*.

Horizon	Depth (cm)	ρ (g cm^{-3})	Organic Carbon (%)	θ_r	θ_s	*A* (cm^{-1})	*n* (-)	K_s (cm d^{-1})
A	0 – 7	1.31	2.75	0.065	0.48	0.016	1.94	95.04
E	7 – 19	1.59	0.75	0.035	0.42	0.015	3.21	311.04
Bh1	19 – 24	1.3	4.92	0.042	0.47	0.016	1.52	38.88
Bh2	24 – 28	1.38	3.77	0.044	0.46	0.028	2.01	864
BC	28 – 50	1.41	0.89	0.039	0.46	0.023	2.99	1209.6
C1	50 – 75	1.52	0.12	0.030	0.42	0.021	2.99	1209.6
C2	75 – 100	1.56	0.08	0.021	0.39	0.021	2.99	1209.6

Part A:
The steady-state flow example corresponds with experimental conditions in a lysimeter experiment described in Seuntjens (2000). The initial condition is defined assuming a constant flux of 0.12 cm day^{-1} and a free-drainage lower boundary condition. The flux corresponds to the long term (1972-1981) actual infiltration rate (precipitation - actual evapotranspiration).

Part B:
The upper boundary condition now involves daily precipitation and evaporation fluxes defined using meteorological data from the Brogel station weather (Belgium) for 1972. Some input data are summarized in the "*HYDRUS-Course-Data.xls*" file.

Reference

Seuntjens, P., 2000. Reactive solute transport in heterogeneous porous media. Cadmium leaching in acid sandy soil. PhD, University of Antwerp, 236 p.

A. Steady-State Water Flow in a Layered Soil Profile

Project Manager

Button "New"
Name: LSP-W1
Description: Steady-State Water Flow (q=0.12 cm/d) in a Layered Soil Profile
Button "OK"
Button "Open"

Main Processes

Heading: Calculate steady-state conditions
Button "Next"

Geometry Information

Length Units: cm
Number of Soil Materials: 7
Depth of the Soil Profile: 100 cm
Button "Next"

Time Information

Time Units: Days
Final Time: 100
Initial Time Step: 0.001
Minimum Time Step: 0.000001
Maximum Time Step: 0.5
Button "Next"

Print Information

Number of Print Times: 10
Button "Select Print Times"
Button "OK"
Button "Next"

Water Flow – Iteration Criteria

Button "Next"

Water Flow – Soil Hydraulic Model

Button "Next"

Water Flow – Soil Hydraulic Parameters

Copy the soil hydraulic parameters from the Excel file (units are cm and day)
Button "Next"

Water Flow – Boundary Conditions

Upper Boundary Condition: Constant Flux
Lower Boundary Condition: Free Drainage
Button "Next"

Water Flow – Constant Boundary Fluxes

Upper Boundary Flux: -0.12 cm/day
Button "Next"

HYDRUS-1D Guide:

Button "OK"

Profile Information – Graphical Editor

Button "Edit condition"
Select with the *Mouse*: nodes from 8 to 19 cm; specify Material 2
nodes from 20 to 24 cm; specify Material 3
nodes from 25 to 28 cm; specify Material 4
nodes from 29 to 50 cm; specify Material 5
nodes from 51 to 75 cm; specify Material 6
nodes from 76 to 100 cm; specify Material 7
Specify initial pressure head of –100 cm
Include observation points at 50 and 100 cm
Save and Exit

Execute HYDRUS-1D

OUTPUT:

Observation Points
Profile Information
Soil Hydraulic Properties
Mass Balance Information

B. Transient Water Flow in a Layered Soil Profile

Project Manager

Select the LSP-W1 project
Button "Copy”
Name: LSP-W2
Description: Transient Water Flow in a Layered Soil Profile
Button "OK"
Button "Open"

Main Processes

Heading: Transient Water Flow in a Layered Soil Profile
Button “OK"

Time Information

Initial Time Step: 0.001
Minimum Time Step: 0.000001
Final Time: 360
Check Time-Variable Boundary Conditions
Number of Time-Variable Boundary Records: 360
Button "Next"

Print Information

Number of Print Times: 18
Button "Select Print Times"
Button "Default"
Button "OK"

Water Flow – Boundary Conditions

Upper Boundary Condition: Atmospheric BC with Surface Run Off
Lower Boundary Condition: Free Drainage
Button "Next"

Variable Boundary Conditions

Open the Excel file with meteorological variables
Select and **Copy** Atmospheric Boundary Conditions
Paste copied values
Button "OK"

Soil Profile Summary

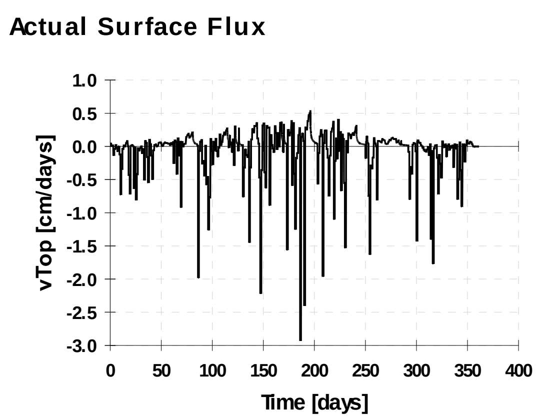
Open the *NOD_INF.OUT* file from the project LSP-W1.h1d using MS Excel
Select and **copy** the last pressure head profile
Paste pressure head profile in h column to define initial conditions.

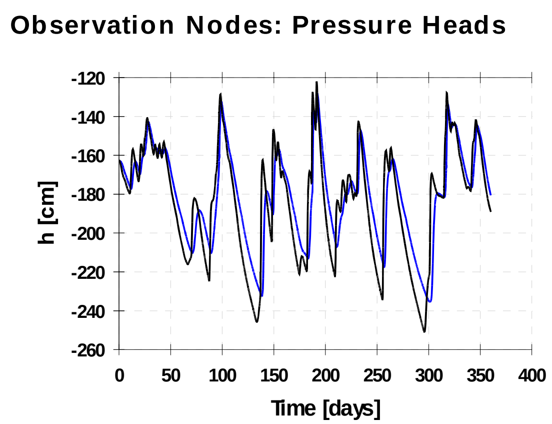
Execute HYDRUS-1D

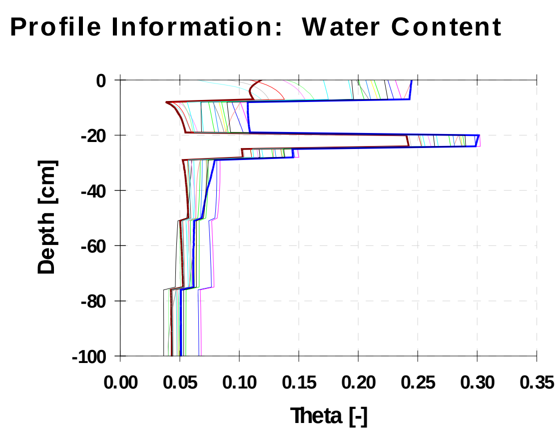
OUTPUT:

Observation Points
Profile Information
Water Flow – Boundary Fluxes and Heads
Soil Hydraulic Properties
Mass Balance Information

Close Project







Tutorial 4

II. Solute Transport in a Layered Soil Profile

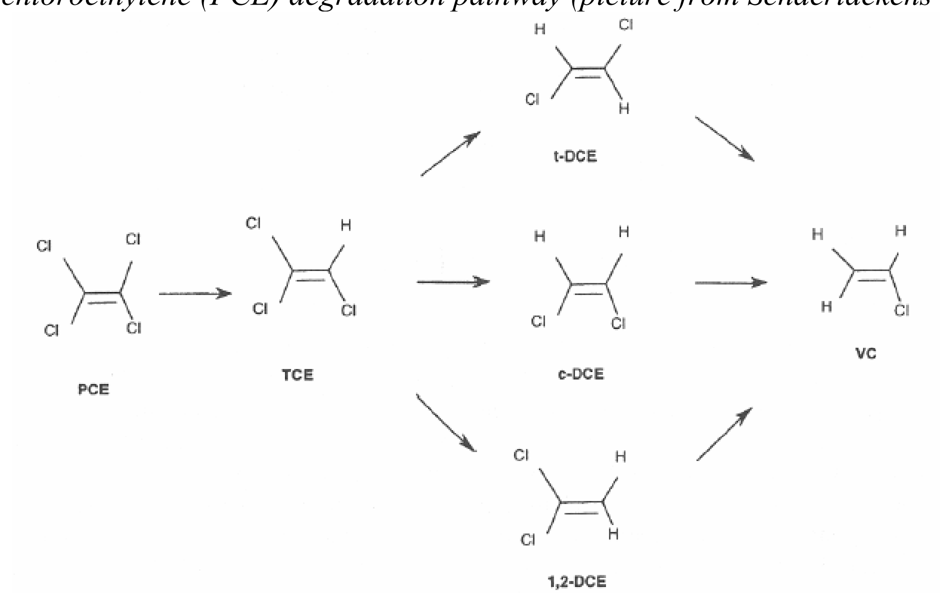
Diederik Jacques, Jirka Šimůnek, and Rien van Genuchten

In the second part of the Tutorial 4 we will use the project "LSP-W2" created in the first part of the Tutorial 4 and assume that there is a spill of a chemical on the first day of simulation at the soil surface. The example is divided into three parts, each of increasing complexity:

A. Tracer Transport
B. Reactive Chemical Transport
C. Transport of PCE and its Daughter Product

For the first run we assume that a nonreactive chemical is spilled on the soil surface. The second and third runs consider the transport of a reactive chemical and that of PCE and its degradation products, respectively. PCE degrades to sequentially form trichloroethylene (TCE), *cis*-1,2-dichloroethylene (*cis*-DCE), *trans*-1,2-dichloroethylene (*trans*-DCE), 1,1-dichloroethylene (1,1-DCE), vinyl chloride (VC) (after Schaerlaekens et al., 1999). VC eventually degrades to ethylene (ETH) which is environmentally acceptable and does not cause direct health effects. HYDRUS-1D can not consider diverging and converging branches. Consequently, all DCE species must be lumped into a single constituent. Some of the input data are again given in the "*HYDRUS-Course-Data.xls*" file.

***Figure** Perchloroethylene (PCE) degradation pathway (picture from Schaerlaekens et al., 1999).*



References

Schaerlaekens, J., Mallants, D., Šimůnek, J., van Genuchten, M.Th., Feyen, J., 1999. Numerical simulation of transport and sequential biodegradation of chlorinated aliphatic hydrocarbons using CHAIN_2D. *Hydrological Processes* 13, 2847-2859.

A. Tracer Transport

Project Manager

Select the LSP-W2 project
Button "Copy"
Name: LSP-S1
Description: Transport of Tracer
Button "OK"
Button "Open"

Main Processes

Heading: Transport of Tracer
Check Solute Transport
Button "Next"

Solute Transport - General Information

Button "Next"

Solute Transport - Transport Parameters

Copy Bulk Densities from the Excel File (1.31, 1.59, 1.3, 1.38, 1.41, 1.52, 1.56)
Dispersivity = 1 cm
Diffusion Coefficient in liquid phase is 1 cm^2/d
Button "Next"

Solute Transport - Reaction Parameters

Button "Next"

Solute Transport - Boundary Conditions

Upper Boundary Condition: Concentration Flux BC
Lower Boundary Condition: Zero Gradient
Button "Next"

Time Variable Boundary Conditions

Precipitation on day 1: 1 cm/d
Evaporation on day 1: 0 cm/d
cTop on day 1: 1.0
Button "Next"

HYDRUS-1D Guide:

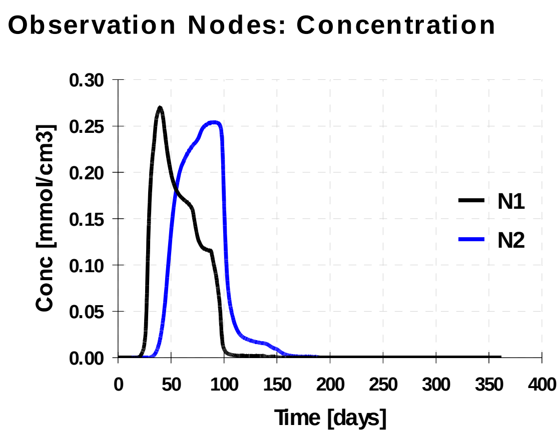
Button "Next"

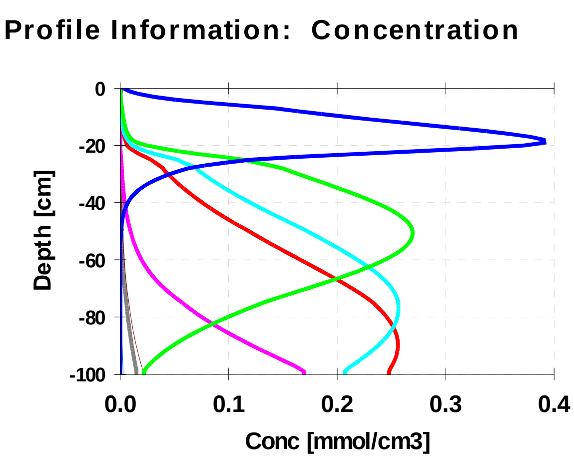
Execute HYDRUS-1D

OUTPUT:

Observation Points
Profile Information
Water Flow – Boundary Fluxes and Heads
Solute Transport Fluxes

Close Project





B. Reactive Solute Transport

Project Manager

Select the LSP-S1 project
Button "Copy"
Name: LSP-S2
Description: Transport of Reactive Solute
Button "OK"
Button "Open"

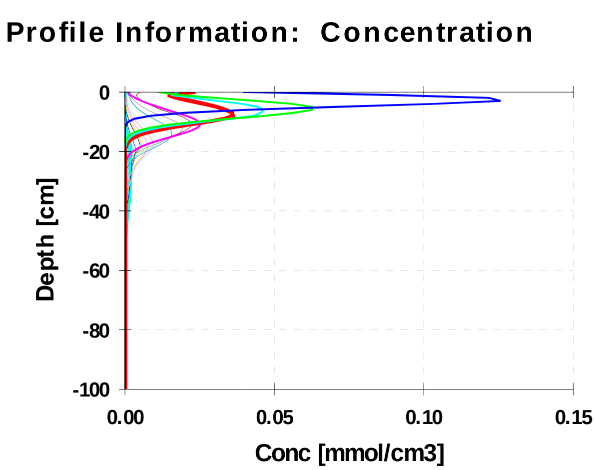
Solute Transport - Reaction Parameters

Distribution coefficient K_d: 0.784 in all layers
Degradation constant SinkWater1': 0.075 in all layers

Execute HYDRUS-1D

OUTPUT:

Observation Points
Profile Information
Mass Balance Information
Solute Transport Fluxes



C. Transport of PCE and its Daughter Products

Project Manager

Select the LSP-S2 project
Button "Copy"
Name: LSP-S3
Description: Transport PCE and its Daughter Products
Button "OK"
Button "Open"

Main Processes

Heading: Transport PCE and its Daughter Products
Button “OK"

Solute Transport - General Information

Number of Solutes: 5

Solute Transport - Transport Parameters

Copy Bulk Densities from the Excel File (1.31, 1.59, 1.3, 1.38, 1.41, 1.52, 1.56)
Dispersivity = 1 cm
Diffusion Coefficient = 1 cm^2/day

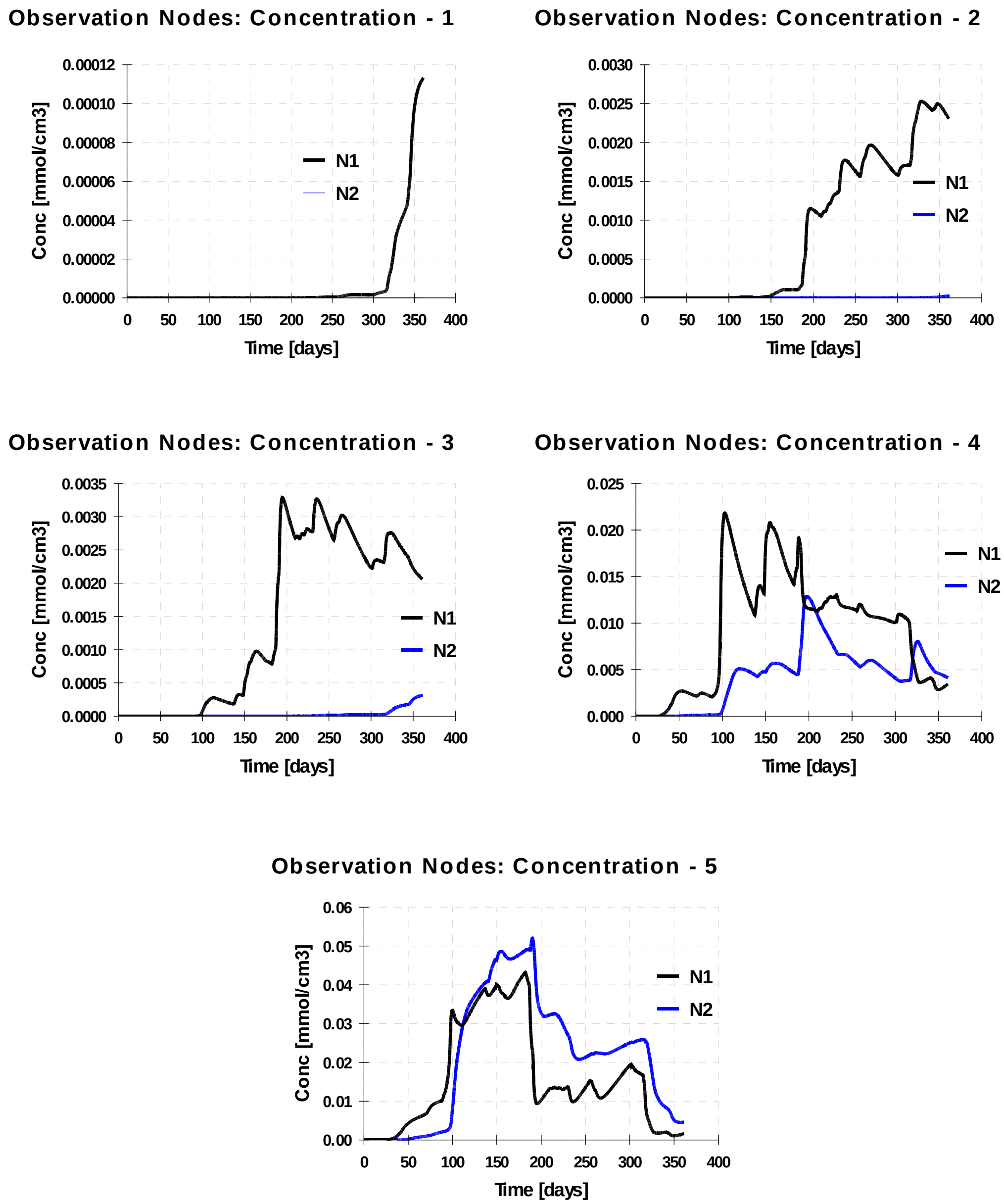
Solute Transport - Reaction Parameters

Solute 1: K_d=0.784, SinkWater1*=0.075 in all layers
Solute 2: K_d=0.277, SinkWater1*=0.07 in all layers
Solute 3: K_d=0.153, SinkWater1*=0.11 in all layers
Solute 4: K_d=0.0106, SinkWater1*=0.03 in all layers
Solute 5: K_d=0.000, SinkWater1*=1e-6 in all layers

Execute HYDRUS-1D

OUTPUT:

Observation Points
Profile Information
Water Flow – Boundary Fluxes and Heads
Solute Transport Fluxes
Mass Balance Information



Transport of (1) PCE, (2) trichloroethylene (TCE), (3) dichloroethylene (DCE), (4) vinyl chloride (VC), and (5) ethylene (ETH).