Food and Agriculture Organization of the United Nations

International Network of Salt-Affected Soils

Optimization of crop irrigation under the risk of salinization using agro-hydrological tools

Session 1: Understanding reactive transport models in soils

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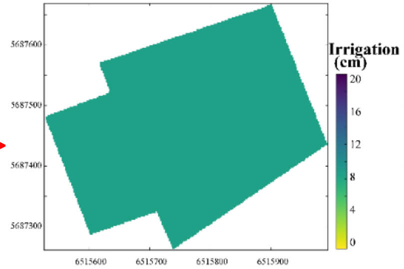
(22/10/2024)

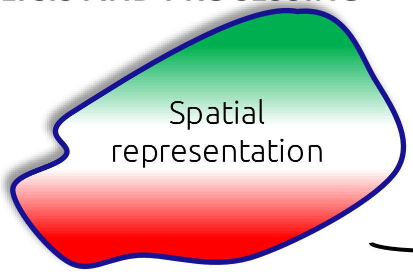
General strategy

Problem statements

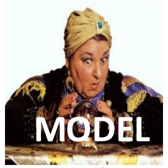
Current situation



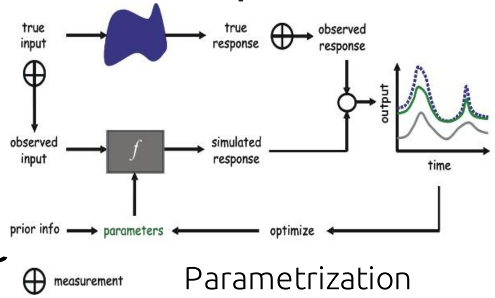
DATA
ANALYSIS AND PROCESSING



Characterization

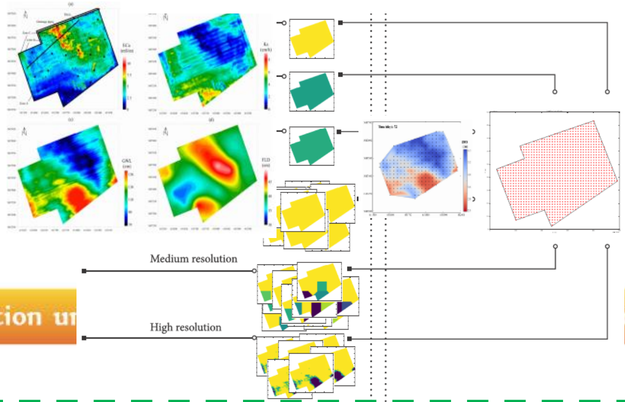


CALIBRATION/EVALUATION

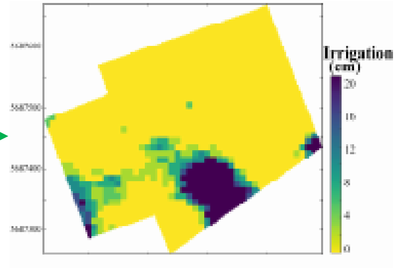


Parametrization

OVERLAY KNOWLEDGE



Knowledge-based solution&application



What observing?

Forcing data

precipitation, net radiation, wind speed, temperature, ...

Monitoring data

flow rate, soil moisture content, solute concentration, soil hydraulic conductivity, groundwater depth (upper and bottom boundary conditions), evapotranspiration, flood depth, root growth and pattern

Knowledge on soil processes

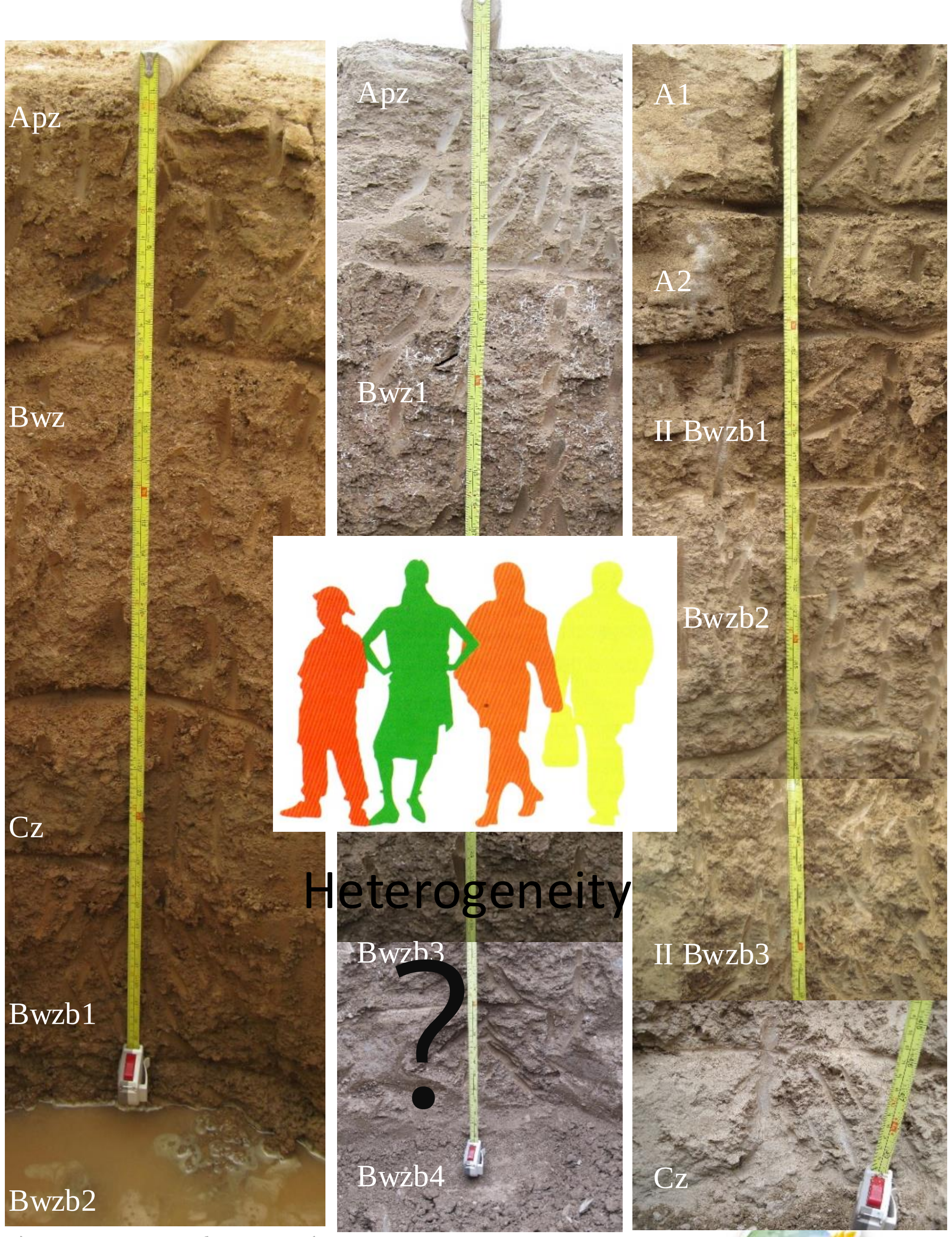
Types of observations?

direct: in situ
in the lab
indirect: Using proxy data, PTFs

Why modeling?

- Part of the action takes place underground
- The spatial and temporal variability is too complex to correctly describe with mathematical formulas
- Various processes are non-linear and / or are stochastic
- Answer different questions: solute movement, water management (irrigation, leaching), crop yield…

✓ To predict (simulate the real world situation)
✓ To understand/simplify the hydrology of a complex system
✓ To constructions or mitigating measures against extremes
✓ To scenario analysis and decision making



(Rezaei et al, 2021)

'All models are wrong...'

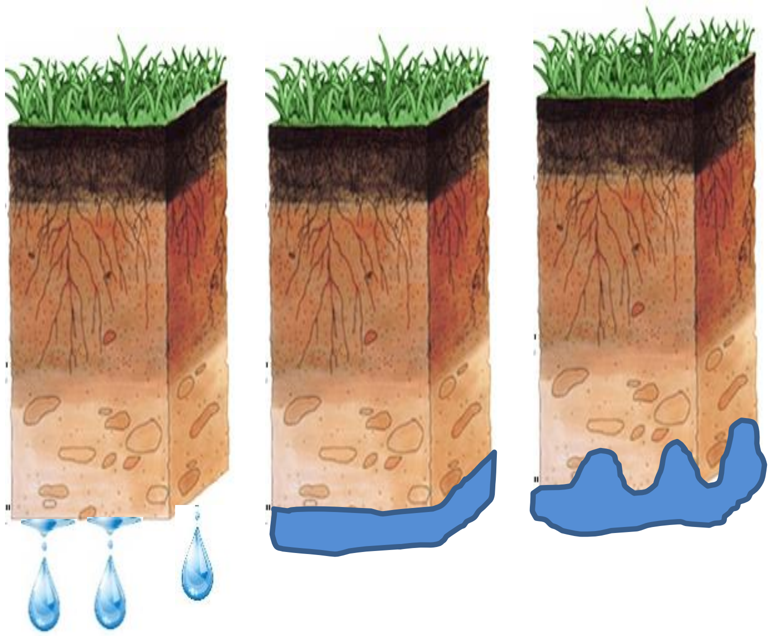
'... but some are useful' (*)

(*) Box and Draper (1987)

"WHAT TYPE OF MODEL MUST BE USED?"
Large dataset or good model?

Modeling approach

Model conceptualization



Root zone depth

Soil layers depth

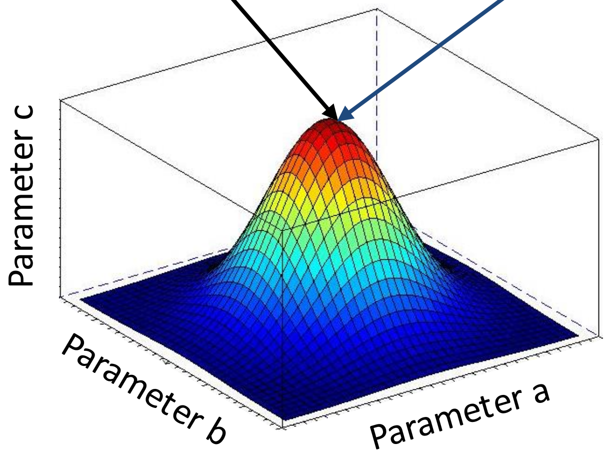
Free drainage/Constant head
variable head

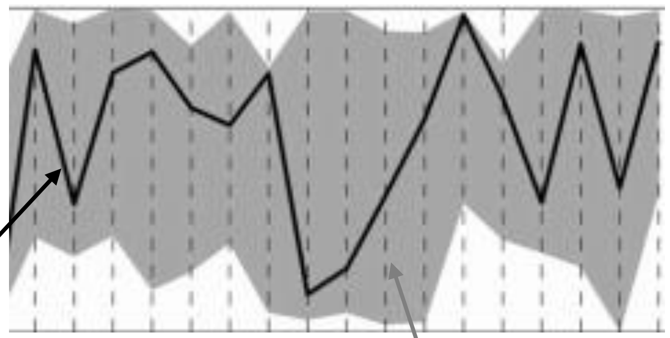
Modeling approach

Model parametrization

Real word parameter set (true value)

Initial/estimated parameter set



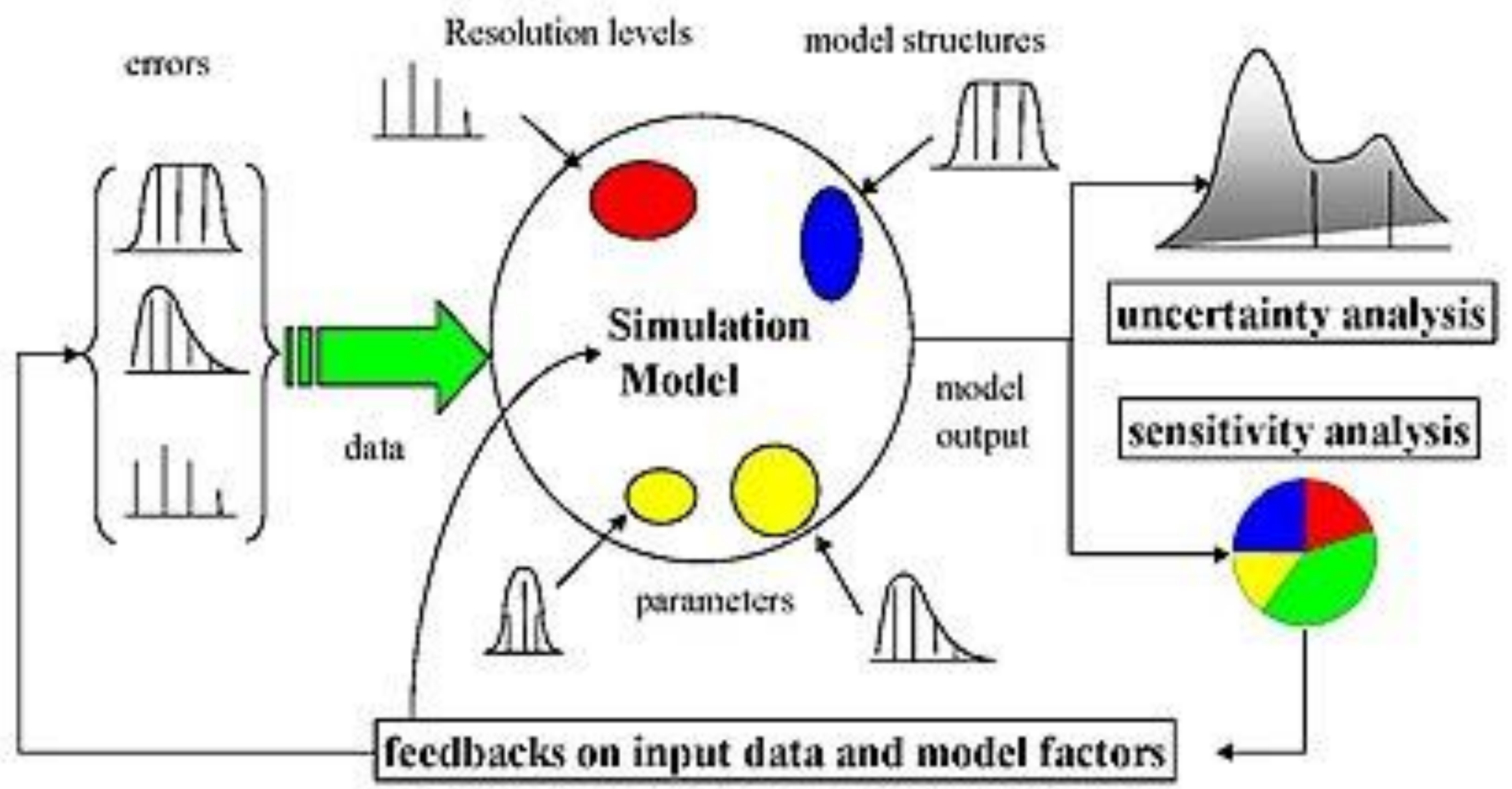


Prediction of true parameter set/observation

Predictions of different parameter sets

Modeling approach

Sensitivity & uncertainty analysis

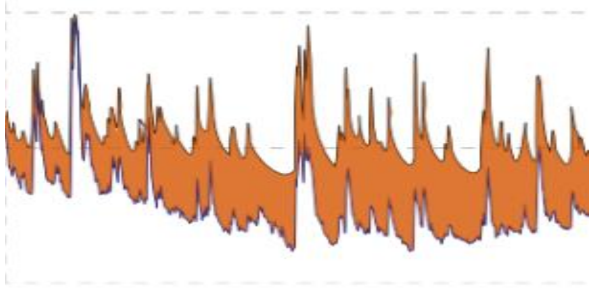


(Saltelli et al, 2019)

Modeling approach

Inverse modeling
Inverse optimization scenarios

Observed data with sensors

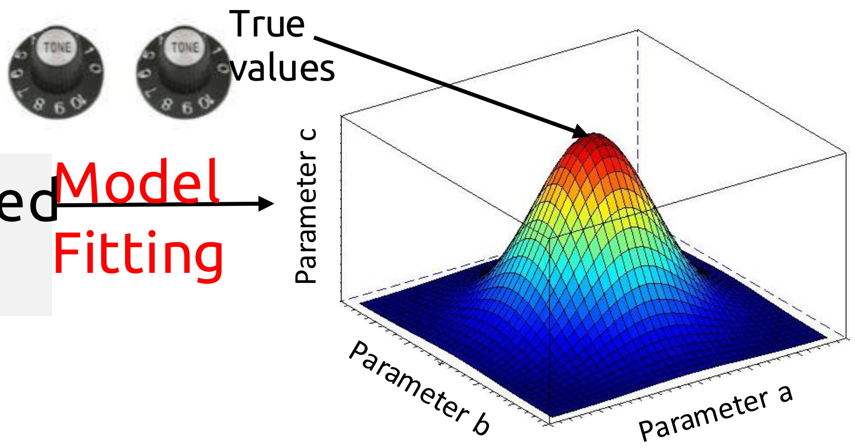


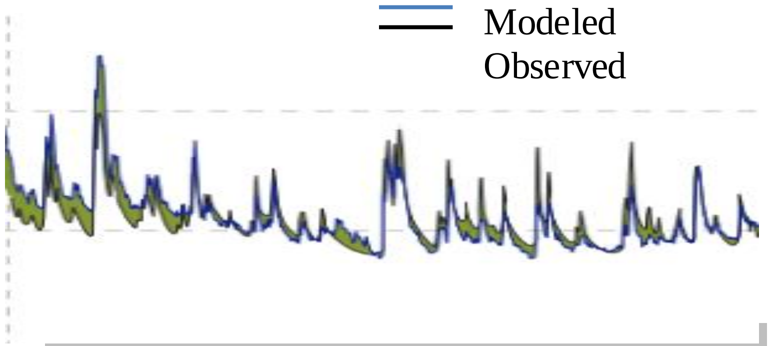
Advanced monitoring

+ Initial/estimated parameter set

Advanced characterization
Boundary condition

Model Fitting





Optimized parameter set
Appropriate bottom boundary

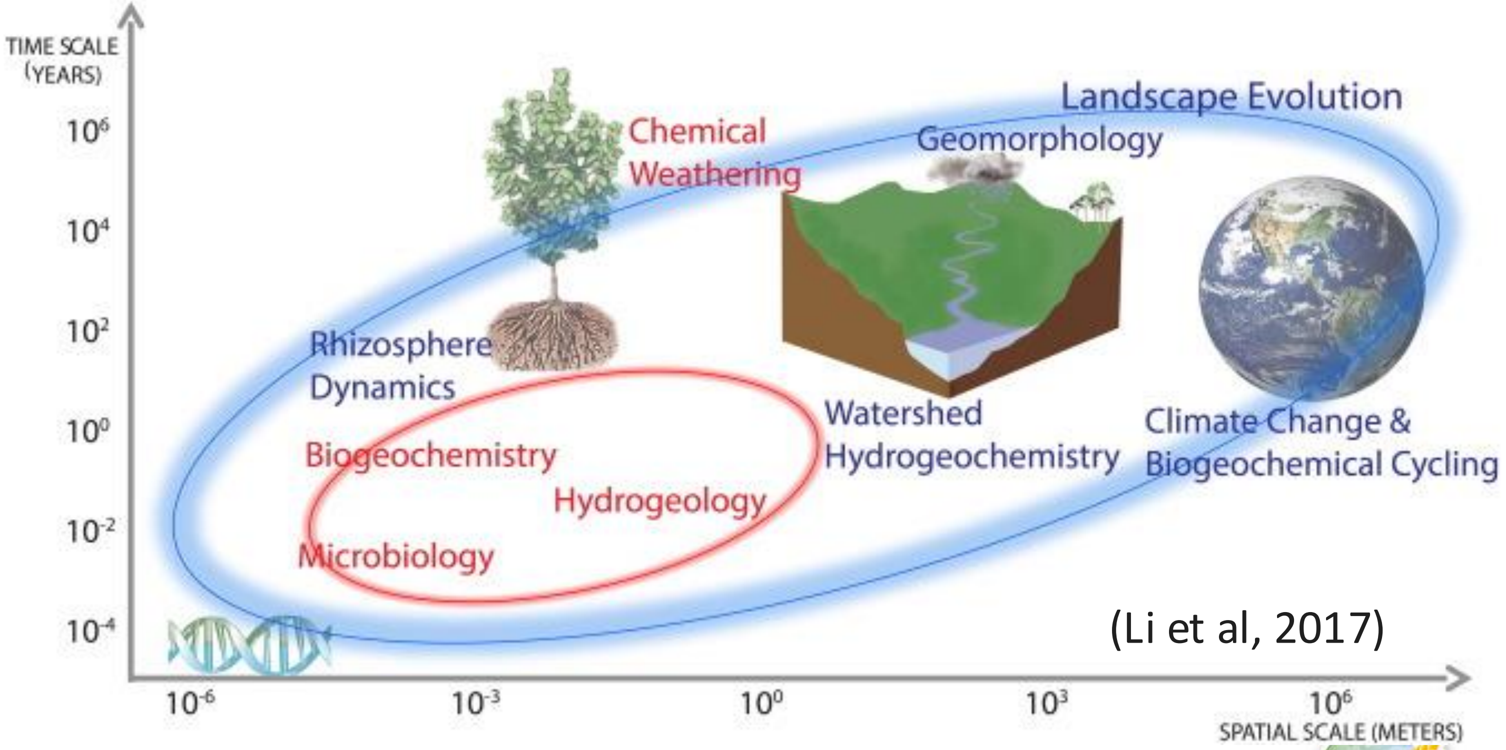
Validation /Evaluation
Independent datasets, Statistical criteria, Soil water & solute stress

“Reactive transport model”

Computer models are integrating chemical species (solutes) reaction with transport of fluids (water phase) through the porous medium. Such models predict the distribution in space (1/2/3D) and time of the chemical reactions that occur along a flowpath.
(Guimarães, 2002; Jung et al., 2009; Wallis et al., 2011).

(1) equilibrium models,
(2) partial equilibrium models, and (3) kinetic models.

Coupling models
Hydrological models
Crop growth models



(Li et al, 2017)

“Reactive transport modelling”

Interactions in Soil Systems

Atmosphere: Influences soil moisture, temperature, and gas exchange

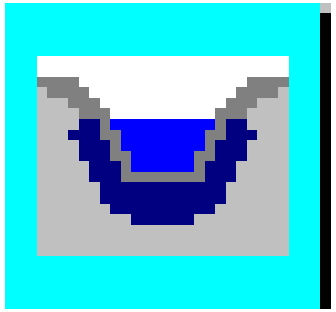
Plants: Affect water uptake, nutrient cycling, and root exudates

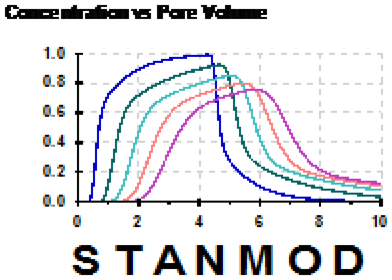
Groundwater: Affects soil saturation, chemical transport, and salinity

Coupling/integrating models

Hydrological models

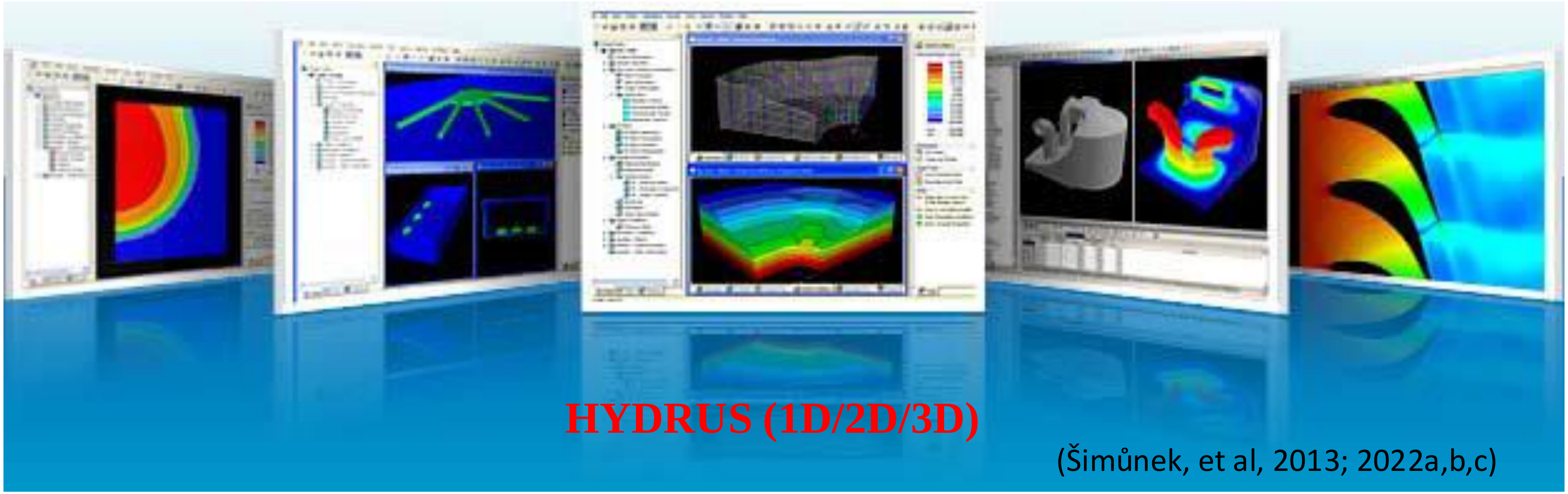
Crop growth models





ISMC International Soil Modeling Consortium

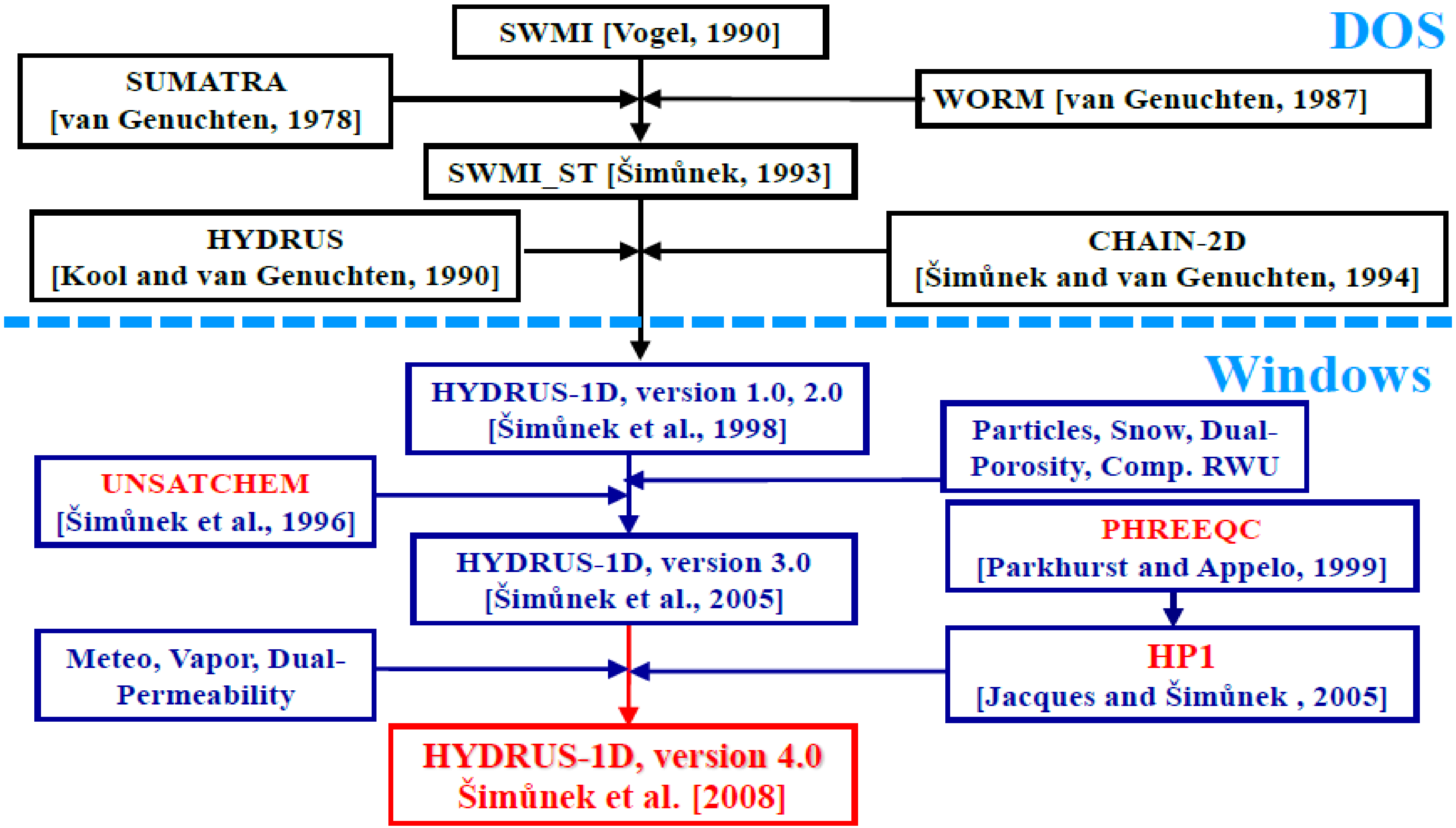
https://soil-modeling.org/resources-links/model-portal



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

- **thousands of users around the world**
- **thousands of applications published**
- **used by scientists, students, and/or practicing professionals**

Brief history and development of Hydrus-1D

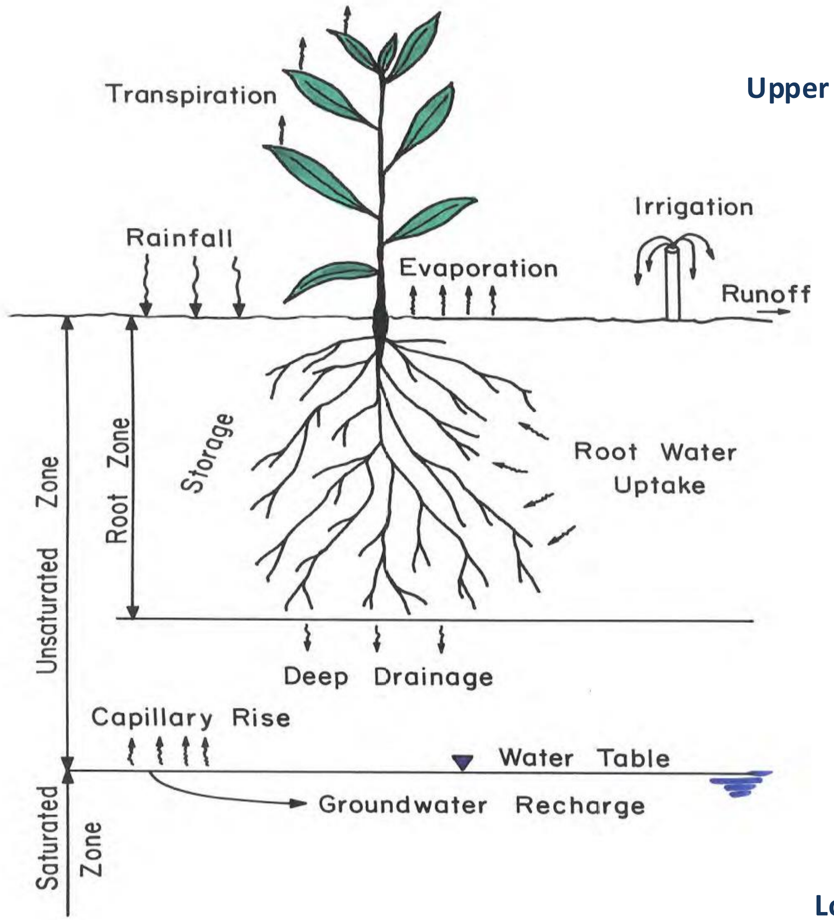


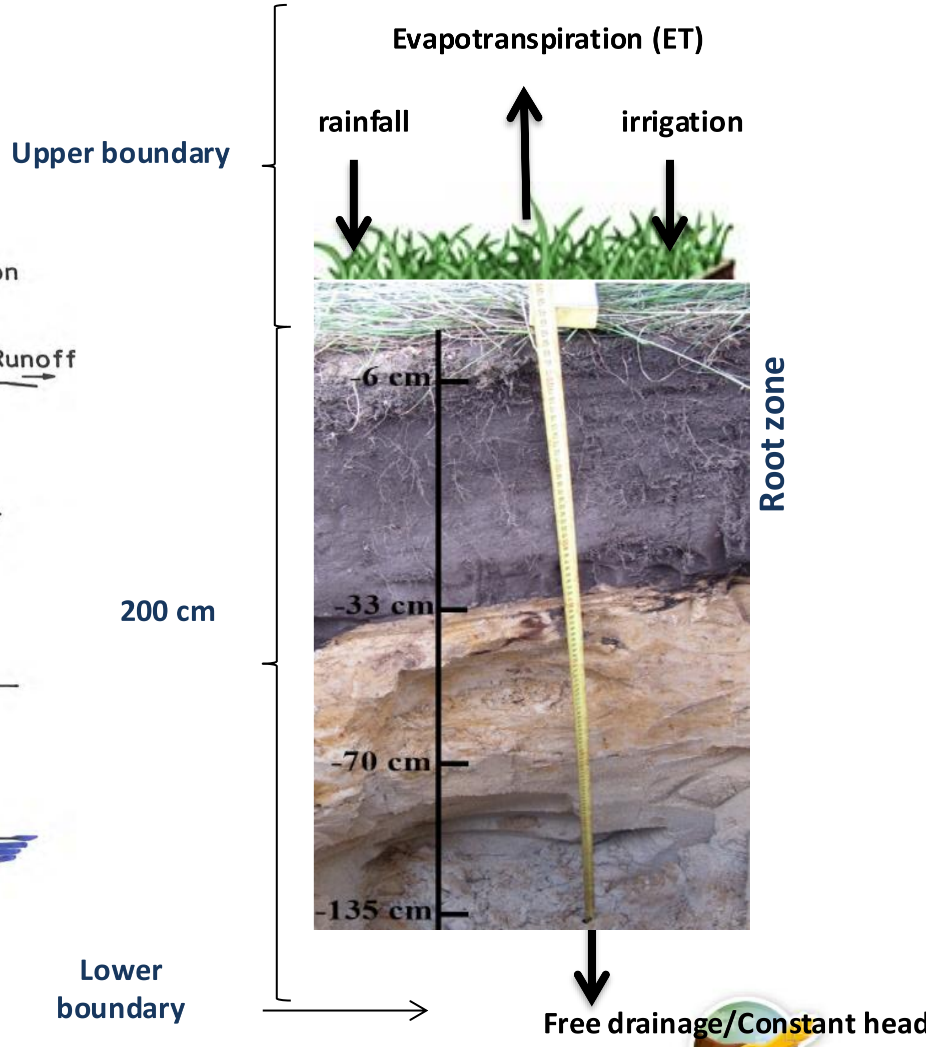
... **Version** 4.16, 2013 and **Version** 4.17, 2018

Version 5.0, 2022

Agricultural Applications

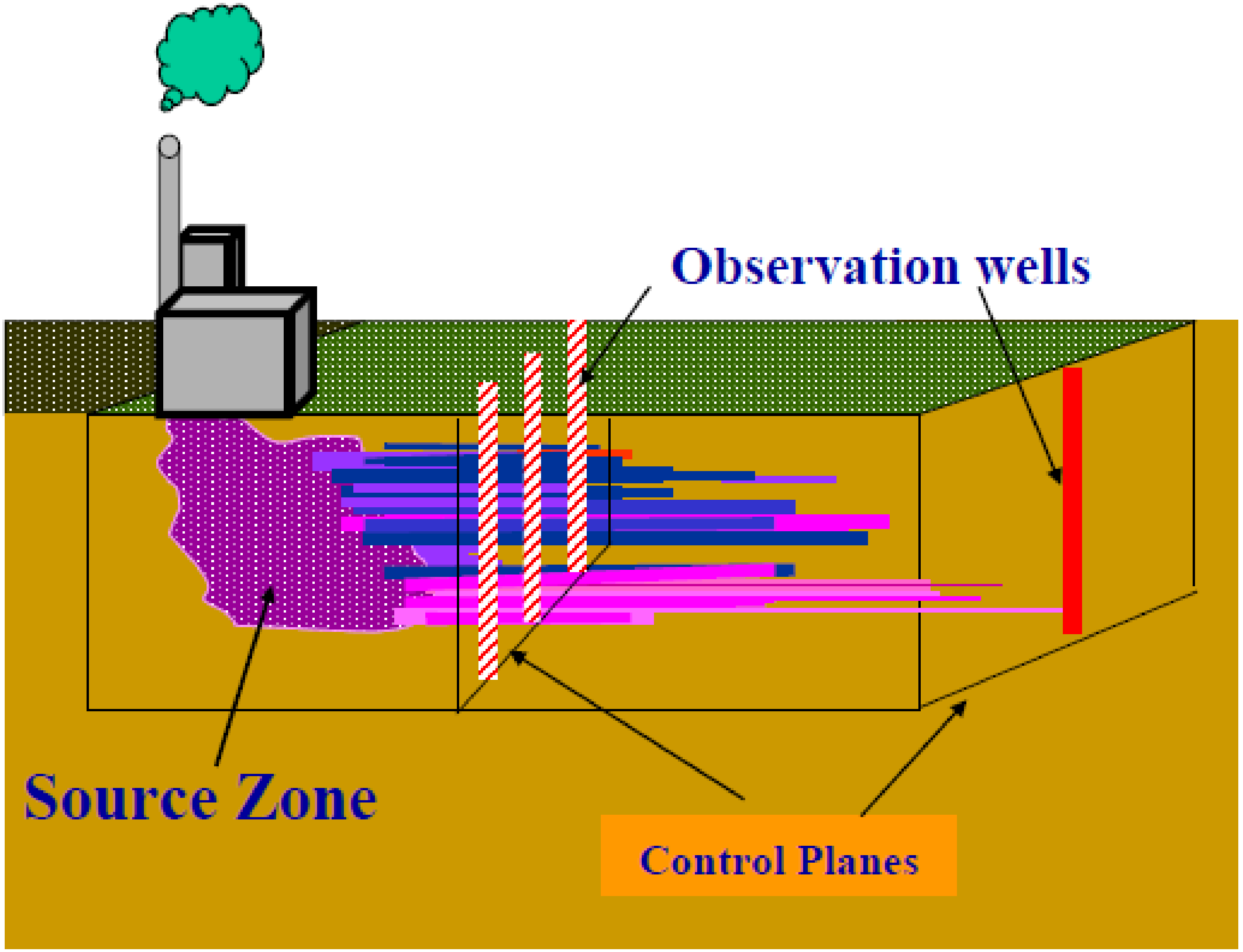
- Precipitation
- Irrigation
- Runoff
- Evaporation
- Transpiration
- Root Water Uptake
- Capillary Rise
- Deep Drainage
- Solute transport
- Fertigation
- Pesticides
- Fumigants
- Colloids
- Pathogens
- Nanoparticles





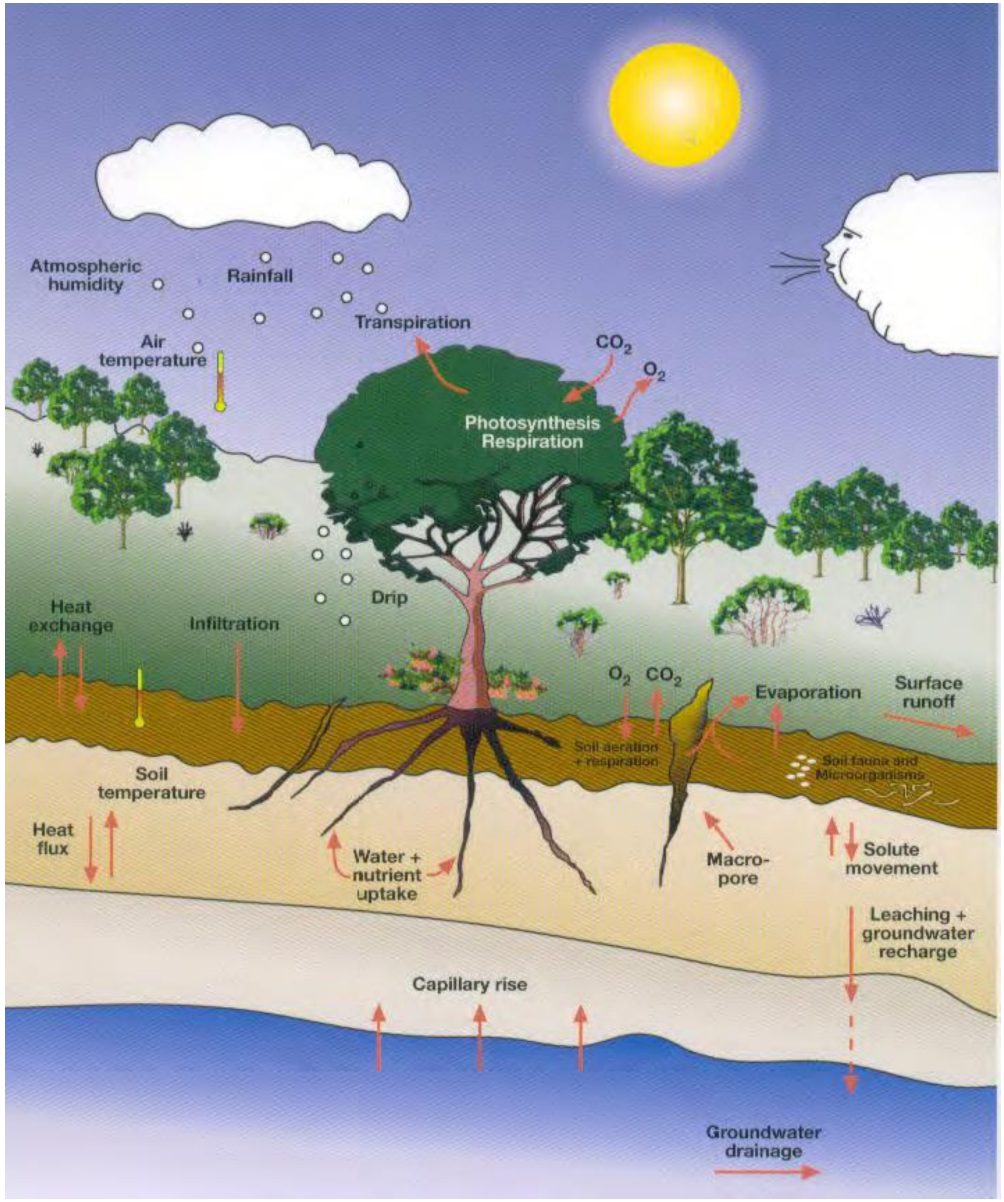
Industrial Applications

- 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-AquiferInteractions

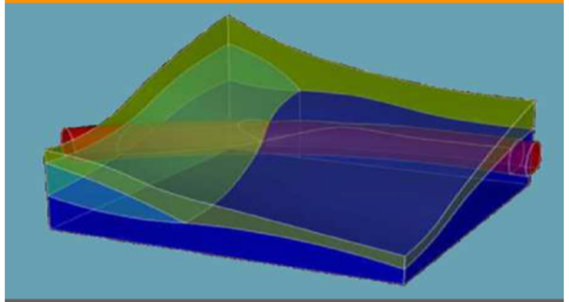


Hillel (2003)

https://www.pc-progress.com/

Brief history and development of Hydrus-1D

Review and Analysis



Core Ideas

- Review of selected capabilities of HYDRUS implemented since 2008
- New standard and nonstandard specialized add-on modules significantly expanded capabilities of the software
- Review of selected applications of

Recent Developments and Applications of the HYDRUS Computer Software Packages

Jiří Šimůnek,* Martinus Th. van Genuchten, and Miroslav Šejna

The HYDRUS-1D and HYDRUS (2D/3D) computer 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 2008, Šimůnek et al. (2008b) 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 manuscript is to review selected capabilities of HYDRUS that have been implemented since 2008. Our review is not limited to listing additional processes that were implemented in the standard computational modules, but also describes many

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Vadose Zone Journal

REVIEW

Special Section: Tribute to Rien van Genuchten, Recipient of the 2023 Wolf Prize for Agriculture

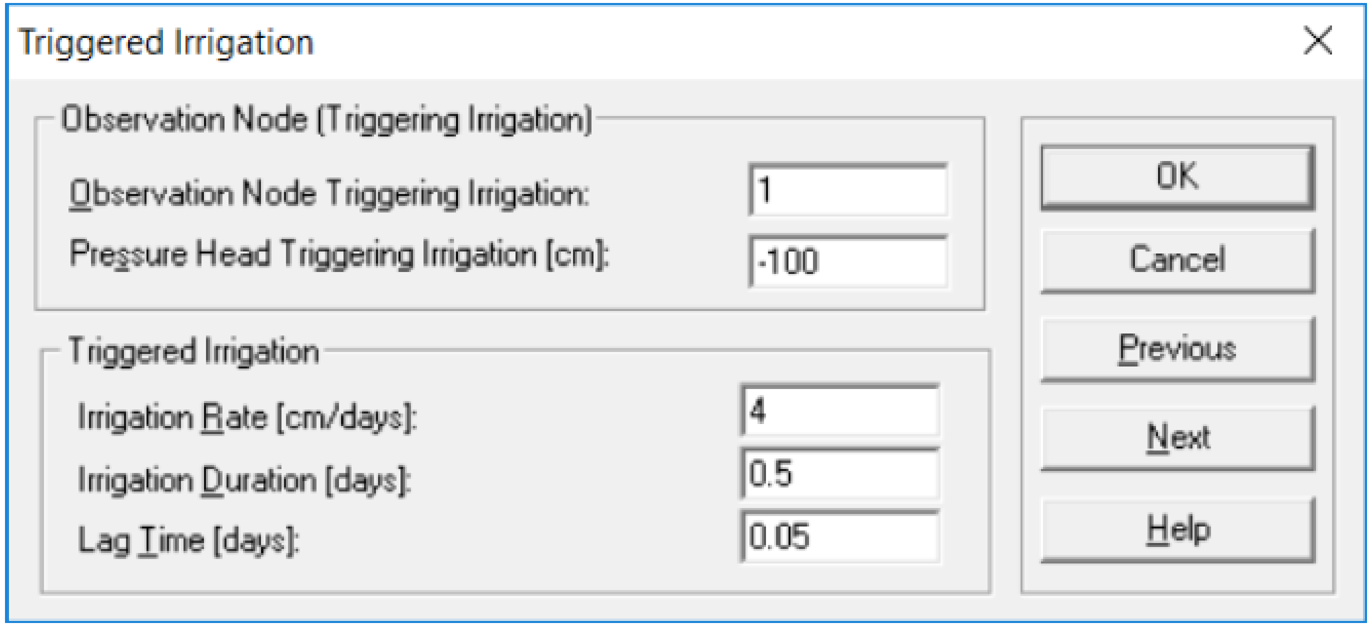
Developments and applications of the HYDRUS computer software packages since 2016

Jiří Šimůnek[1] | Giuseppe Brunetti[2] | Diederik Jacques[3] | Martinus Th. van Genuchten[4,5] | Miroslav Šejna[6]

Development of HYDRUS-1D

Version 4.16, February 2013

- Triggered irrigation, Irrigation Scheduling



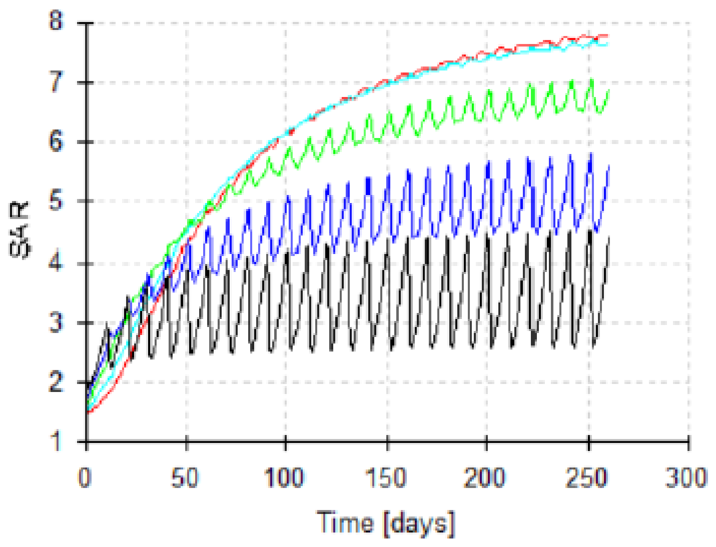
Rezaei, M., De Pue, J., Seuntjens, P., Joris, I., Cornelis, W. 2017. Quasi 3D modelling of vadose zone soil-water flow for optimizing irrigation strategies: challenges, uncertainties and efficiencies. *Environmental modelling and software*. 93: 59-77.

Development of HYDRUS-1D

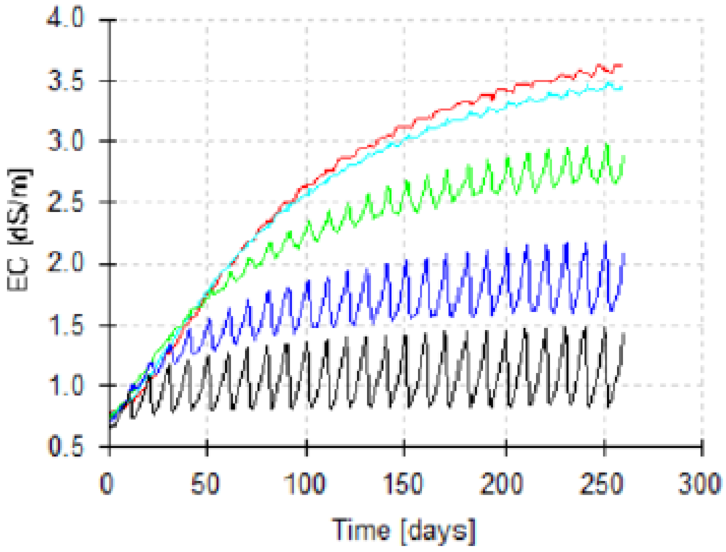
Version 4.17, 2017

- Graph of major ions, EC, and SAR in observation nodes

Observation Nodes: SAR

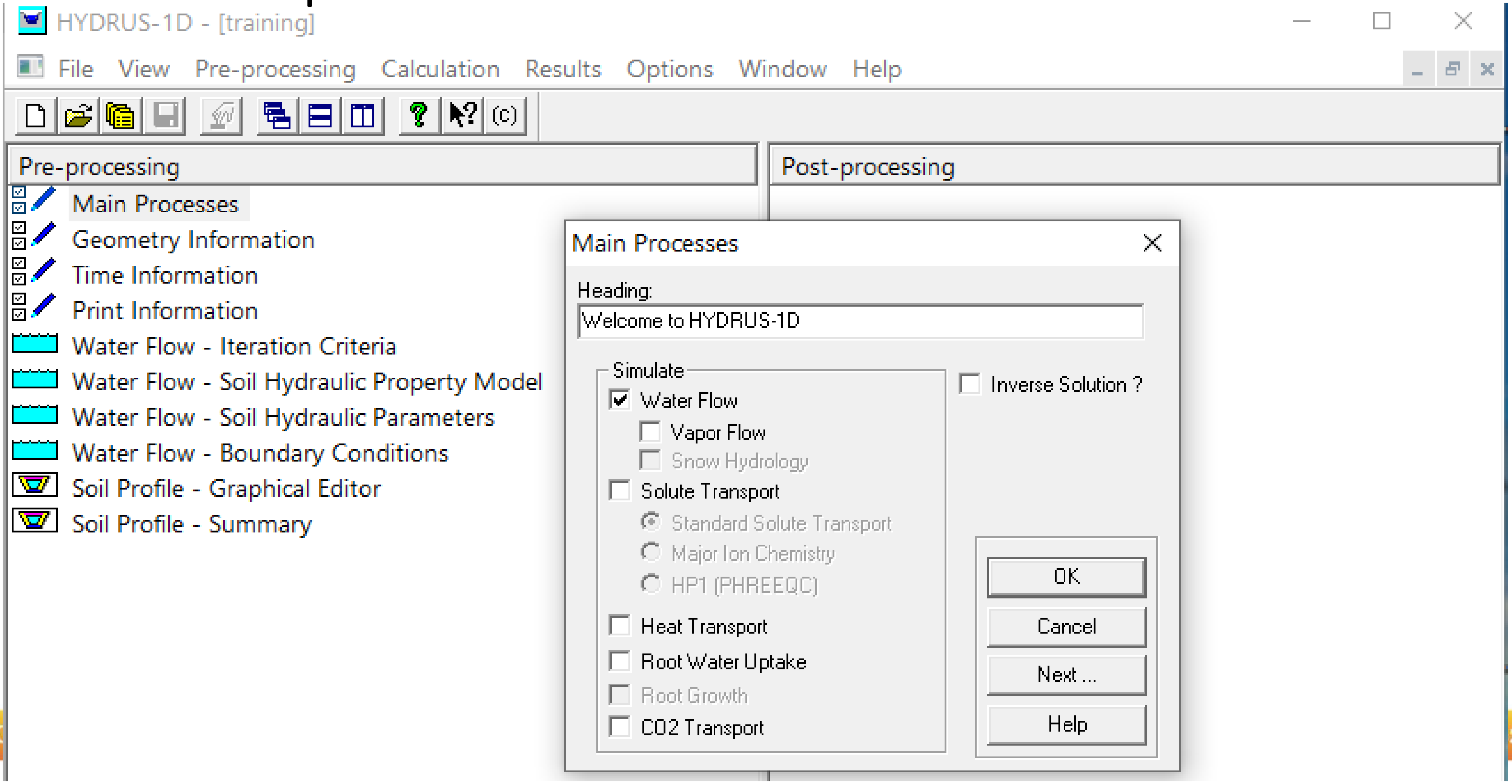


Observation Nodes: Electric Conductivity



Key Features of Hydrus-1D

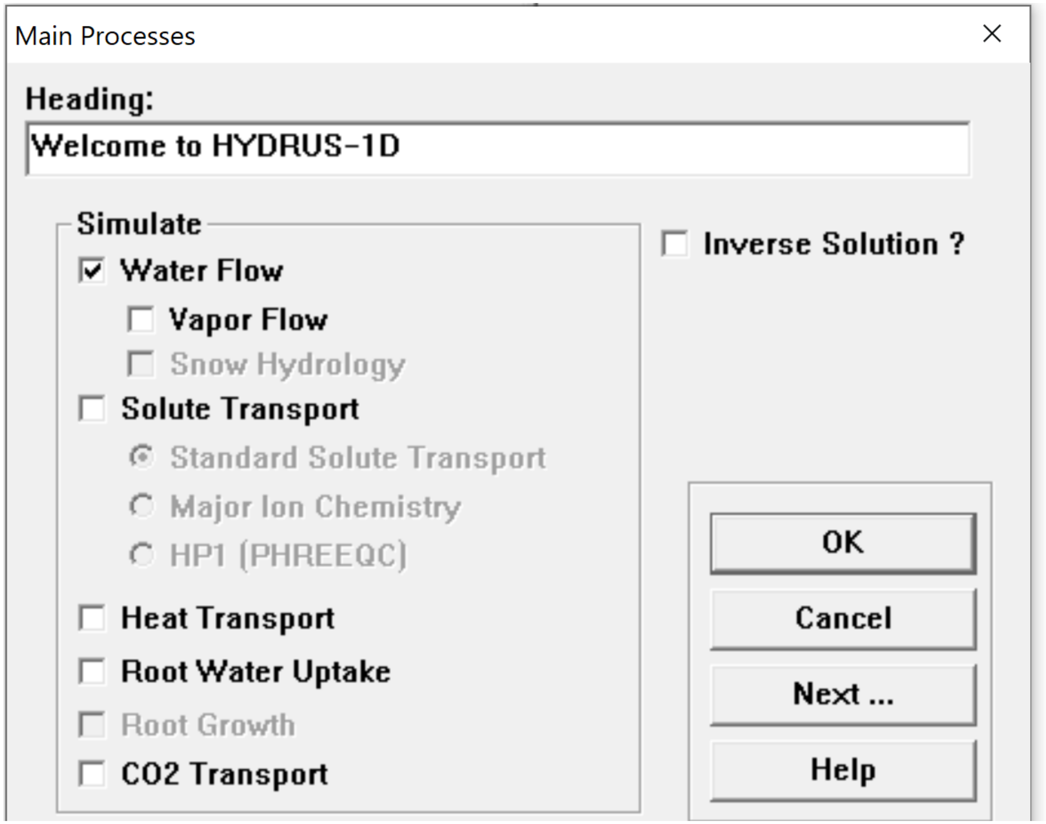
- Modeling water flow (saturated and unsaturated).
- Solute transport (including reactive and non-reactive solutes).
- Heat transport and coupling with water/solute movement.
- Root water and nutrient uptake.



HYDRUS-1D Modules

Standard Modules (fully supported by and distributed with HYDRUS-1D GUI):

- Inverse – Marquardt-Levenberg algorithm to optimize soil hydraulic, solute transport and reaction, and heat transport parameters.
- UnsatChem– carbon dioxide transport and production, and reactions and transport of major ions (Šimůnek and Suarez, 1993, 1994).
- HP1 – coupling with PHREEQC, allowing to consider the transport and general biogeochemical reactions between many different ions (Jacques and Šimůnek, 2005).



HYDRUS-1D Modules: UNSATCHEM

1	Aqueous components	7	Ca^{2+}, Mg^{2+}, Na^{+}, K^{+}, SO_4^{2-}, Cl^{-}, NO_3^{-}
2	Complexed species	10	$CaCO_3^{o}$, $CaHCO_3^{+}$, $CaSO_4^{o}$, $MgCO_3^{o}$, $MgHCO_3^{+}$, $MgSO_4^{o}$, $NaCO_3^{-}$, $NaHCO_3^{o}$, $NaSO_4^{-}$, KSO_4^{-}
3	Precipitated species	6	$CaCO_3$, $CaSO_4 \cdot 2H_2O$, $MgCO_3 \cdot 3H_2O$, $Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O$, $Mg_2Si_3O_{7.5}(OH) \cdot 3H_2O$, $CaMg(CO_3)_2$
4	Sorbed species (exchangeable)	4	Ca, Mg, Na, K
5	CO_2-H_2O 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

HYDRUS-1D Modules

Non-Standard Modules (not fully supported by and not distributed with HYDRUS-1D GUI):

- Centrifugal Forces: considers centrifugal forces, in addition to gravitation and capillarity (Šimůnek and Nimmo, 2005).
- Freezing/Thawing – considers the effects of freezing and thawing on water flow and solute/heat transport processes (Hansson et al., 2004).
-
- C-Ride (C-hitch) – considers particle transport and particle-facilitated solute transport (Šimůnek et al., 2006).
- Fumigant – considers additional factors important for the fate and transport of fumigants (e.g., tarp; Spurlock et al., 2013).

HYDRUS-1D Modules

Non-Standard Modules:

Colloid Transport with Changing Water Contents: considers the effects of changes in the water content on particle transport and attachment/detachment to/from solid-water and air-water interfaces (e.g., Bradford et al., 2015).

Isotope Transport: accounts for isotope transport (Stumpp et al., 2012). Neglects fractionation processes and does not increase the relative concentration of isotopes (their δ content) at the upper boundary due to evaporation.

Root Growth: simulates root growth and its dependence on various environmental factors (Hartmann and Šimůnek, 2015).

Governing Equations

Variably-Saturated Water Flow (Richards Equation)

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

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

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

HYDRUS – Main Processes

Water Flow:

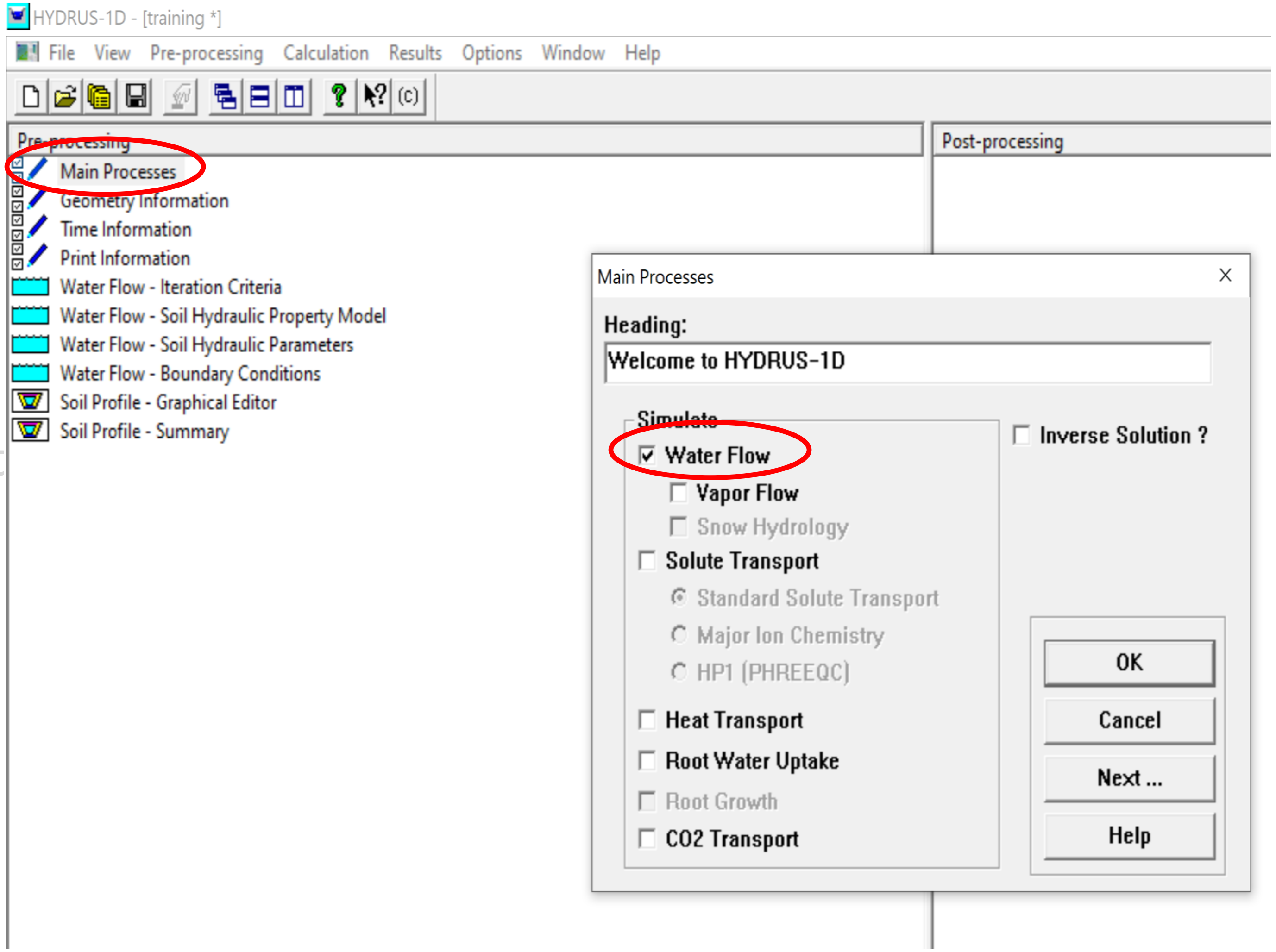
Richards equation for variably-saturated water flow

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)



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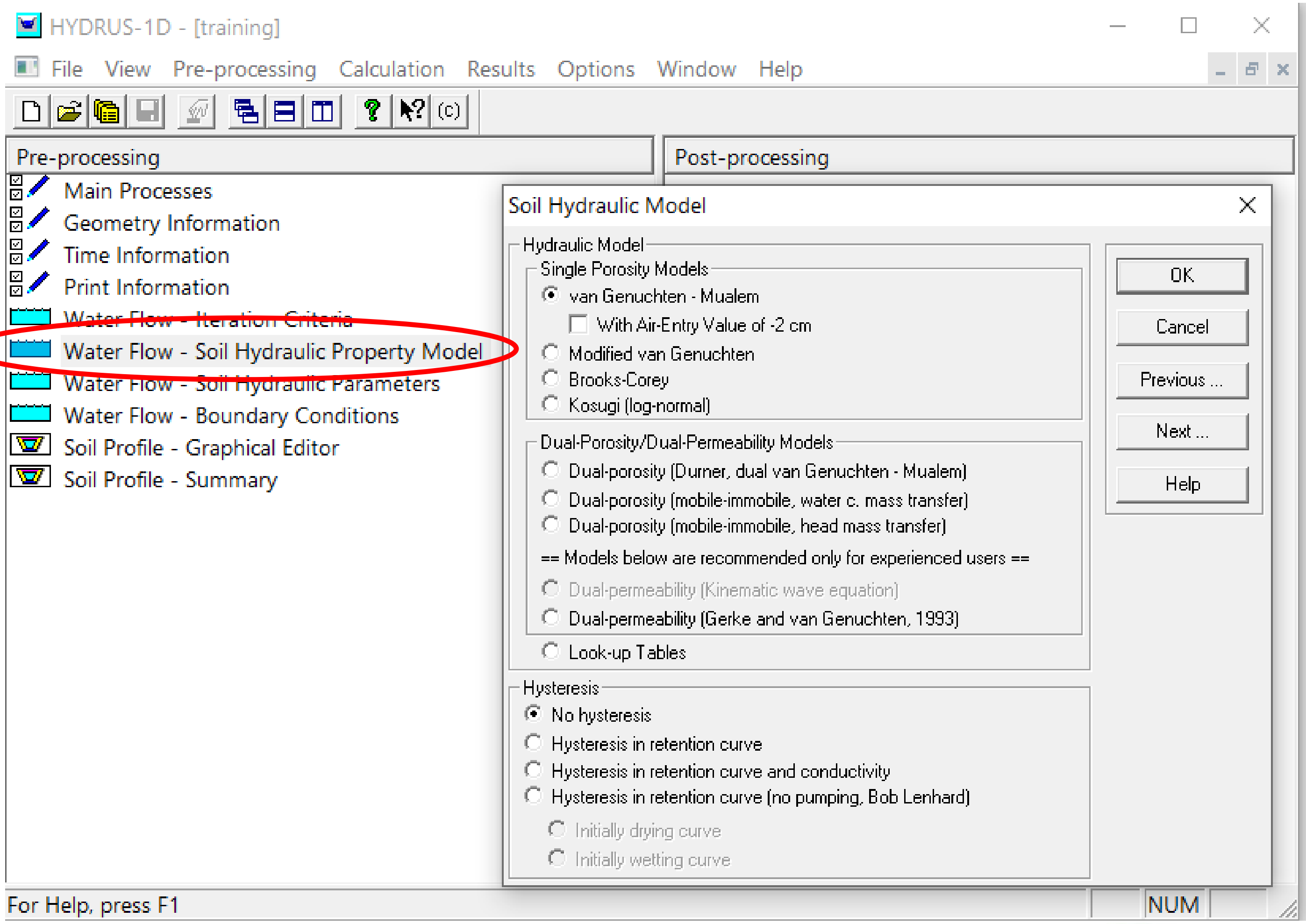

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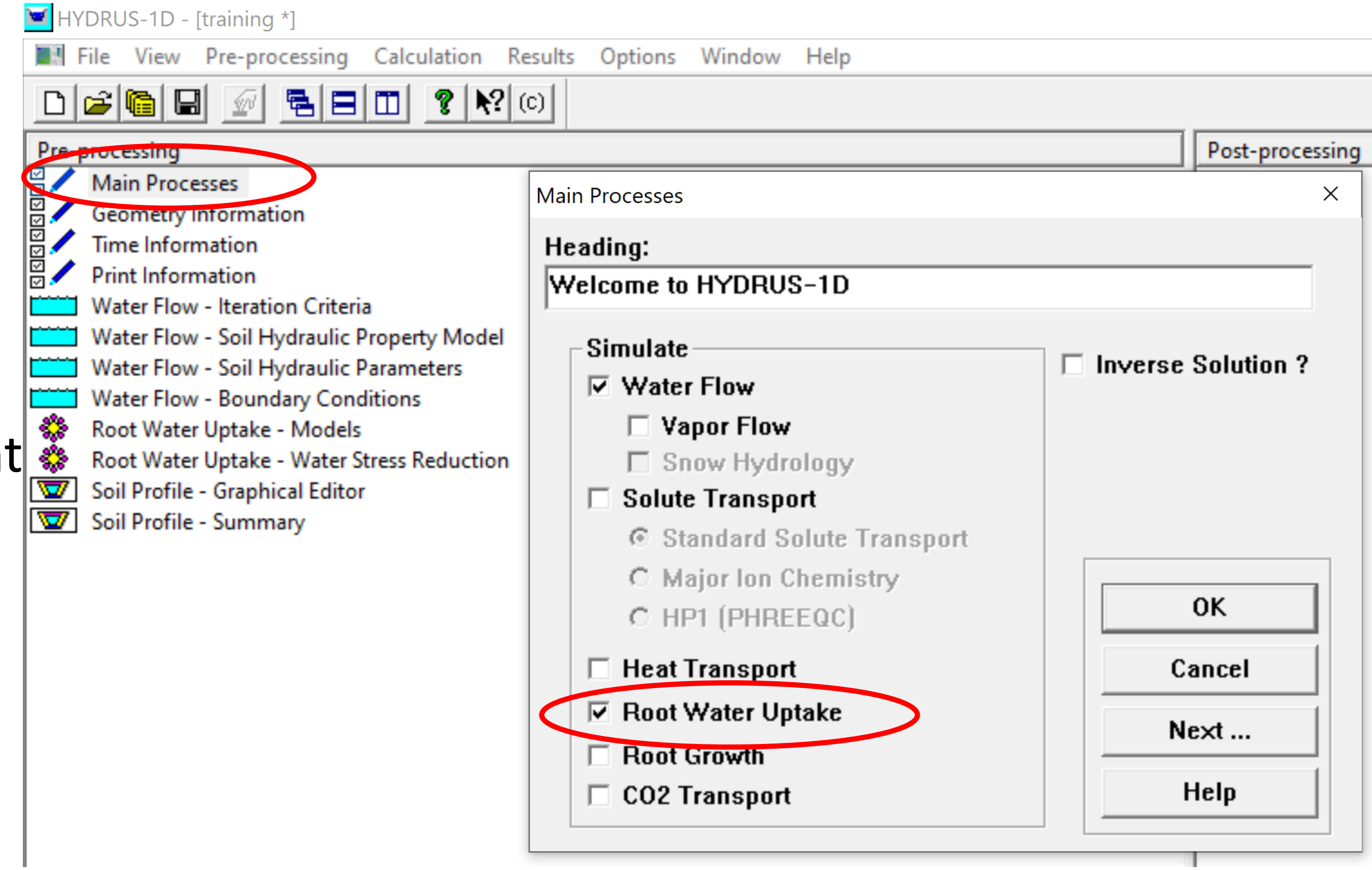

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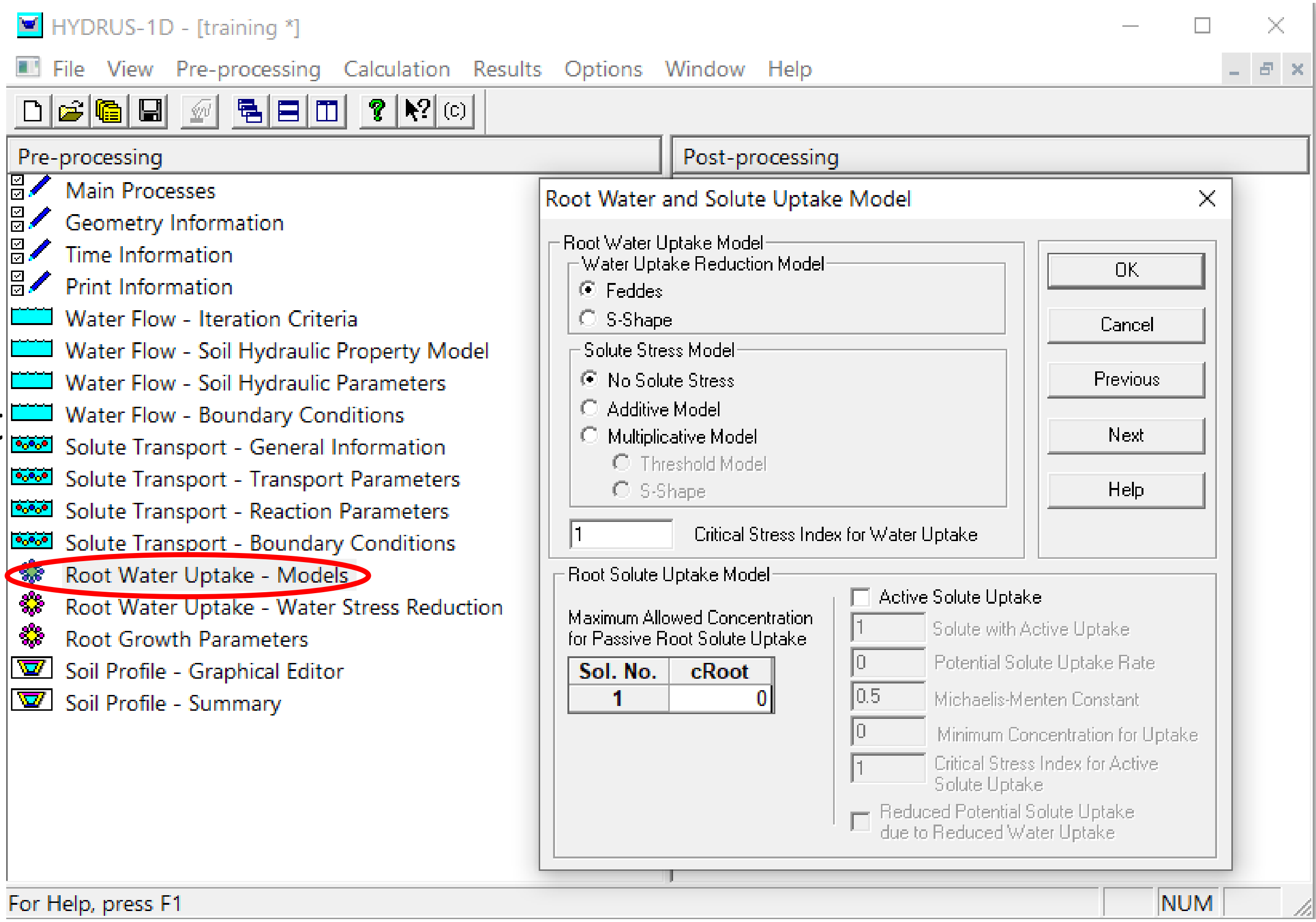

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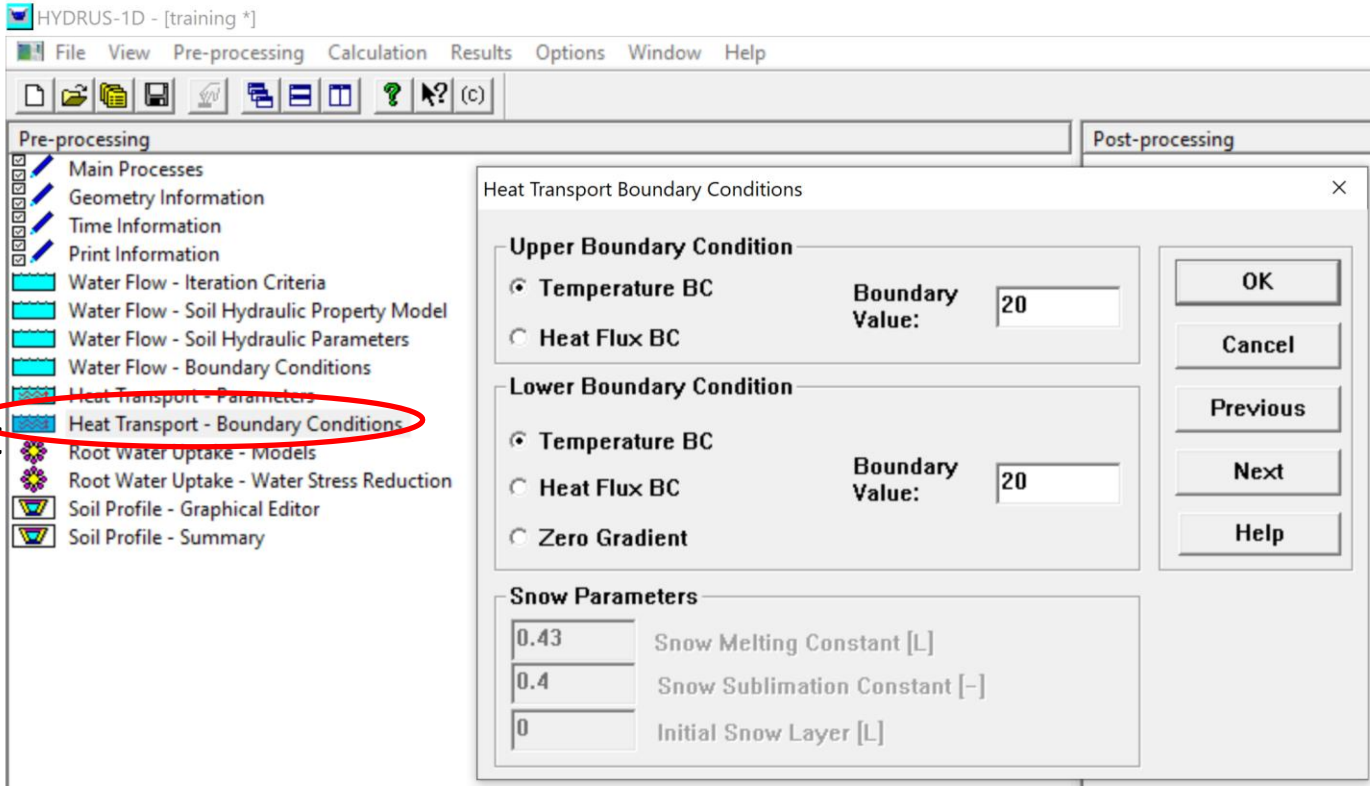
Preferential flow

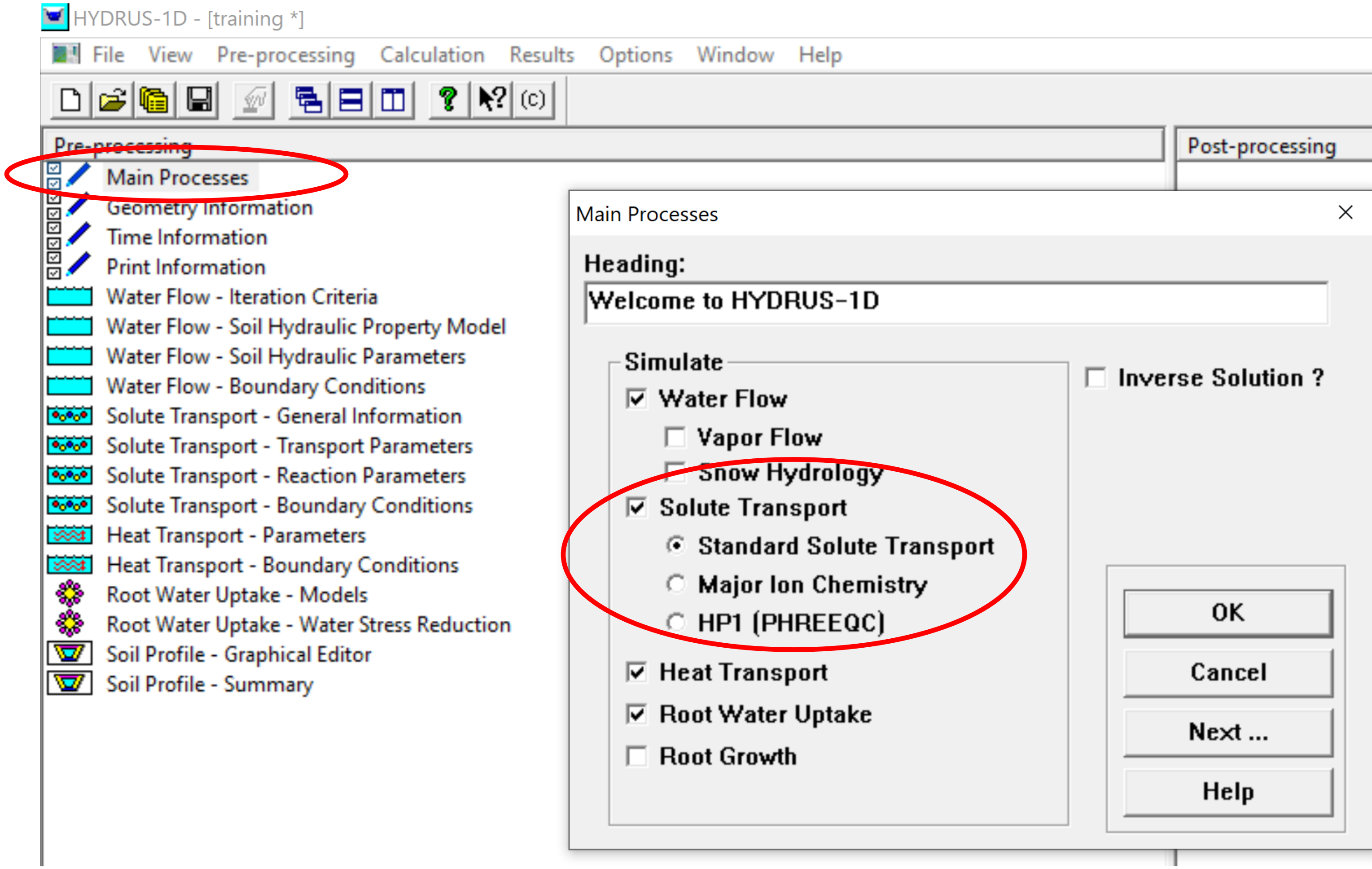
Isothermal and thermal liquid and vapor flow



HYDRUS – Main Processes

Solute Transport (standard mode):

- 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)



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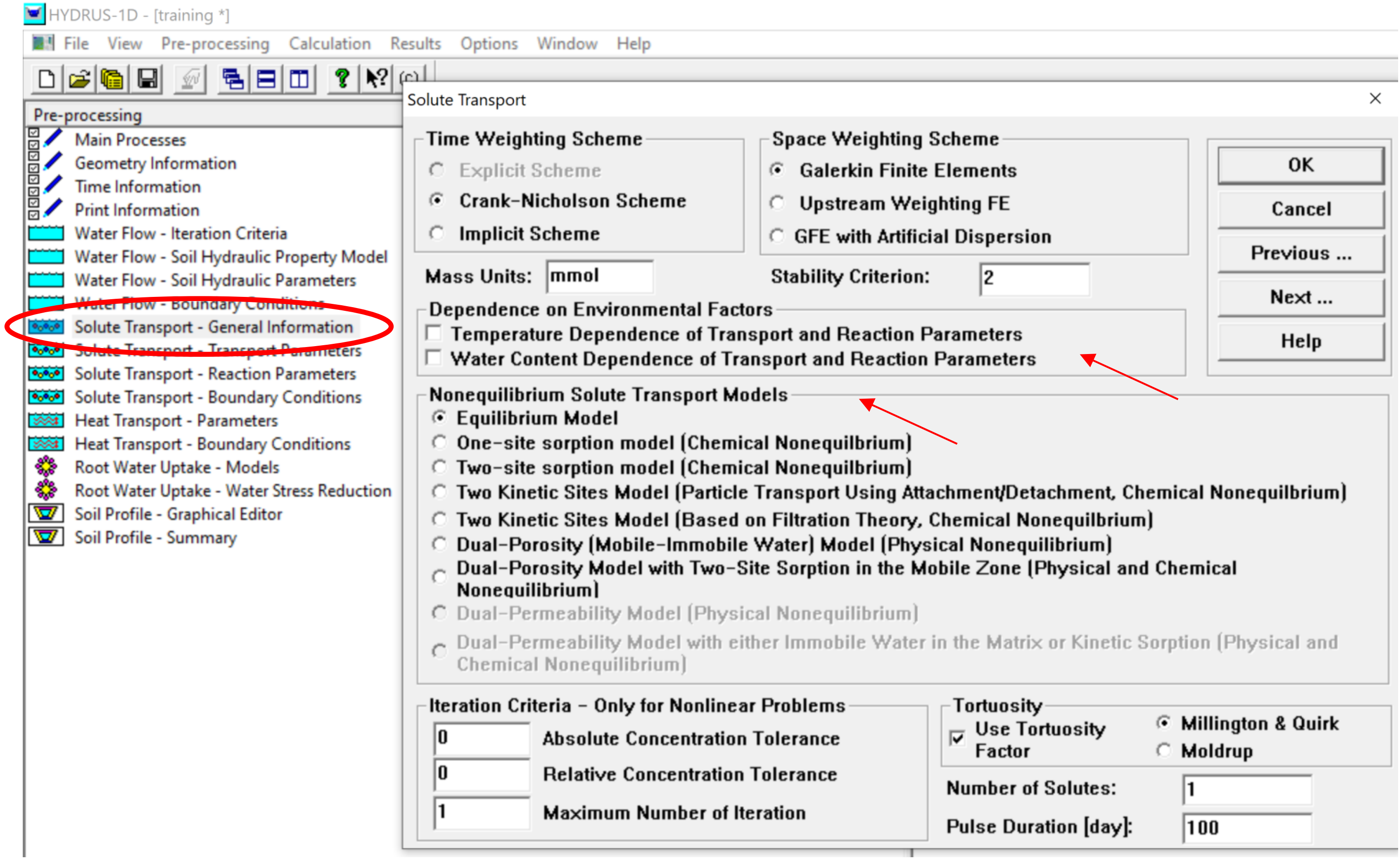

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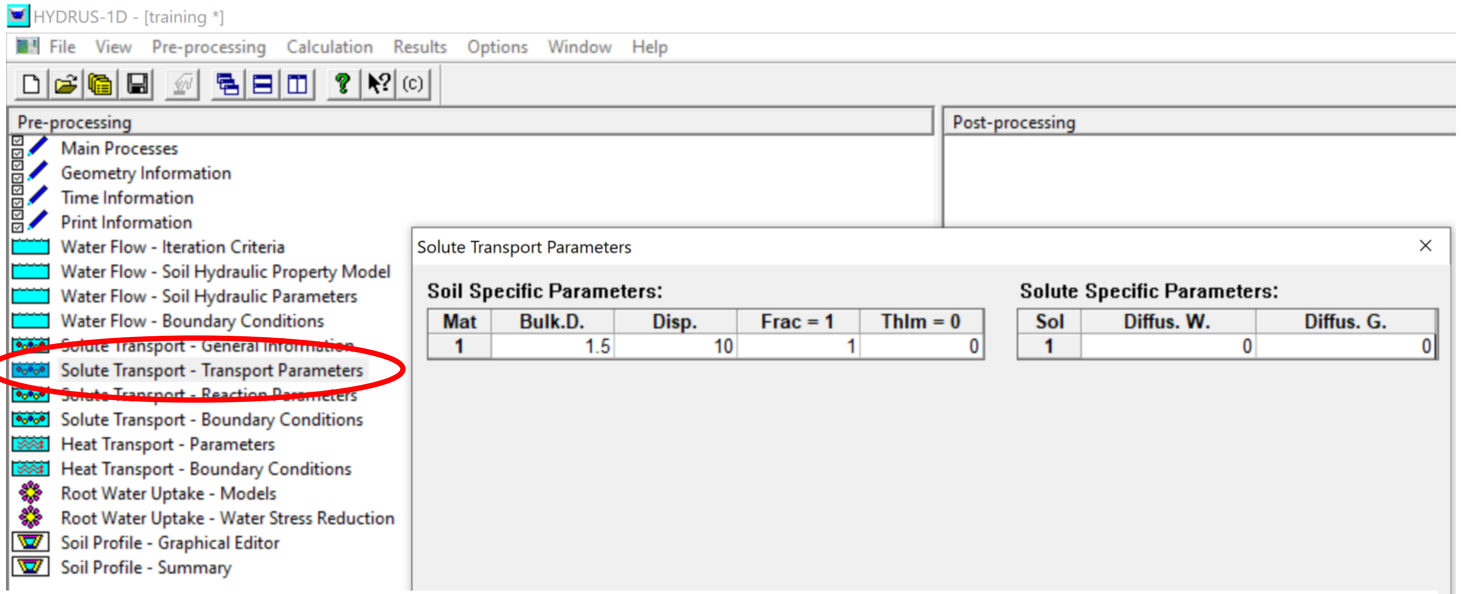

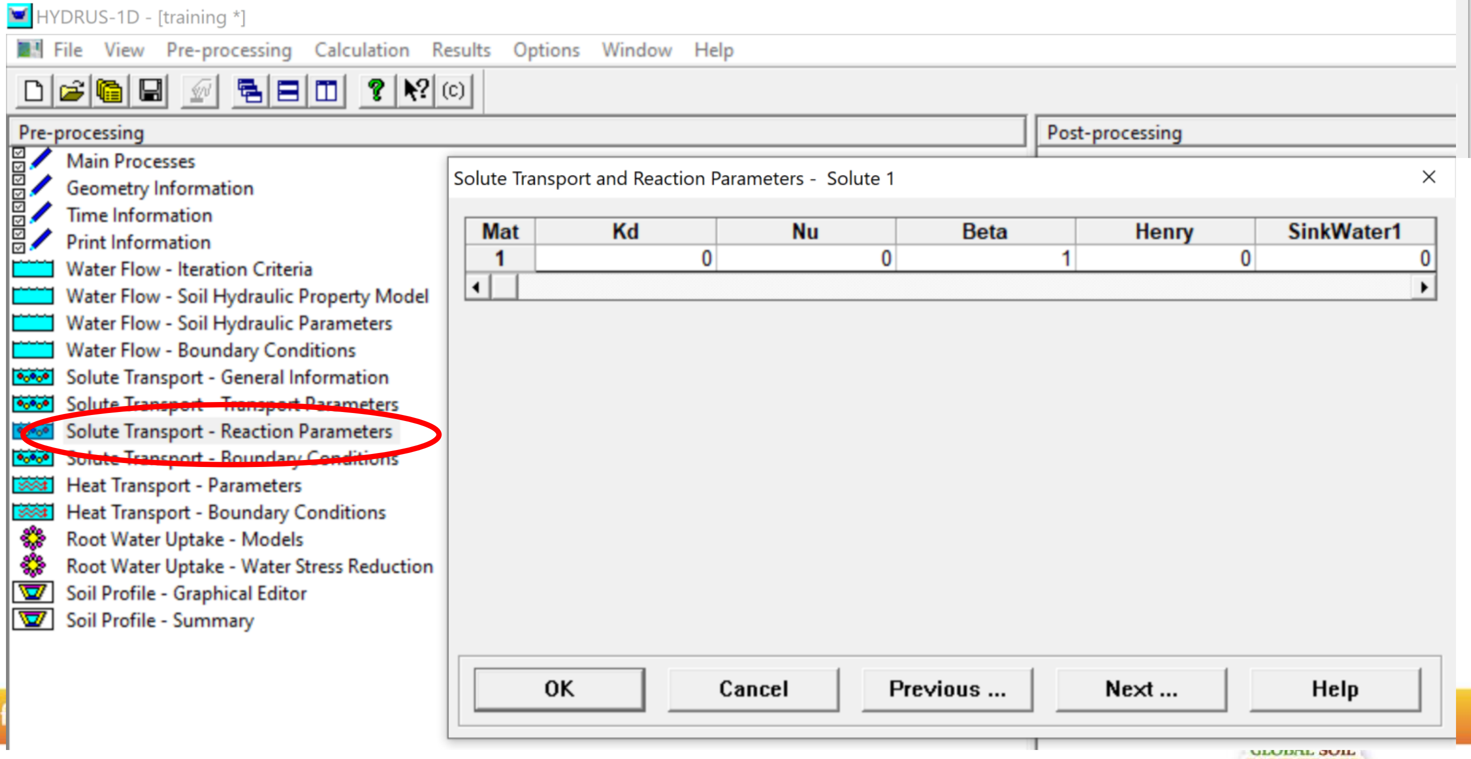

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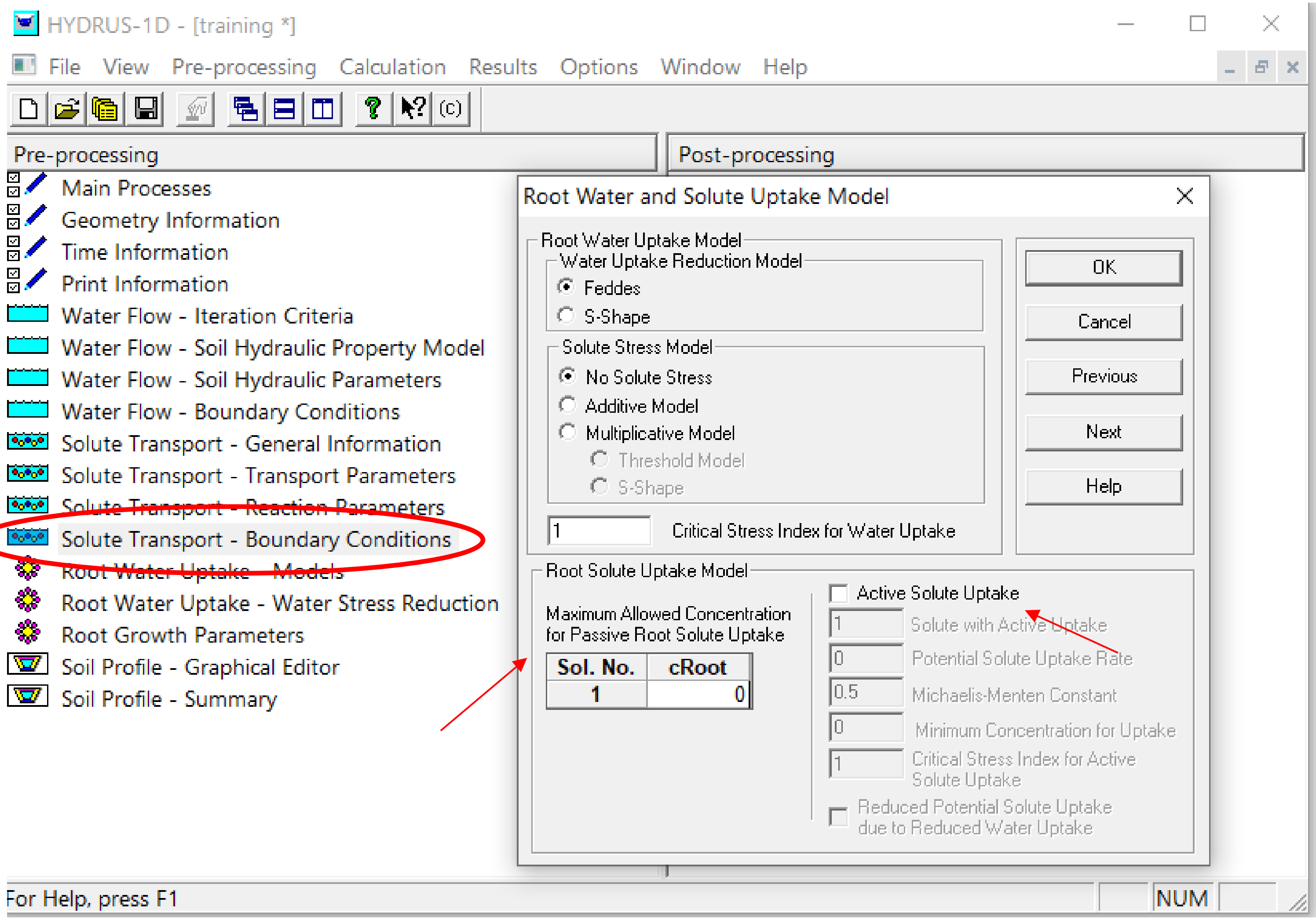

HYDRUS – Main Processes

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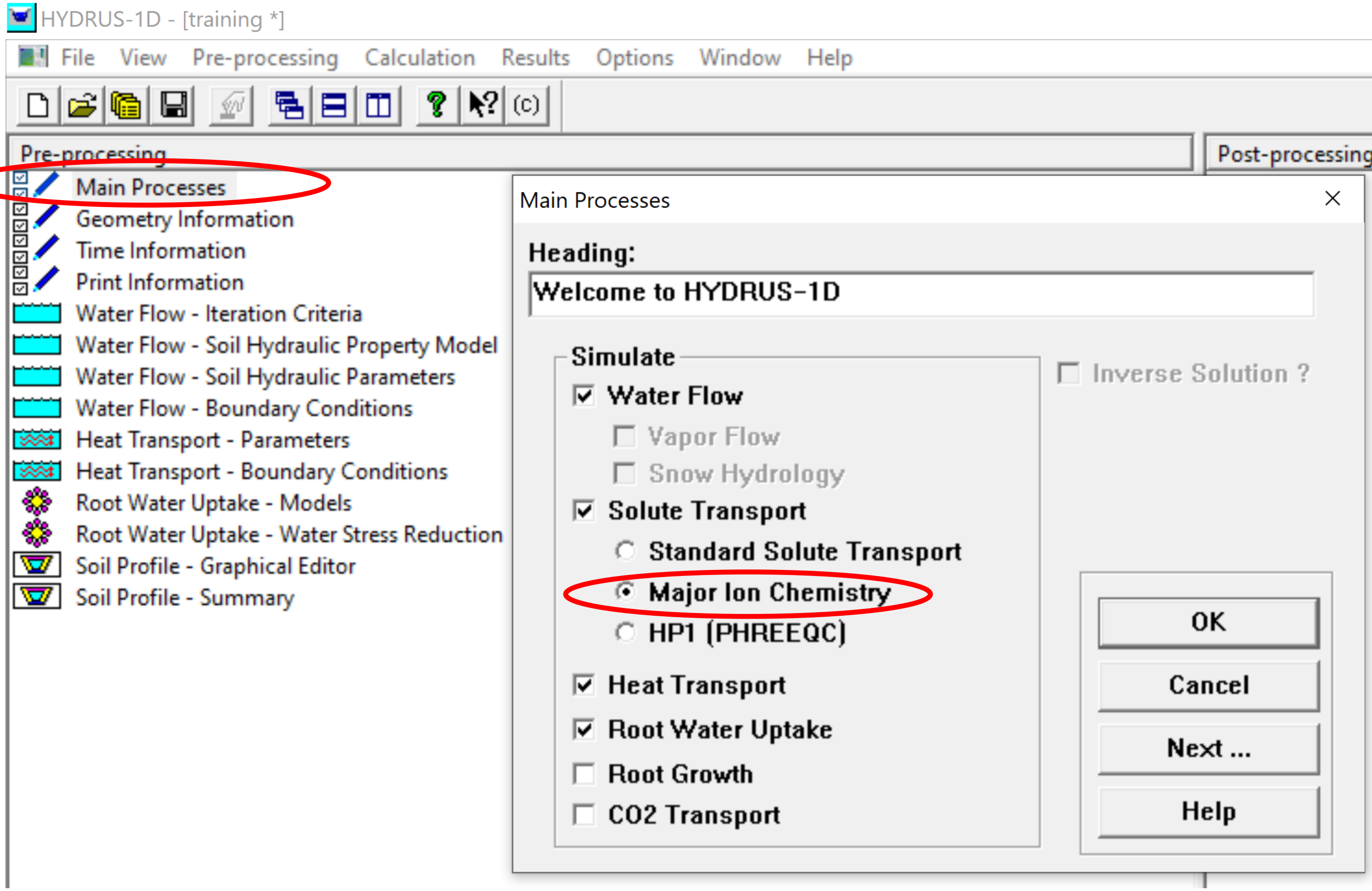

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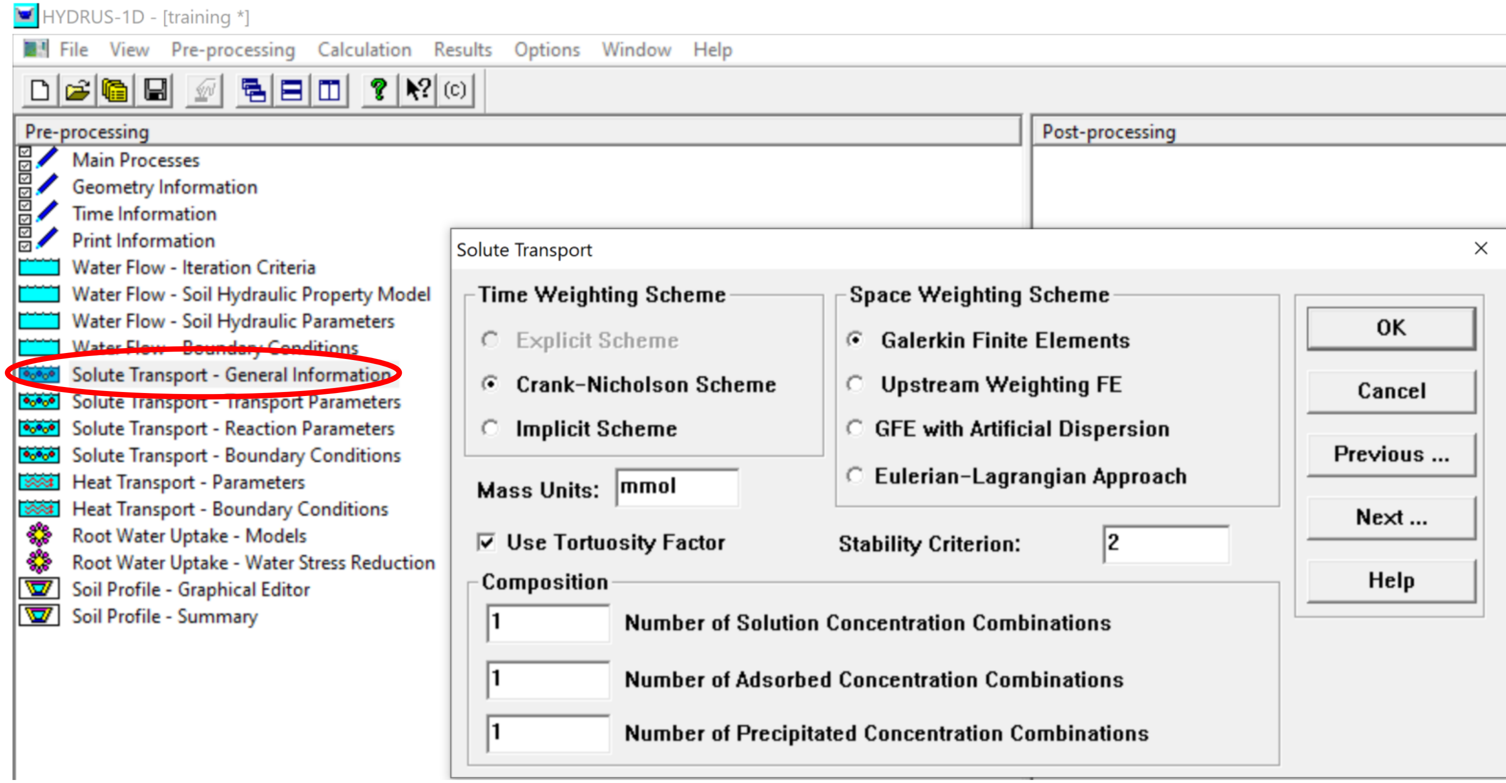
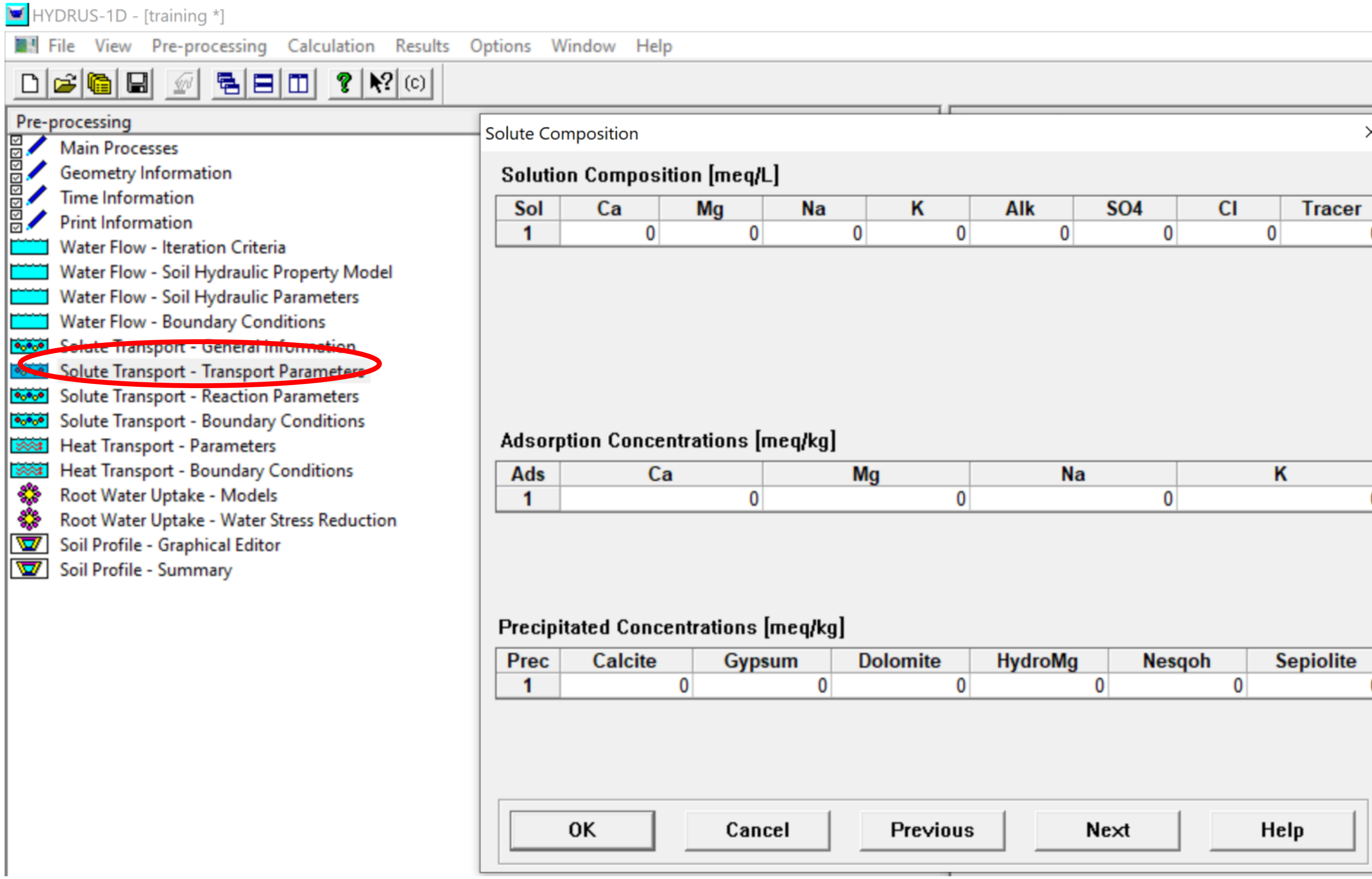


HYDRUS – Main Processes

Solute Transport (UNSATCHEM):

- 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
- Physical and chemical nonequilibrium solute transport
- Zero-order production, First-order degradation
- Sink term, accounting for nutrient uptake by plant roots (active and passive)



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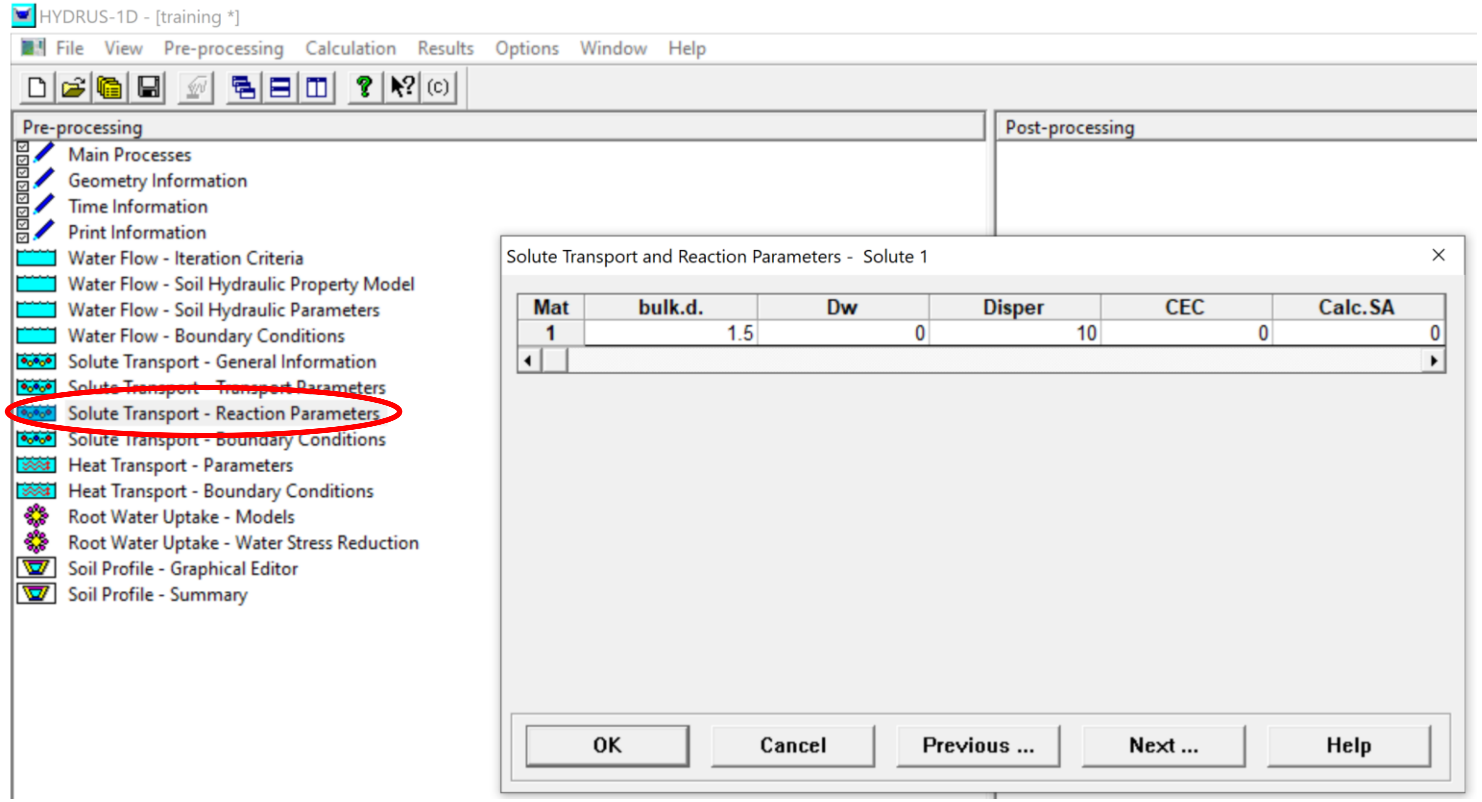

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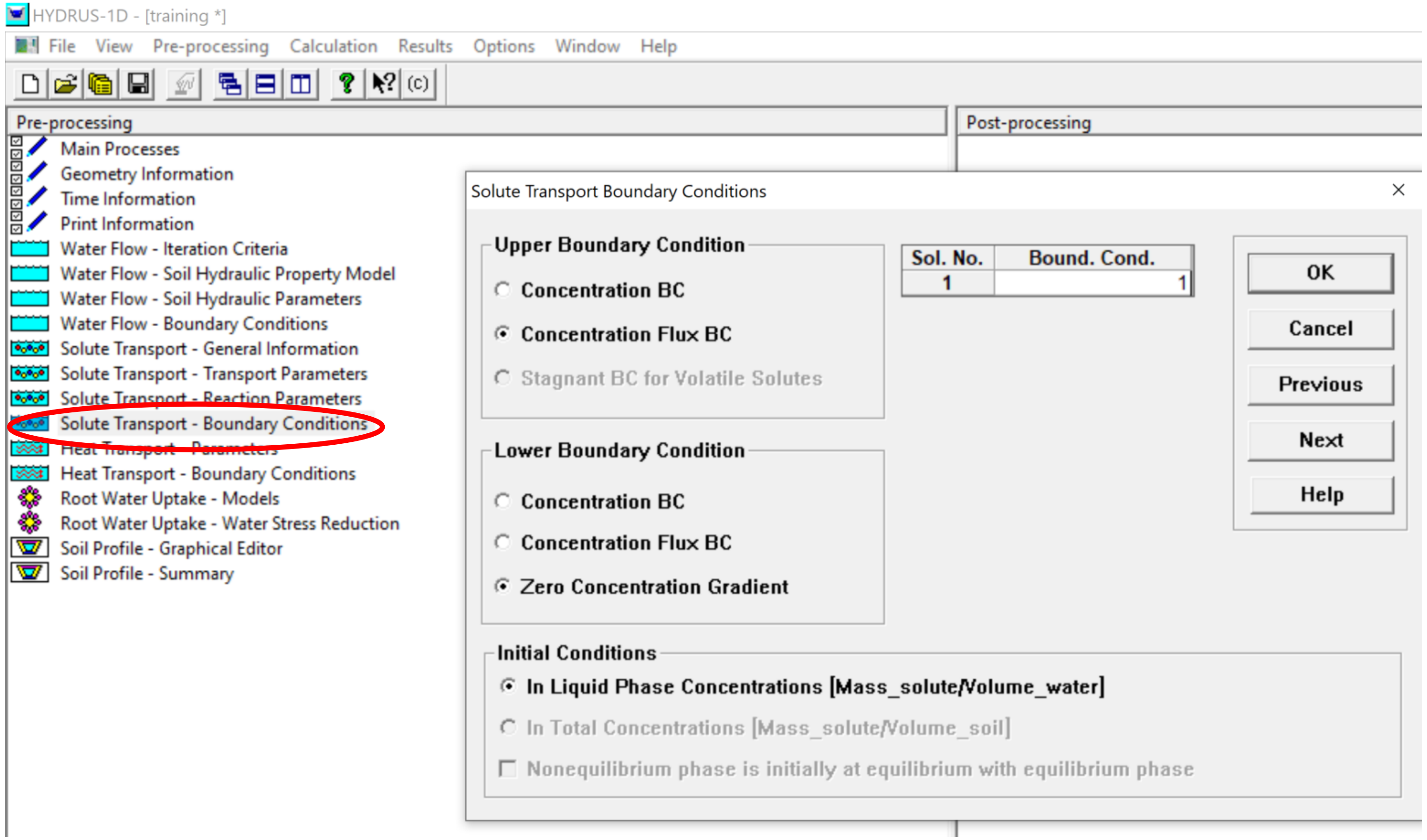
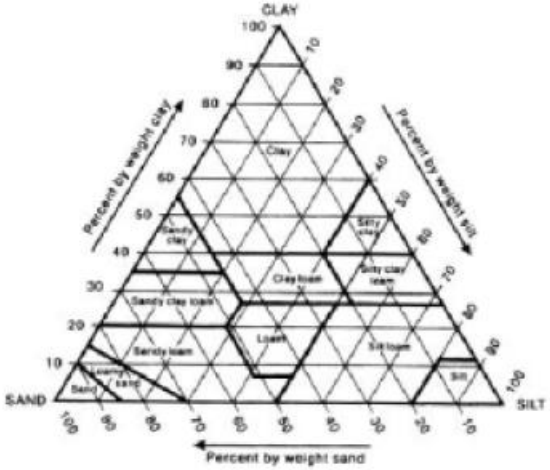


HYDRUS – Main Processes: PTFs by Carsel and Parrish (1988)

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

Texture	θ_r	θ_s	α 1/cm	n	K_s 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
Silt	0.034	0.46	0.016	1.37	6.00
Silt Loam	0.067	0.45	0.020	1.41	10.80
Sandy Clay Loam	0.100	0.39	0.059	1.48	31.44
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
Clay	0.068	0.38	0.008	1.09	4.80



USDA Soil Textural Triangle

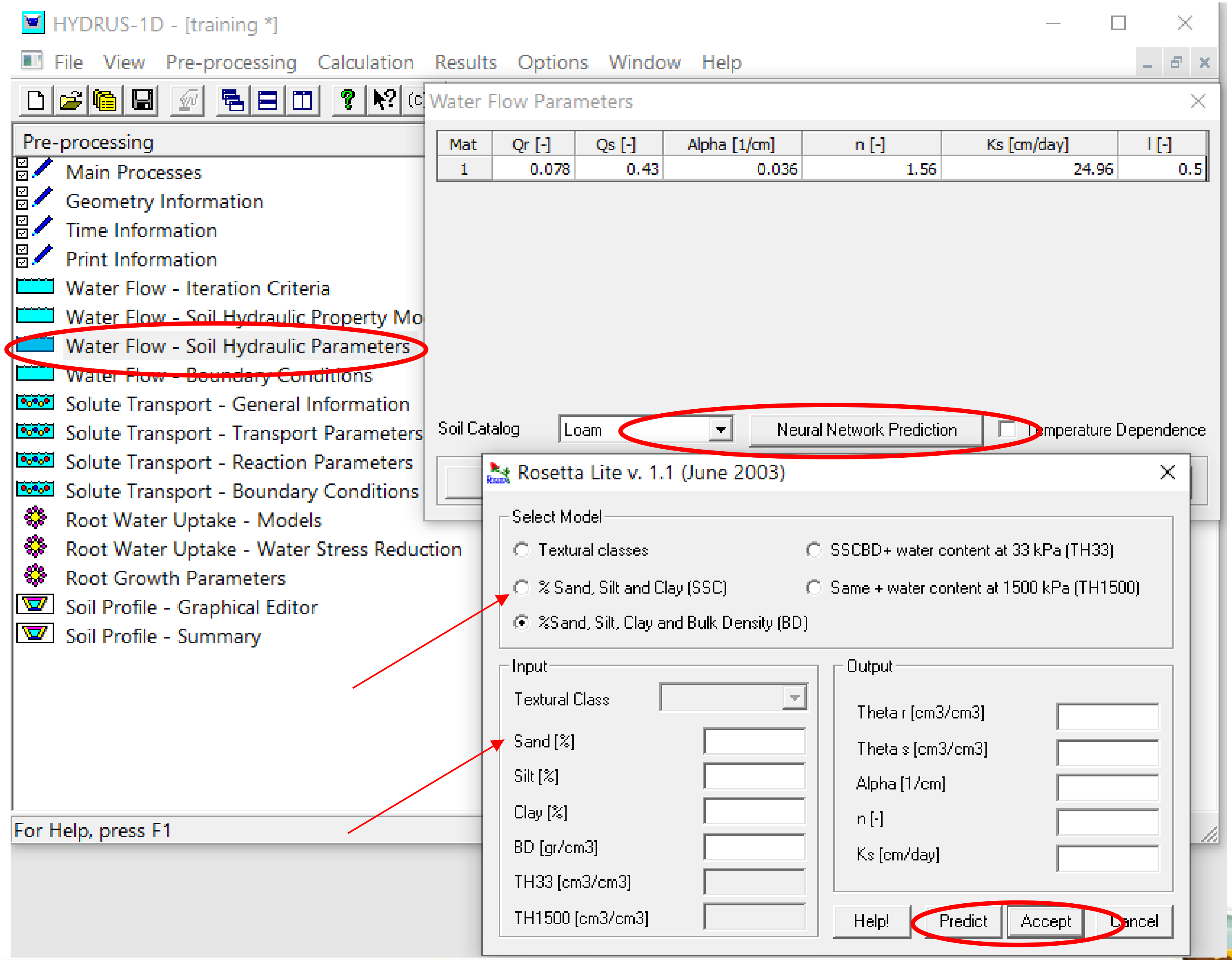
HYDRUS – Main Processes: ROSETTA

- **Soil hydraulic parameters**

(van Genuchten, 1980)

- **Soil texture parameters**

(Schaap et al, 2001)



Example 1: HYDRUS 1D

Water flow and solute transport into a Four-Layered Soil Profile

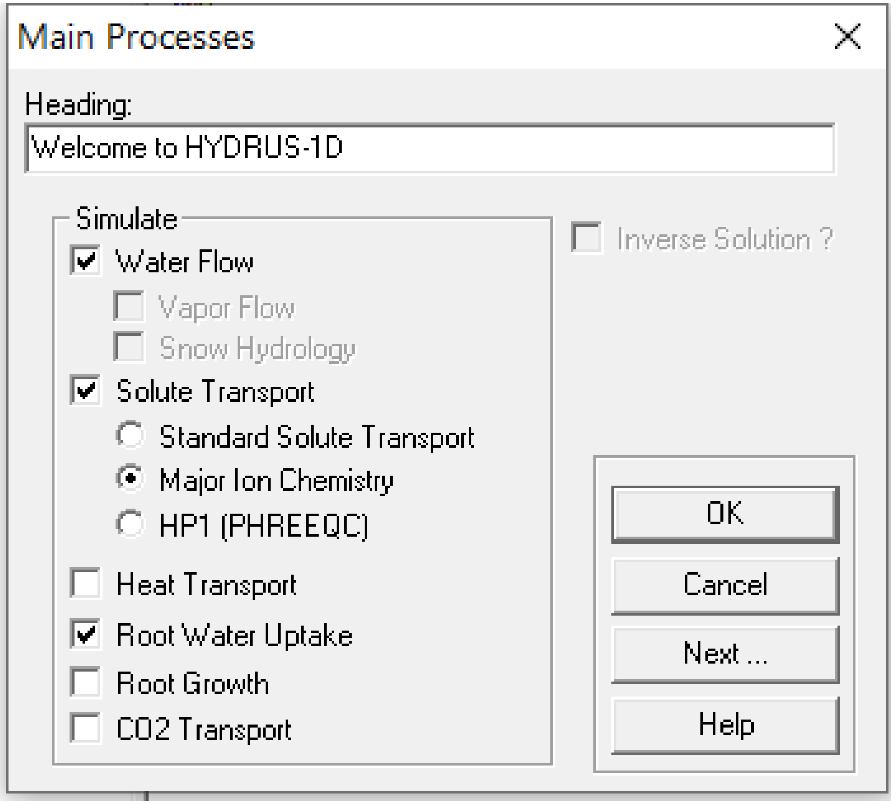
Geometry: 100 cm, 4 layers
Upper boundary: atmospheric BC with surface layer
Bottom boundary: free drainage

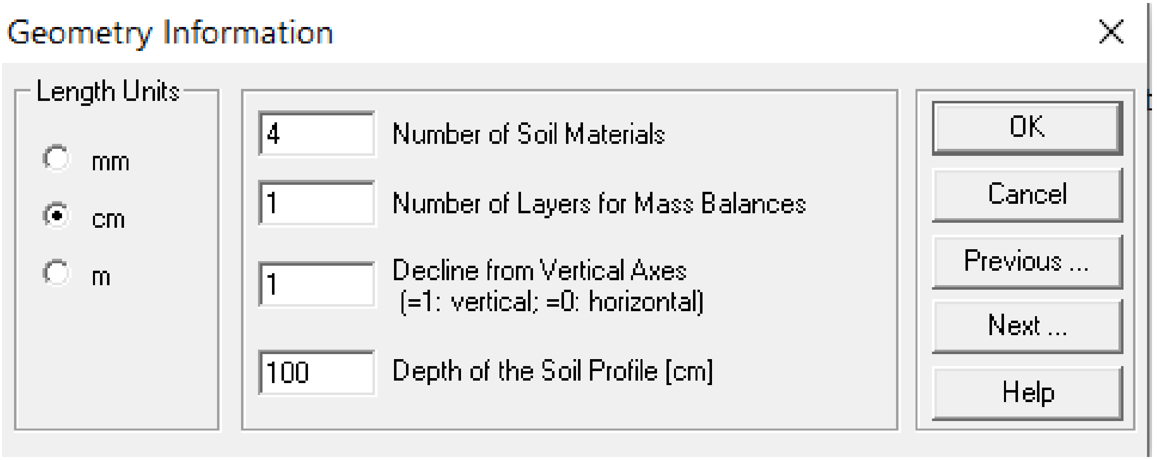
Type the **Name** of the project: "nim2-9"

- Type the **Description** of the project: "Water flow and solute transport ".
- Length Unit: cm
- Assuming: 8,500 m^3 of water, including leaching and water requirement for irrigating wheat to achieve optimal and potential yield.
- apply 20 cm of water as pre-irrigation for leaching purposes (day 30).
- 5 irrigation events are applied using furrow irrigation on the following dates: November 26 (day 96), December 16 (day 116) - January 5 (day 136), January 25 (day 156), and March 2 (day 190).

Example 1: HYDRUS 1D

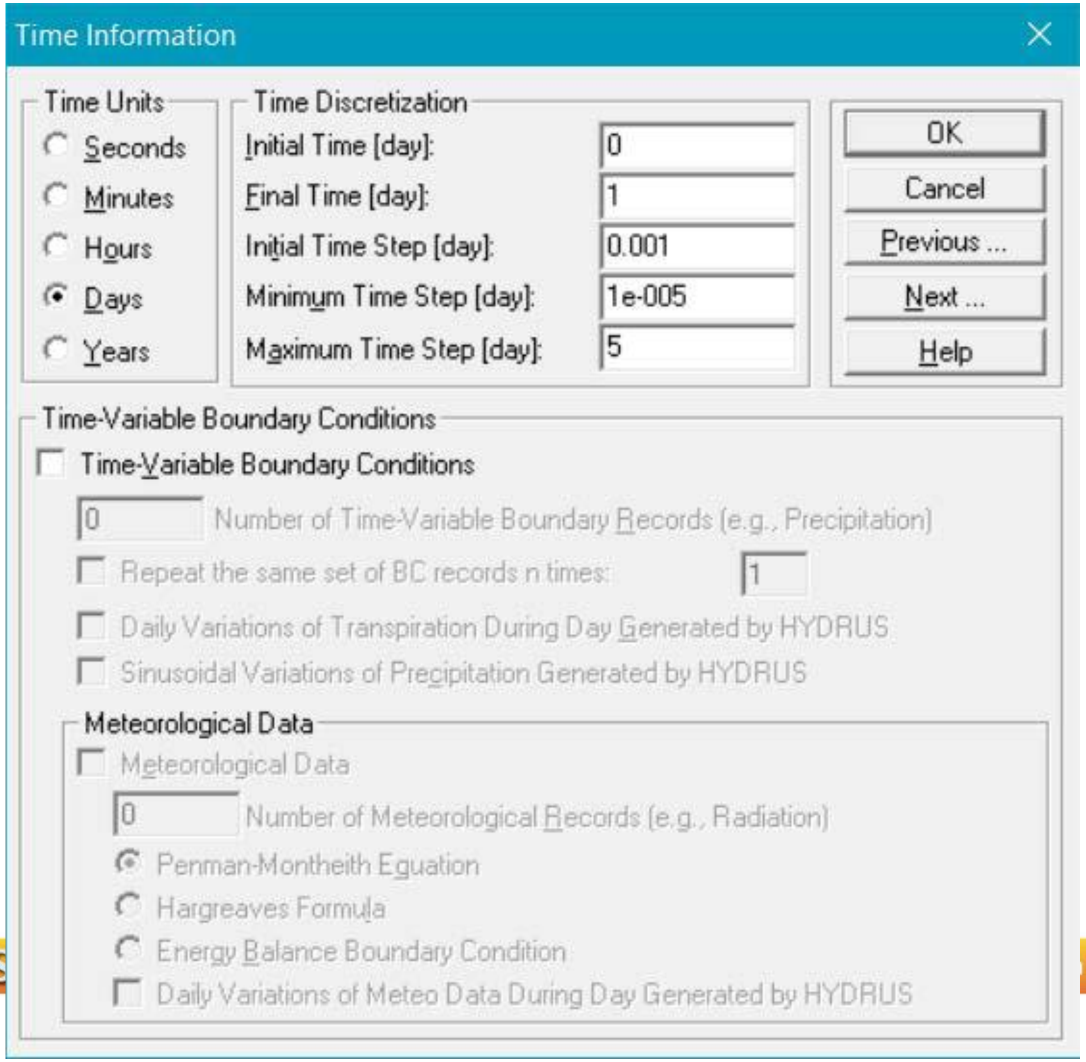
Water flow and solute transport into a Four-Layered Soil Profile

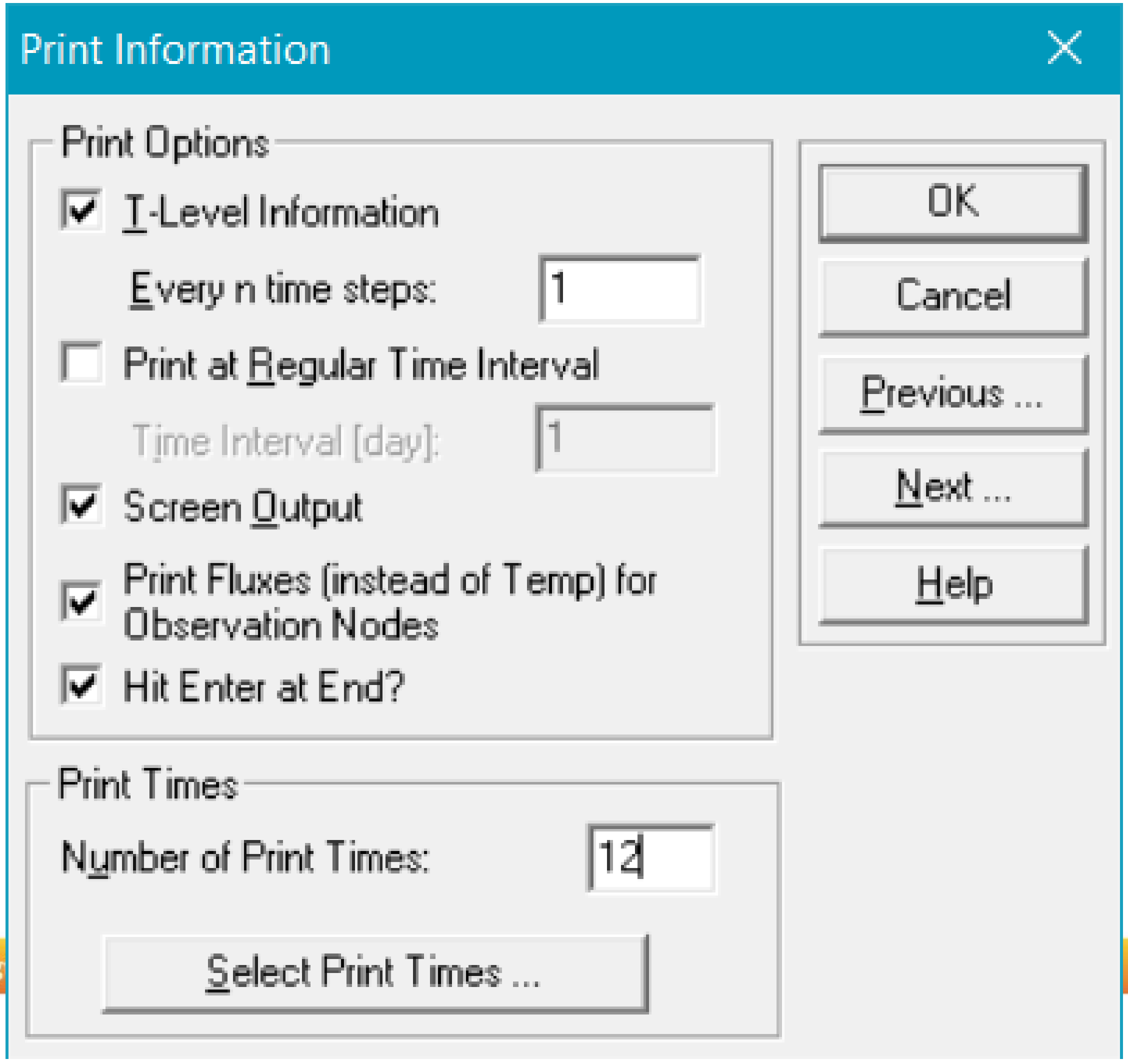




Example 1: HYDRUS 1D

Water flow and solute transport into a Four-Layered Soil Profile





Example 1: HYDRUS 1D

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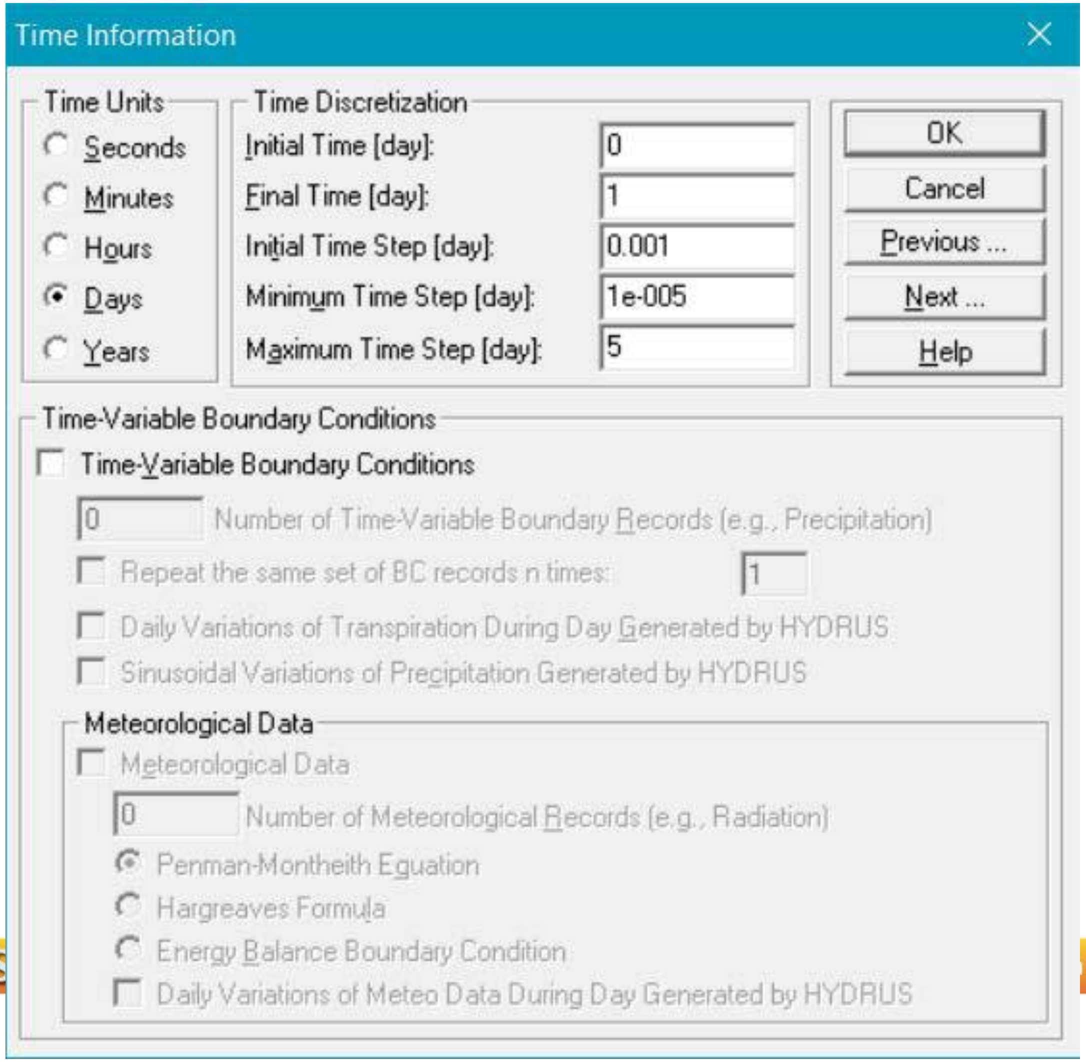
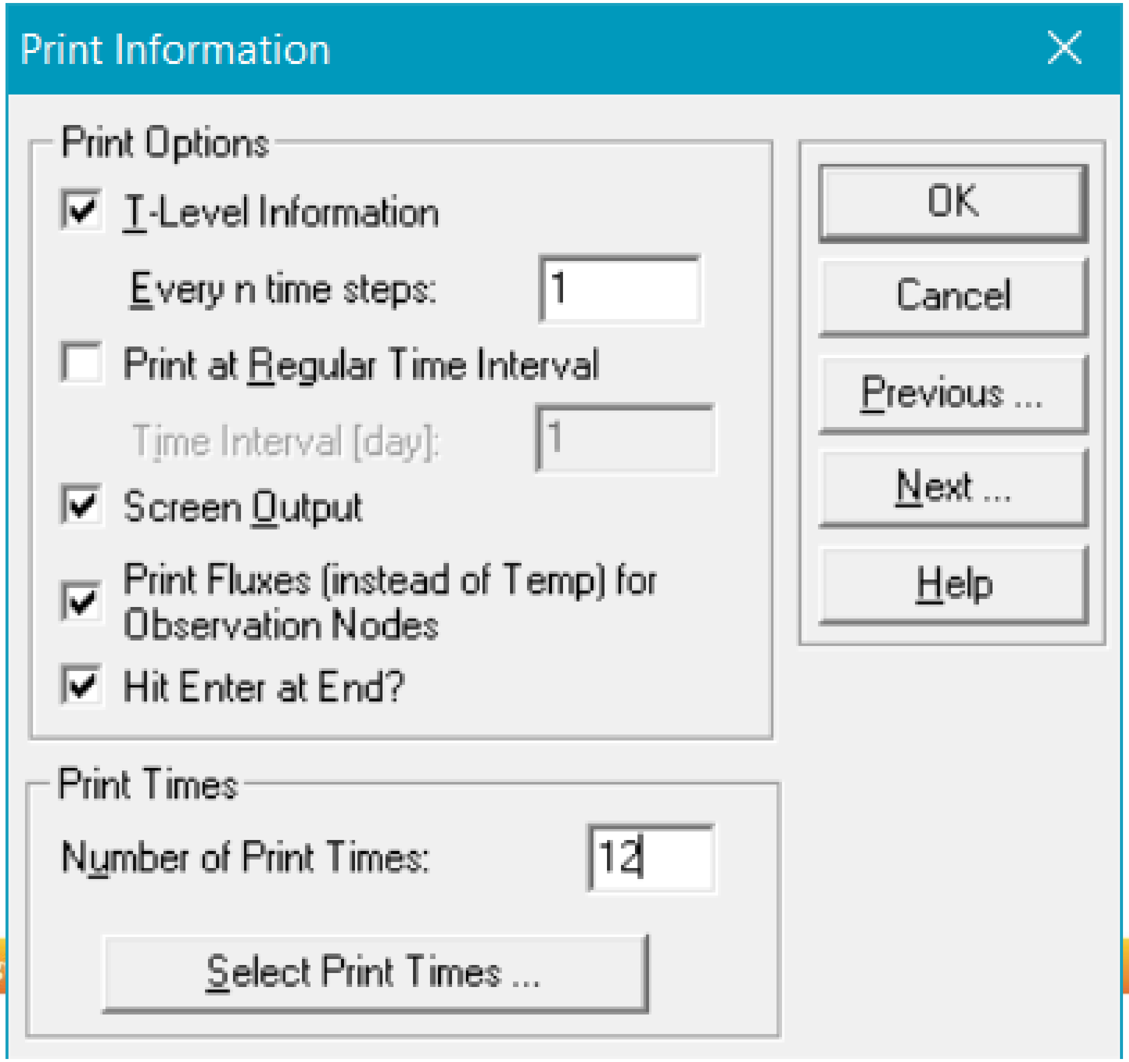
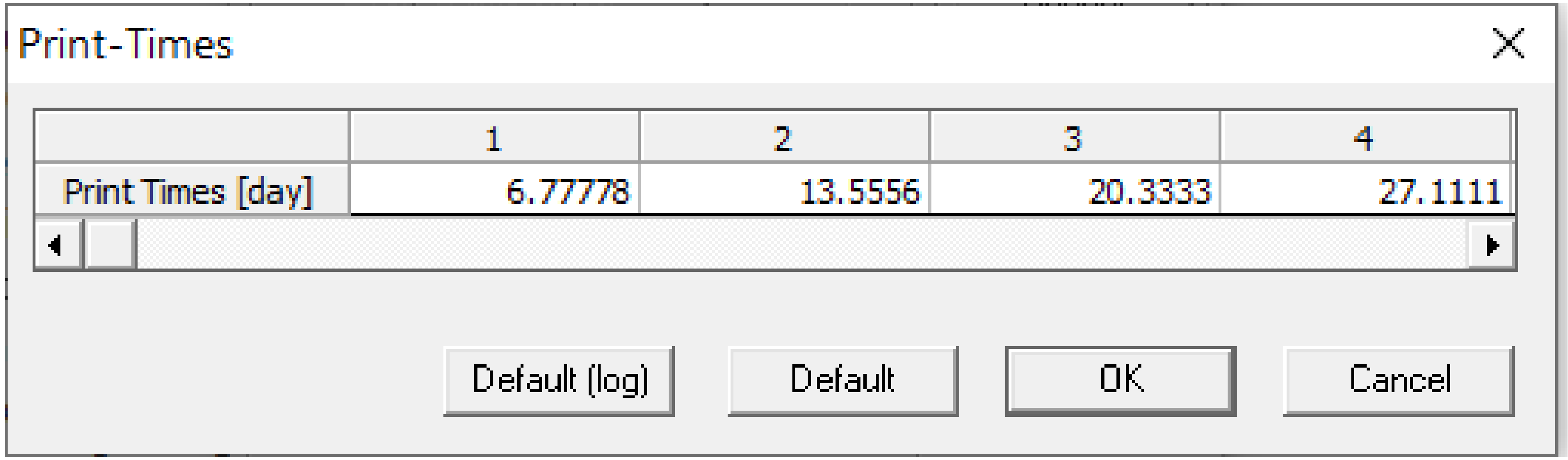




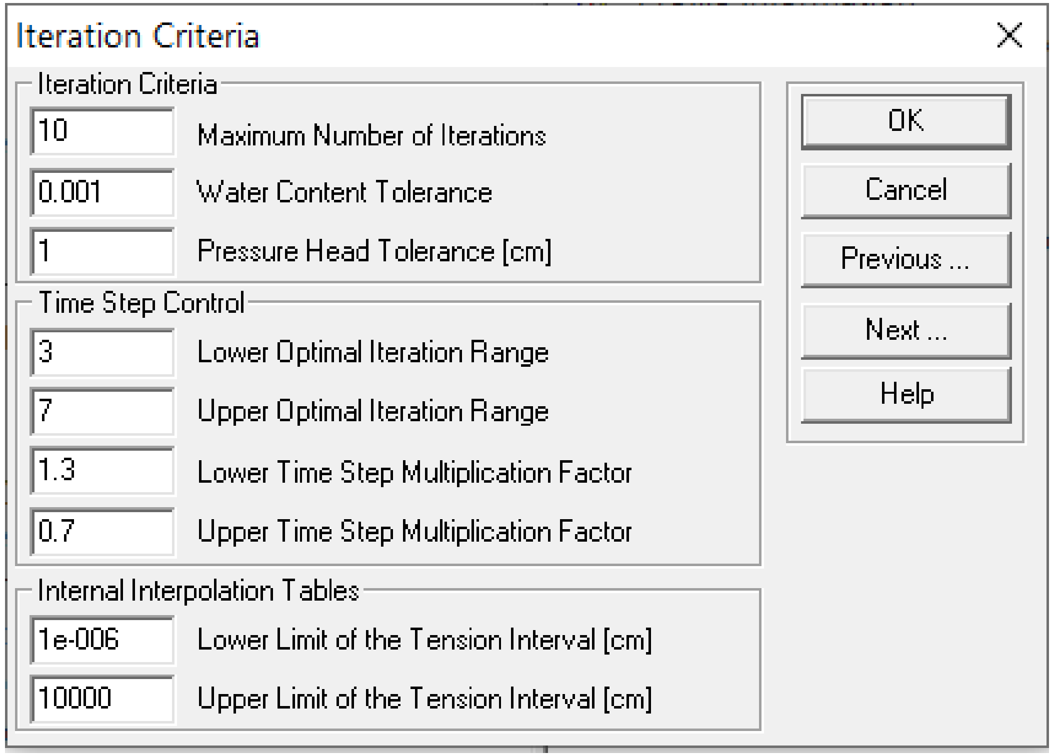
Example 1: HYDRUS 1D

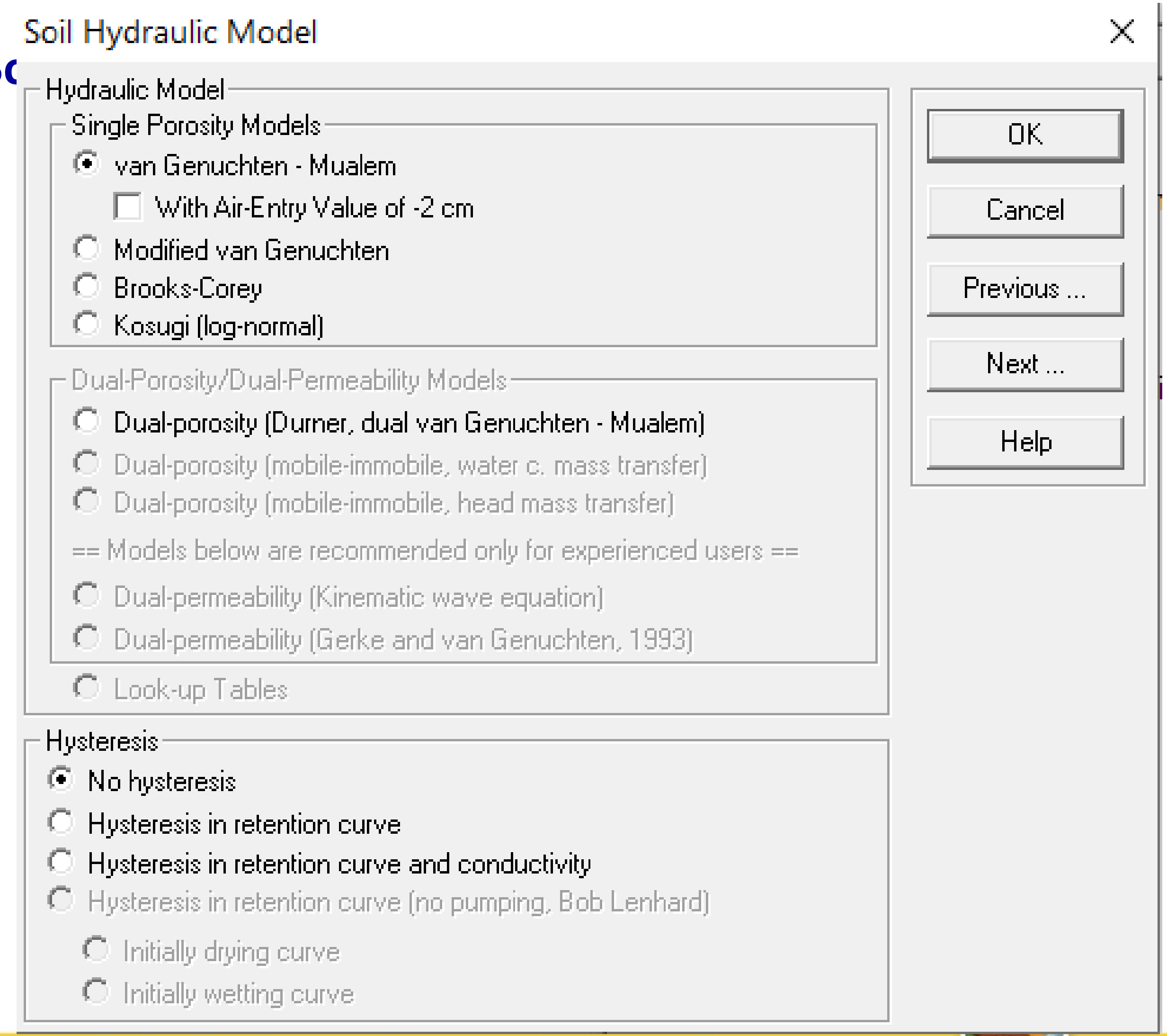
Water flow and solute transport into a Four-Layered Soil Profile



Example 1: HYDRUS 1D

Water flow and solute transport into a Four-Layered Sc





Example 1: HYDRUS 1D

Water flow and solute transport into a Fou

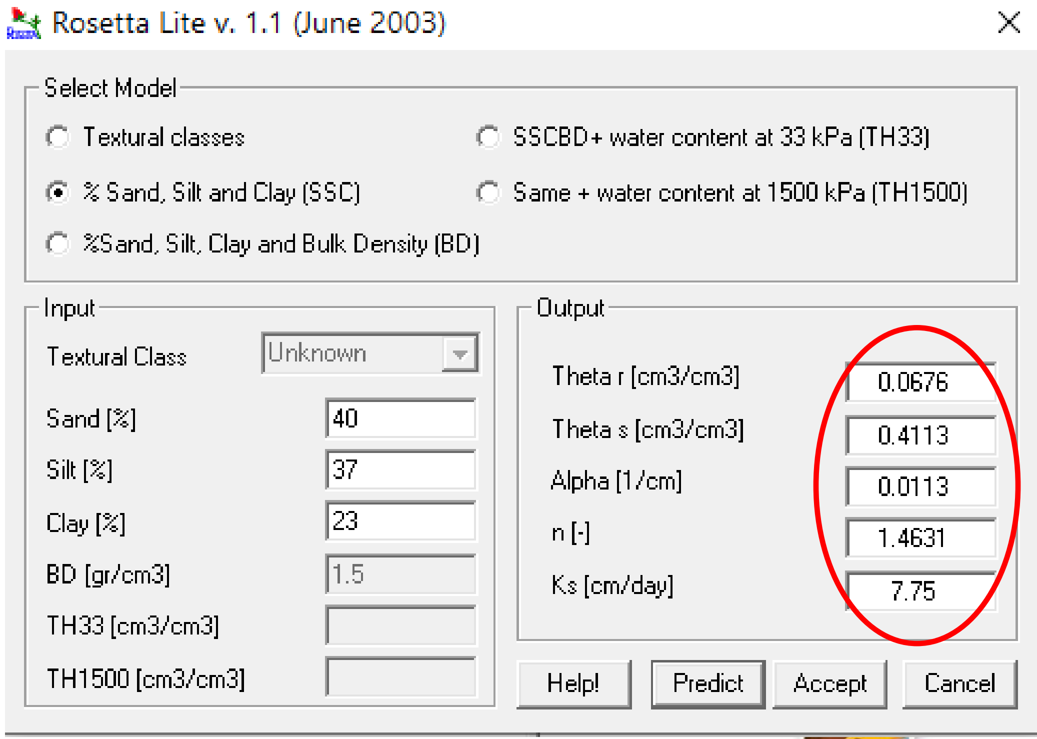
n	α	θ_s	θ_r	K_s	SAR	sand	silt	Clay	pH	EC	Depth	
	cm^{-1}	cm^3/cm^3		cm/day		%				ds/m	cm	
1.3065	0.0073	0.417	0.116	5.835	13.6	40	37	23	7.7	21.5	0-13	Nim2-9
1.3484	0.0049	0.426	0.120	4.395	8.7	40	57	3	7.8	7.8	13-28	
1.3105	0.00702	0.417	0.116	5.630	10.4	40	39	21	7.8	7.4	28-64	
1.3105	0.00702	0.417	0.116	6.1	11.6	66	26	8	7.9	6.6	61-90	

Water Flow Parameters

Mat	Qr [-]	Qs [-]	Alpha [1/cm]	n [-]	Ks [cm/day]	l [-]
1	0.11628	0.417347	0.007338	1.30657	5.835	0.5
2	0.120837	0.426867	0.004993	1.34848	4.39529	0.5
3	0.116604	0.417571	0.007024	1.31053	5.835	0.5
4	0.116604	0.417571	0.007024	1.31053	6.11	0.5

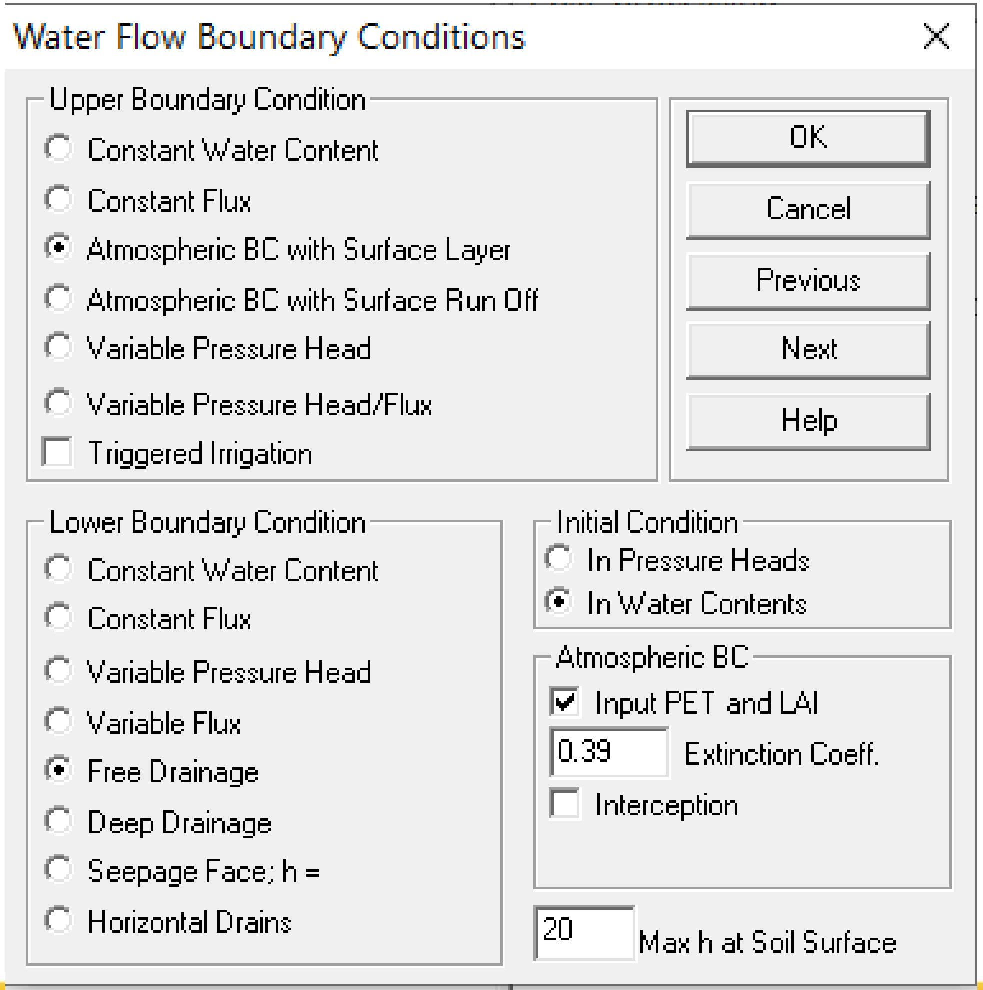
Soil Catalog | Neural Network Prediction | Temperature Dependence

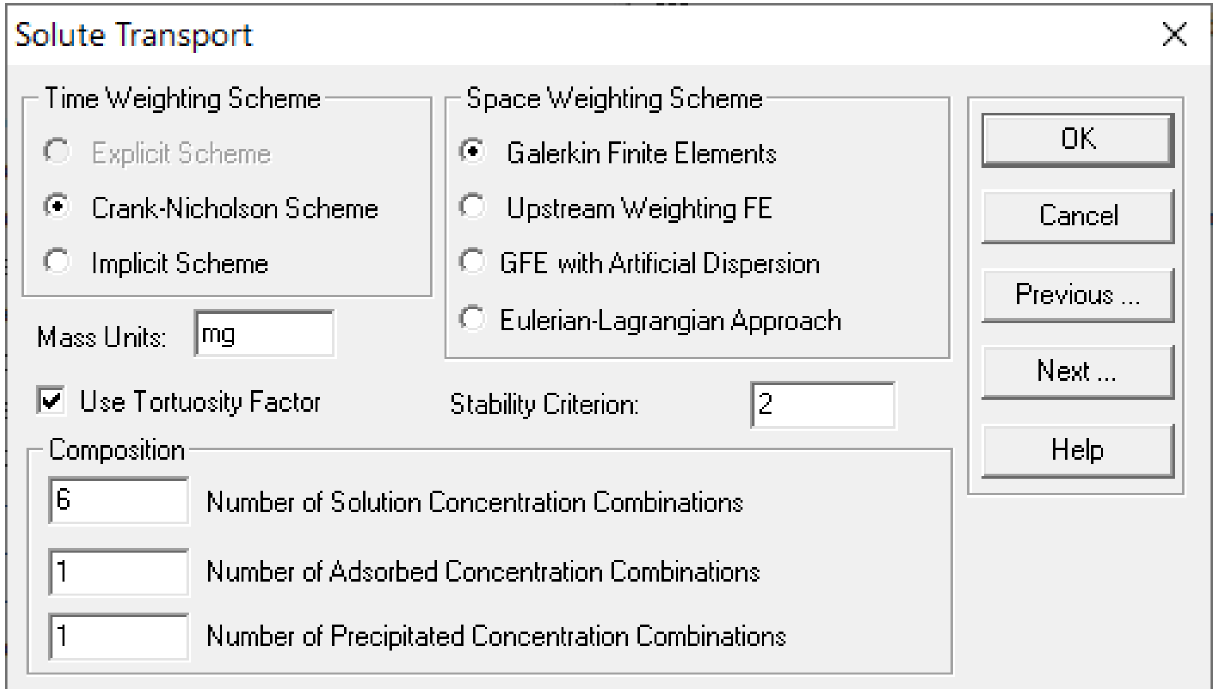
OK | Cancel | Previous ... | Next ... | Help



Example 1: HYDRUS 1D

Water flow and solute transport into a Four-Layered Soil Profile





Example 1: HYDRUS 1D

Water flow and solute transport into a Four-Layered Soil Profile

layer	Ca^{2+}	Mg^{2+}	Na^{+}	Cl^{-}	SO_4^{2-}	CO_3^{2-}	HCO_3^{-}
	Meq/l						
Soil layer 1	170	17	125	150	0.8	0.5	2.16
Soil layer 2	54	5.4	45	54	0.8	0.5	1.68
Soil layer 3	41	4.1	47	56.4	1	1	2.04
Soil layer 4	30	3.8	45	50.4	0.5	0.5	1.54
Irrigation Water	1.8	4.1	6.69	0.17	3.41	5.5	3.02
Rain	0.01	0.01	0.01	0.01	0	0	0.04

Solute Composition

Solution Composition [meq/L]

Sol	Ca	Mg	Na	K	Alk	SO4	Cl	Tracer
1	170	17	125	0.1	2.66	0.8	150	1E+030
2	54	5.4	45	0.1	2.18	0.8	54	1E+030

Solute Composition

Solution Composition [meq/L]

Sol	Ca	Mg	Na	K	Alk	SO4	Cl	Tracer
3	41	4.1	47	0.2	2.05	1	56.4	1E+030
4	30	3.8	45	0.2	3.52	0.5	50.4	1E+030
5	1.8	4.1	6.69	0.17	3.41	5.5	3.02	1E+030
6	0.01	0.01	0.01	0.01	0	0	0.04	0

Adsorption Concentrations [meq/kg]

Ads	Ca	Mg	Na	K
1	0	0	0	0

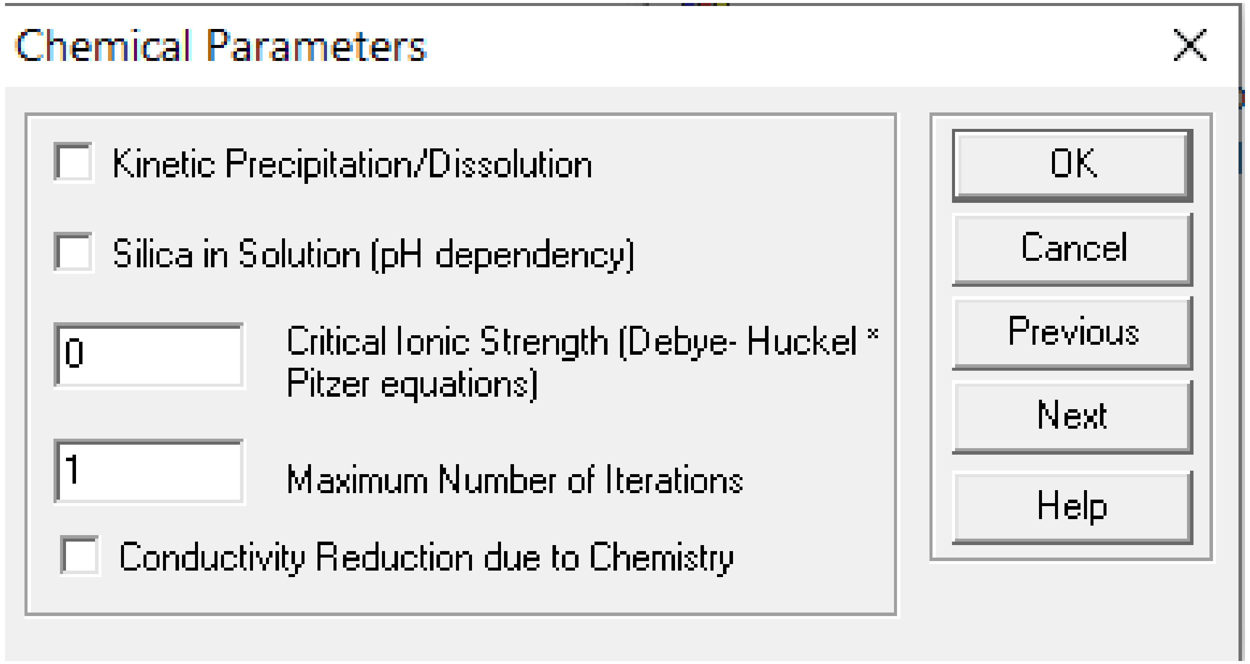
Precipitated Concentrations [meq/kg]

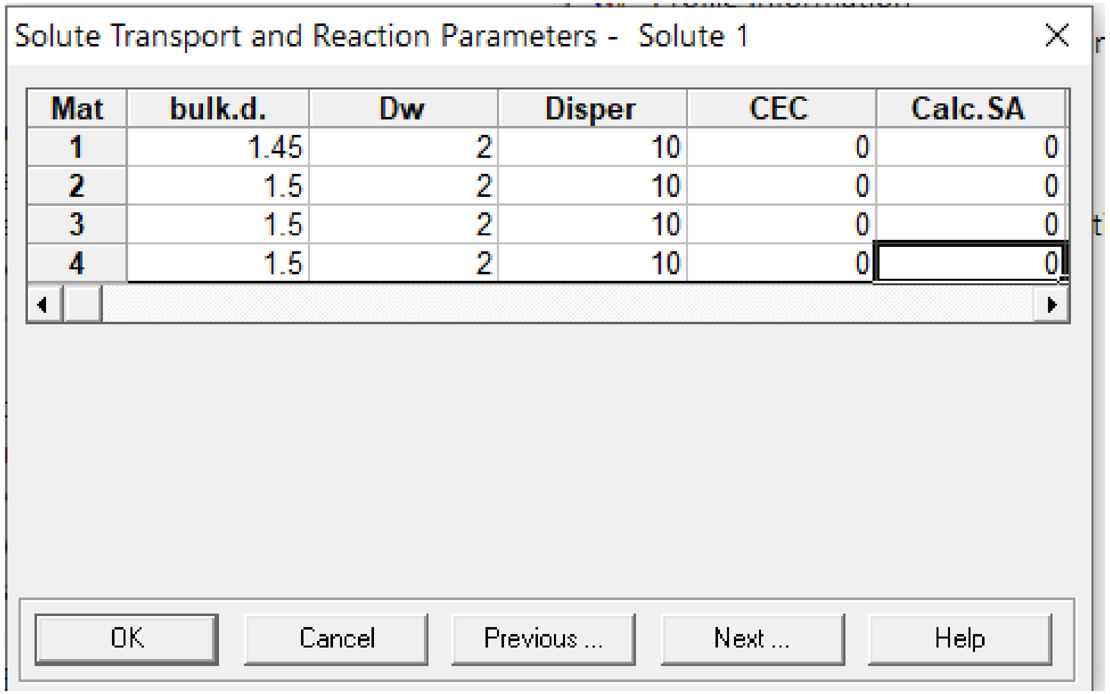
Prec	Calcite	Gypsum	Dolomite	HydroMg	Nesqoh	Sepiolite
1	0	0	0	0	0	0

OK Cancel Previous Next Help

Example 1: HYDRUS 1D

Water flow and solute transport into a Four-Layered Soil Profile

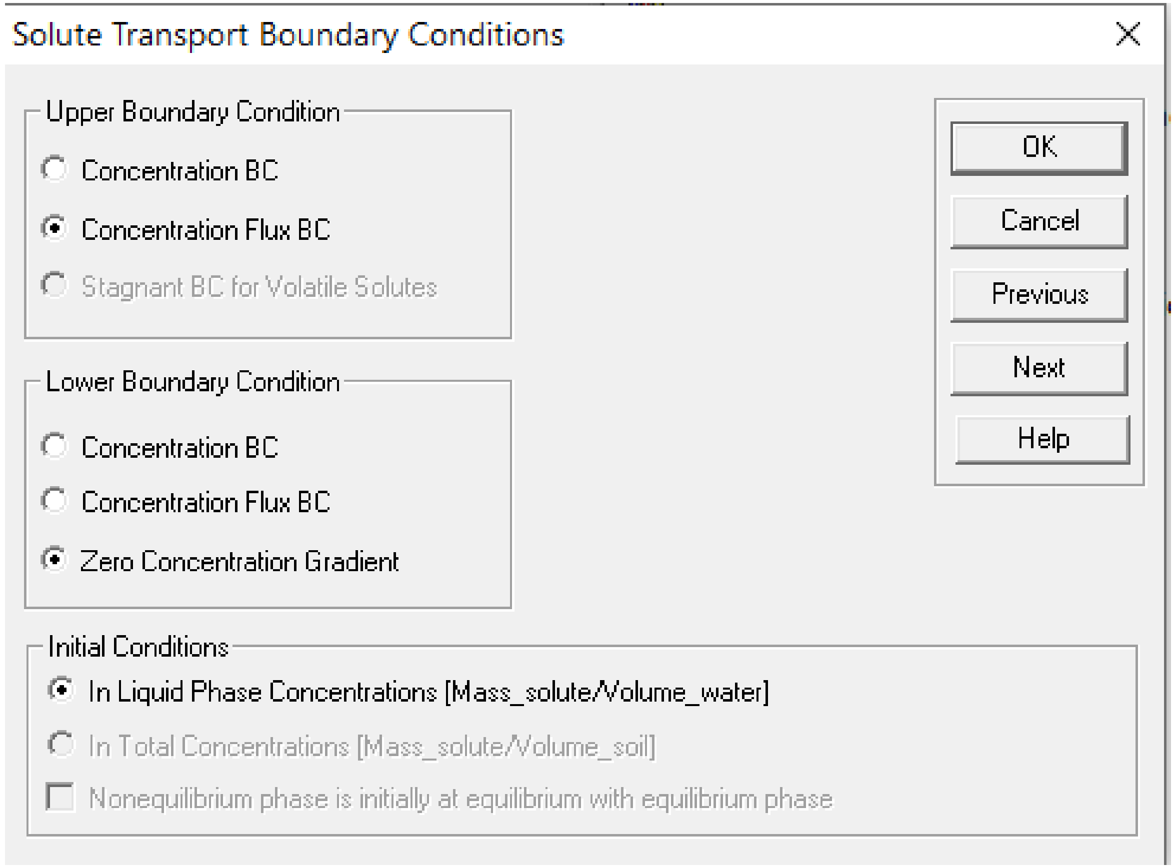


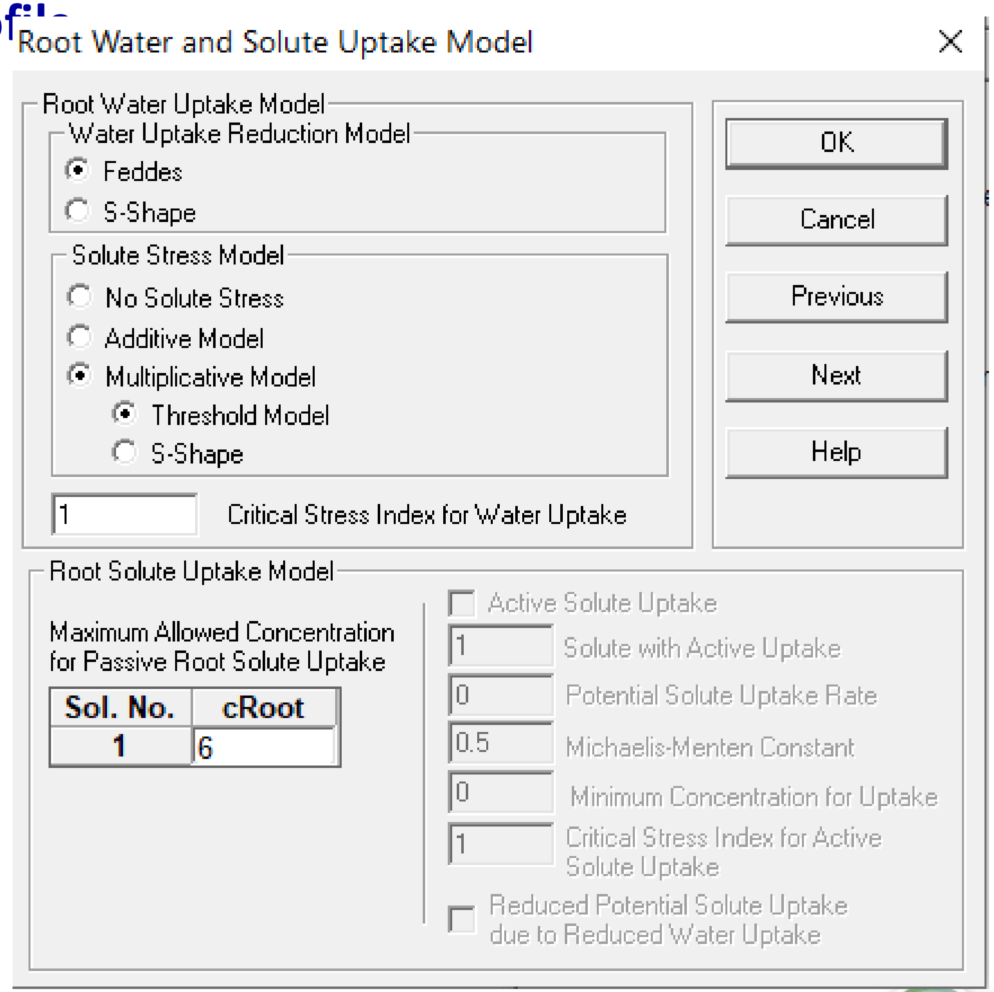


Mat	bulk.d.	Dw	Disper	CEC	Calc.SA
1	1.45	2	10	0	0
2	1.5	2	10	0	0
3	1.5	2	10	0	0
4	1.5	2	10	0	0

Example 1: HYDRUS 1D

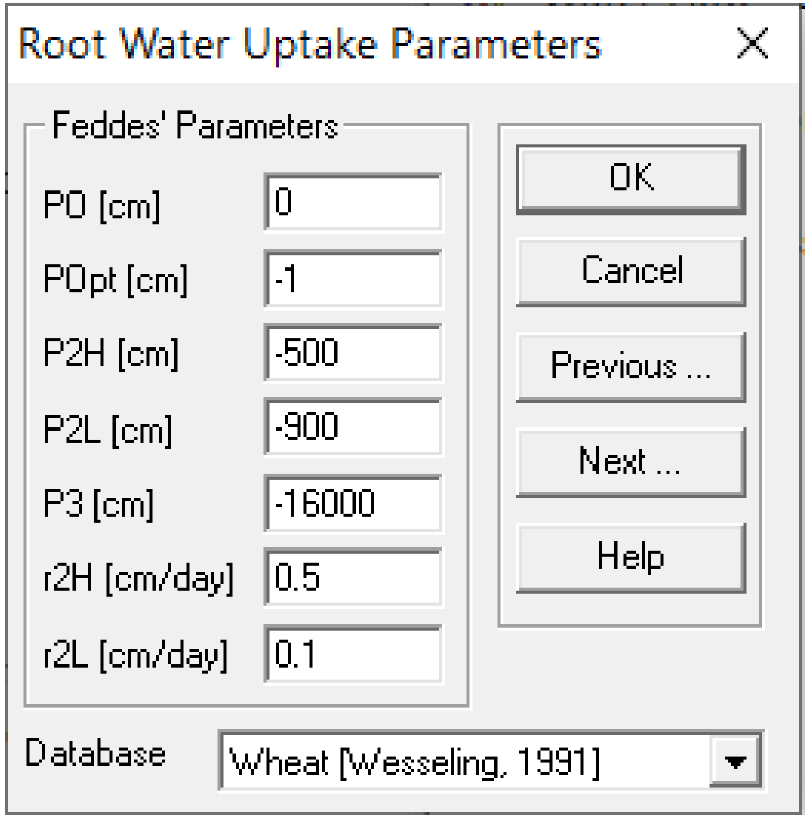
Water flow and solute transport into a Four-Layered Soil Profi...

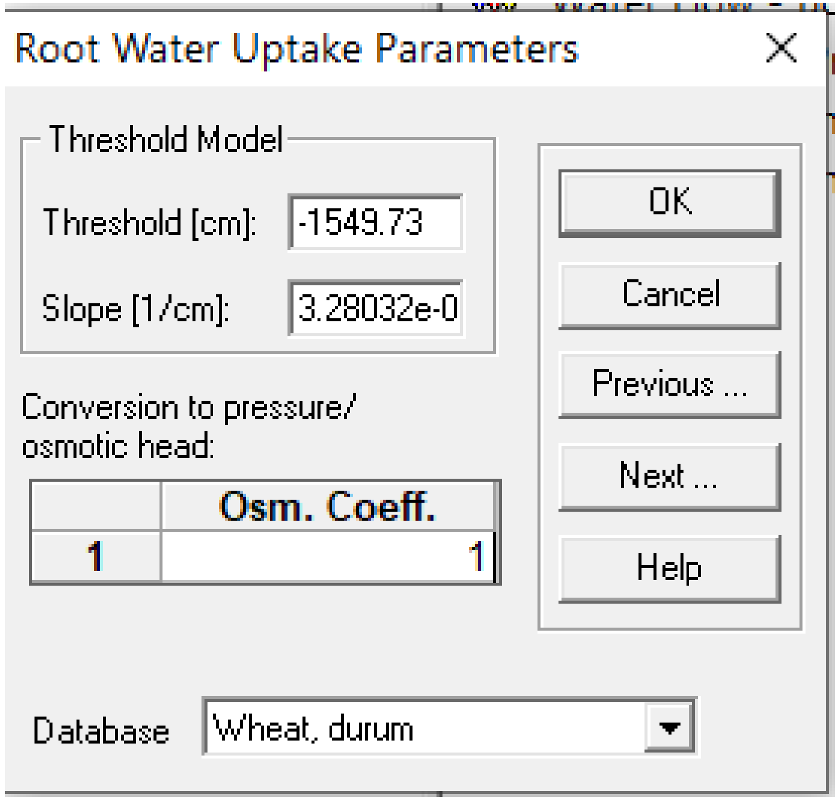




Example 1: HYDRUS 1D

Water flow and solute transport into a Four-Layered Soil Profile





Example 1: HYDRUS 1D

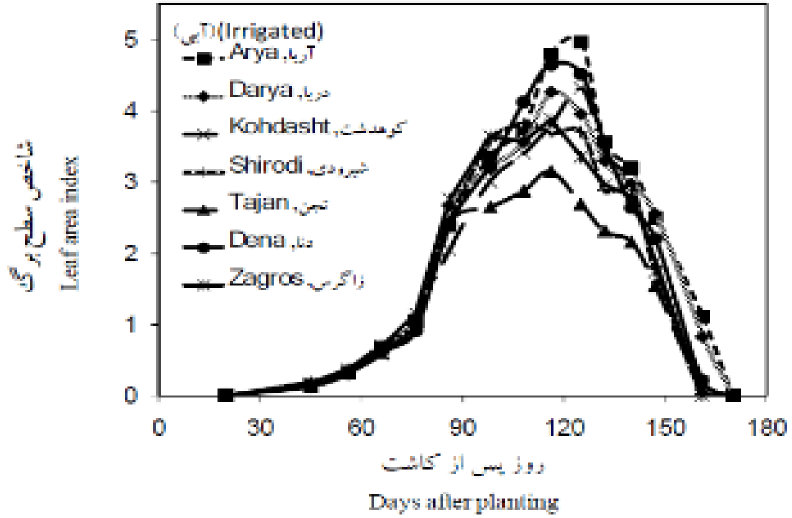
Water flow and solute transport into a Four-Layered Soil Profile

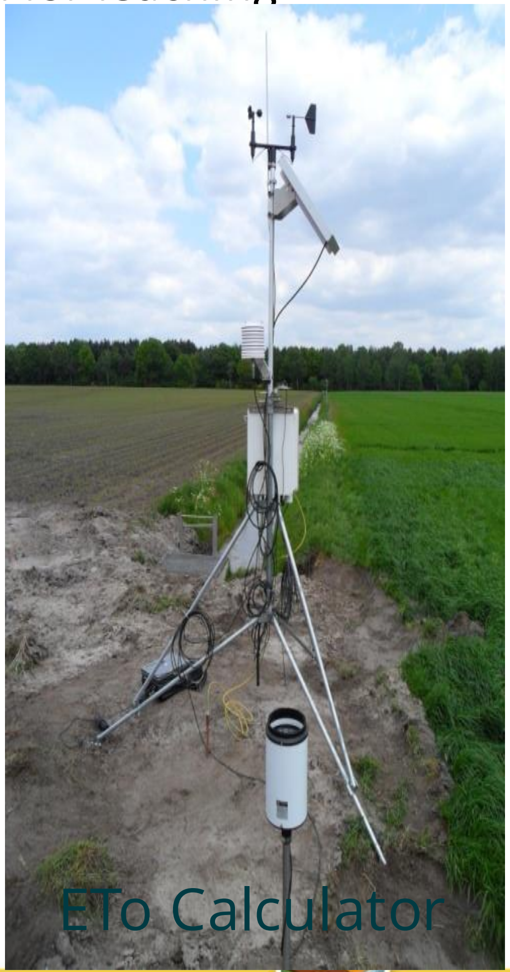
Time Variable Boundary Conditions

	Time [day]	Precip. [cm/day]	potET [cm/day]	hCritA [cm]	LAI	cTop	cBot
1	1	0	0.32	100000	0	0	0
2	2	0	0.33	100000	0	0	0
3	3	0.1	0.37	100000	0	6	0
4	4	0.43	0.37	100000	0	6	0
5	5	0.011	0.36	100000	0	6	0
6	6	0.003	0.36	100000	0	6	0
21	21	0.081	0.33	100000	0	6	0
22	22	0.041	0.32	100000	0	6	0
23	23	0.21	0.29	100000	0	6	0
24	24	0.141	0.26	100000	0	6	0
25	25	0.371	0.29	100000	0	6	0
26	26	0.982	0.31	100000	0	6	0
27	27	0	0.3	100000	0	0	0
28	28	0.03	0.34	100000	0	6	0
29	29	0.31	0.34	100000	0	6	0
30	30	20.93	0.27	100000	0	5	0
31	31	0.86	0.29	100000	0	6	0
32	32	0.63	0.26	100000	0	6	0
33	33	0.87	0.28	100000	0	6	0
34	34	0	0.28	100000	0	0	0

OK | Cancel | Previous ... | Next ... | Help ... | Add Line | Delete Line | Default Time

- 20 cm of water as pre-irrigation for leaching purposes (day 30).
- 5 irrigation events
- (day 96), (day 116), (day 136),
- (day 156), (day 190).





Example 1: HYDRUS 1D

Water flow and solute transport into a Four-Layered Soil Profile

HYDRUS-1D guide

Do you want to run PROFILE application ?

Previous | Next | Cancel | OK

Soil Profile Summary

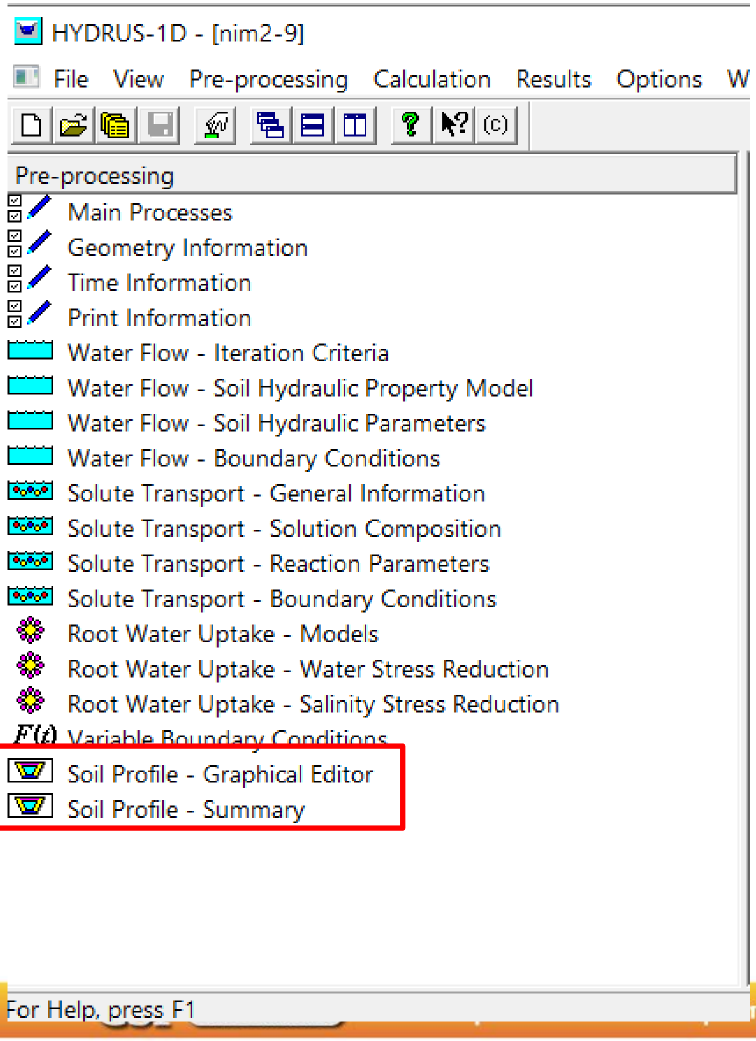
	z [cm]	theta	Root [1/cm]	nConc	nAds	nPrec	Mat
1	0	0.2	0	1	1	1	1
2	1	0.2	0.0833333	1	1	1	1
3	2	0.2	0.166667	1	1	1	1
4	3	0.2	0.25	1	1	1	1
5	4	0.2	0.333333	1	1	1	1
6	5	0.2	0.416667	1	1	1	1
7	6	0.2	0.5	1	1	1	1
8	7	0.2	0.583333	1	1	1	1
9	8	0.2	0.666667	1	1	1	1
10	9	0.2	0.75	1	1	1	1
11	10	0.2	0.833333	1	1	1	1
12	11	0.2	0.916667	1	1	1	1
13	12	0.2	1	1	1	1	1
14	13	0.2	1	1	1	1	2
15	14	0.2	0.916667	1	1	1	2

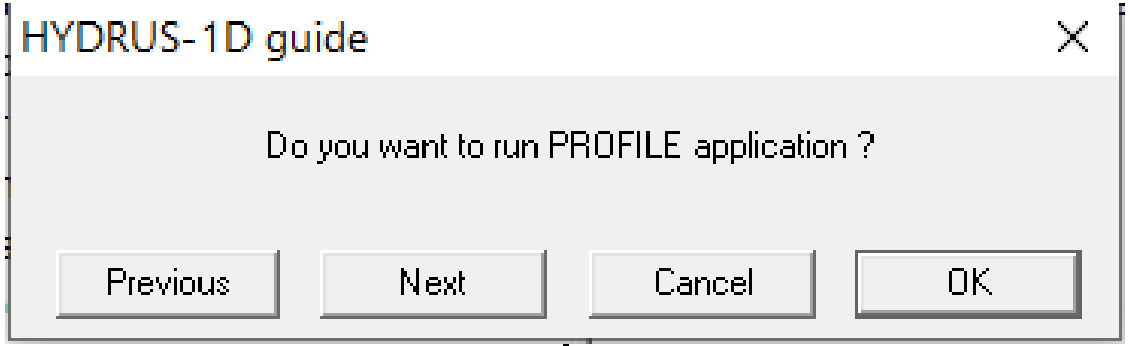
Set to Default Values | Set Initial Conditions Equal to Field Capacity

OK | Cancel | Previous | Next | Help

Example 1: HYDRUS 1D

Water flow and solute transport into a Four-Layered Soil Profile





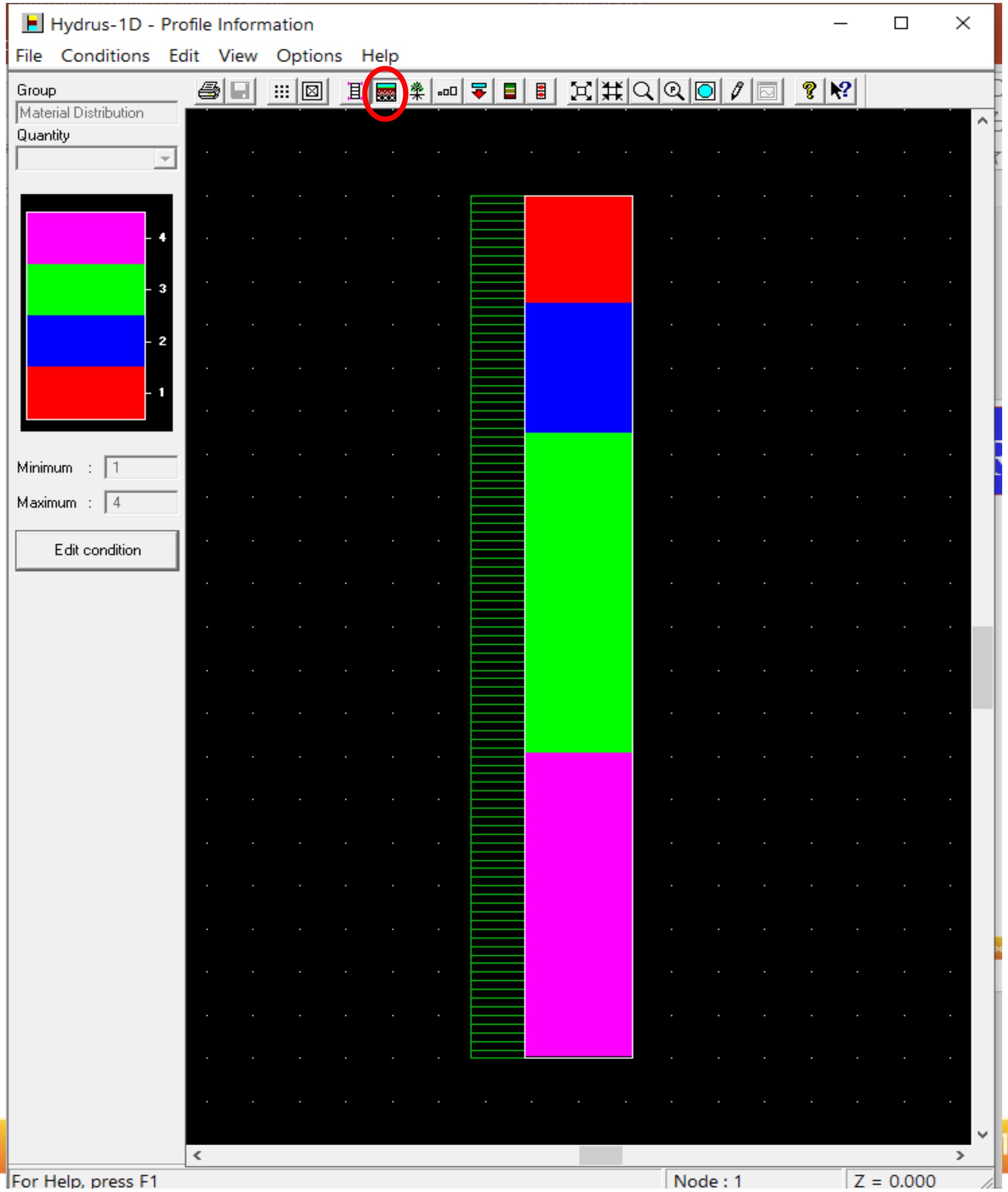
Soil Profile – Graphical Editor

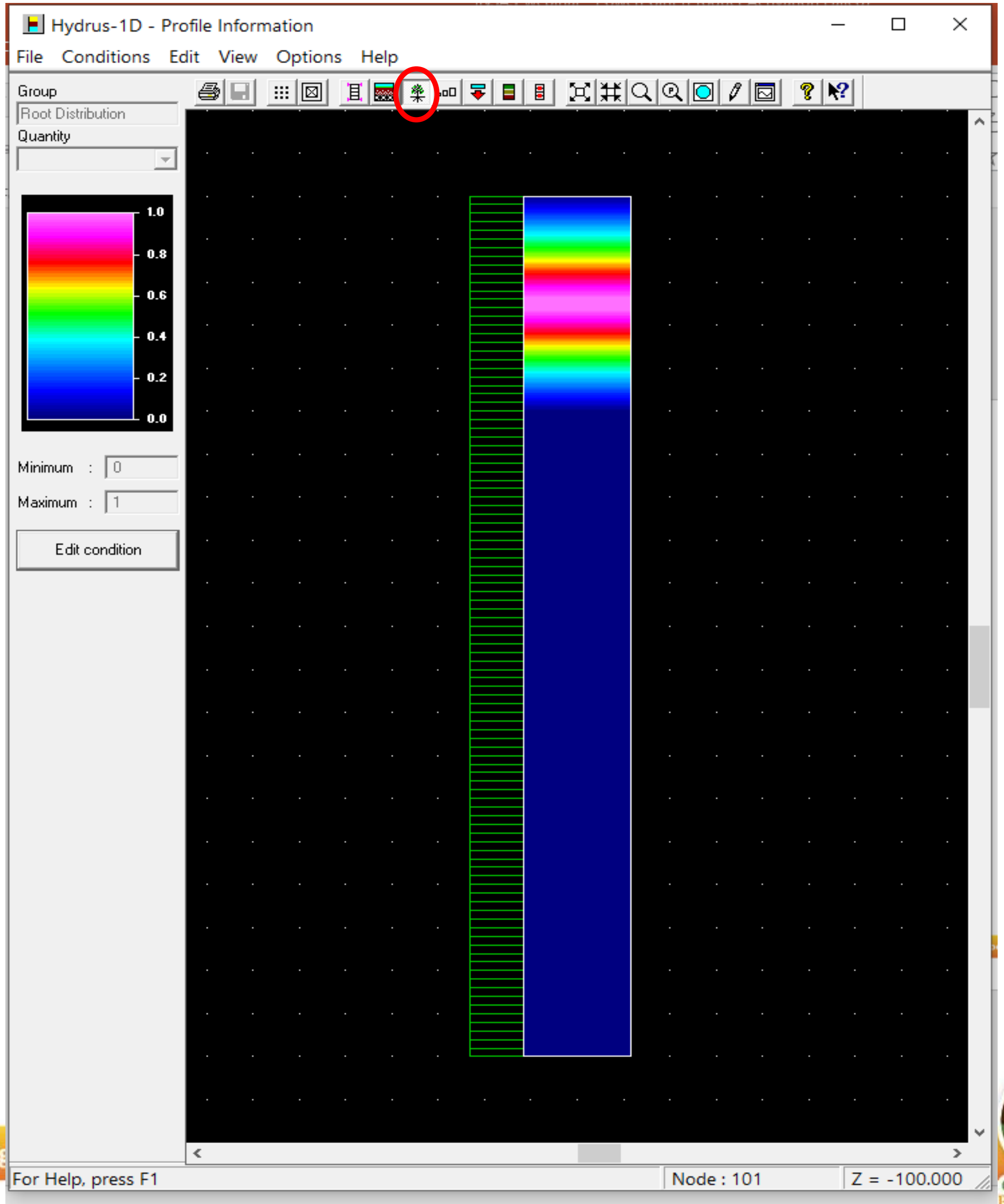
Menu: Conditions->Initial Conditions->water content, or press the Red Arrow() on the Toolbar (top to bottom=0.2)

Menu: Conditions -> Observation Points

Button "Insert", Insert nodes at 2, 13, 25, and 51 cm

Example 1: HYDRUS 1D





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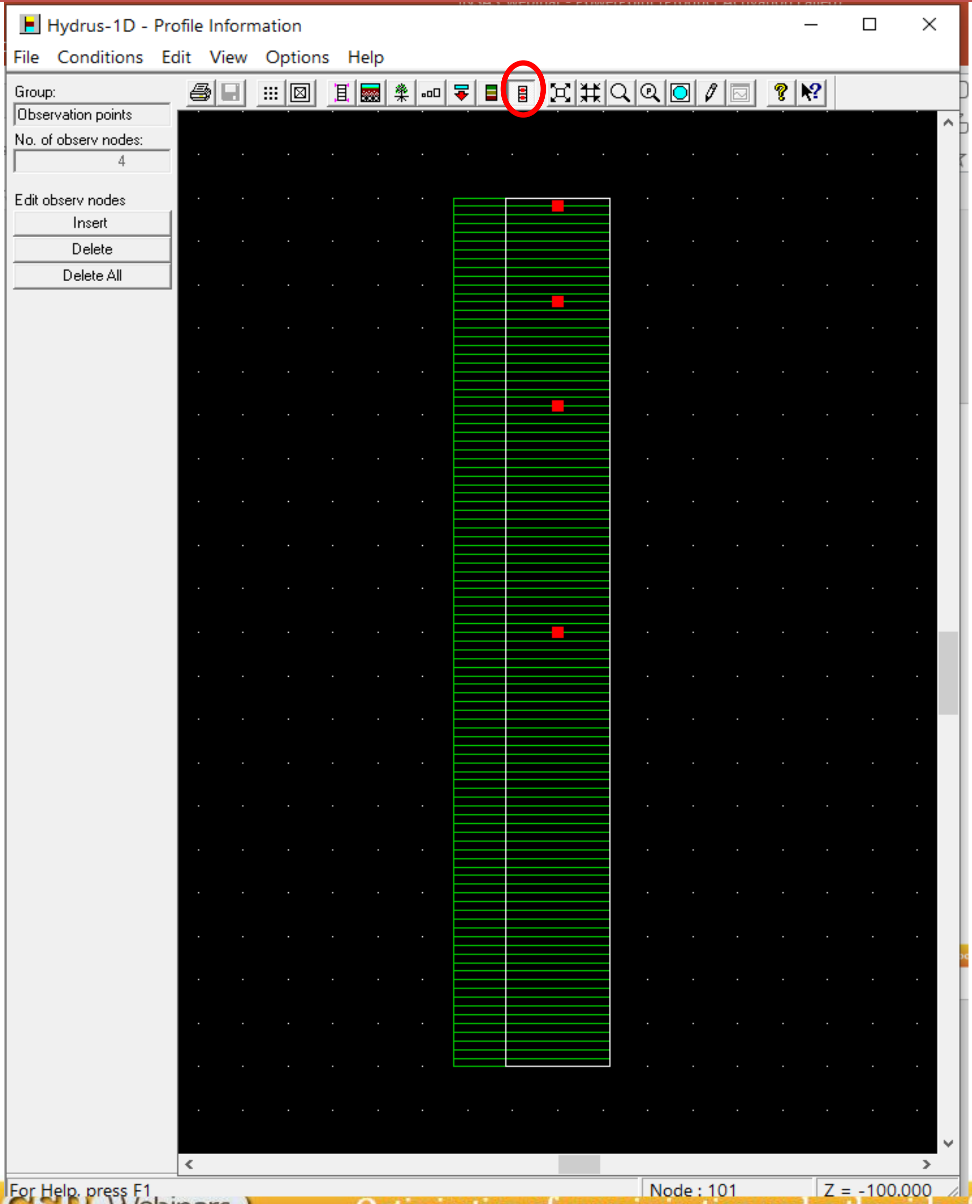

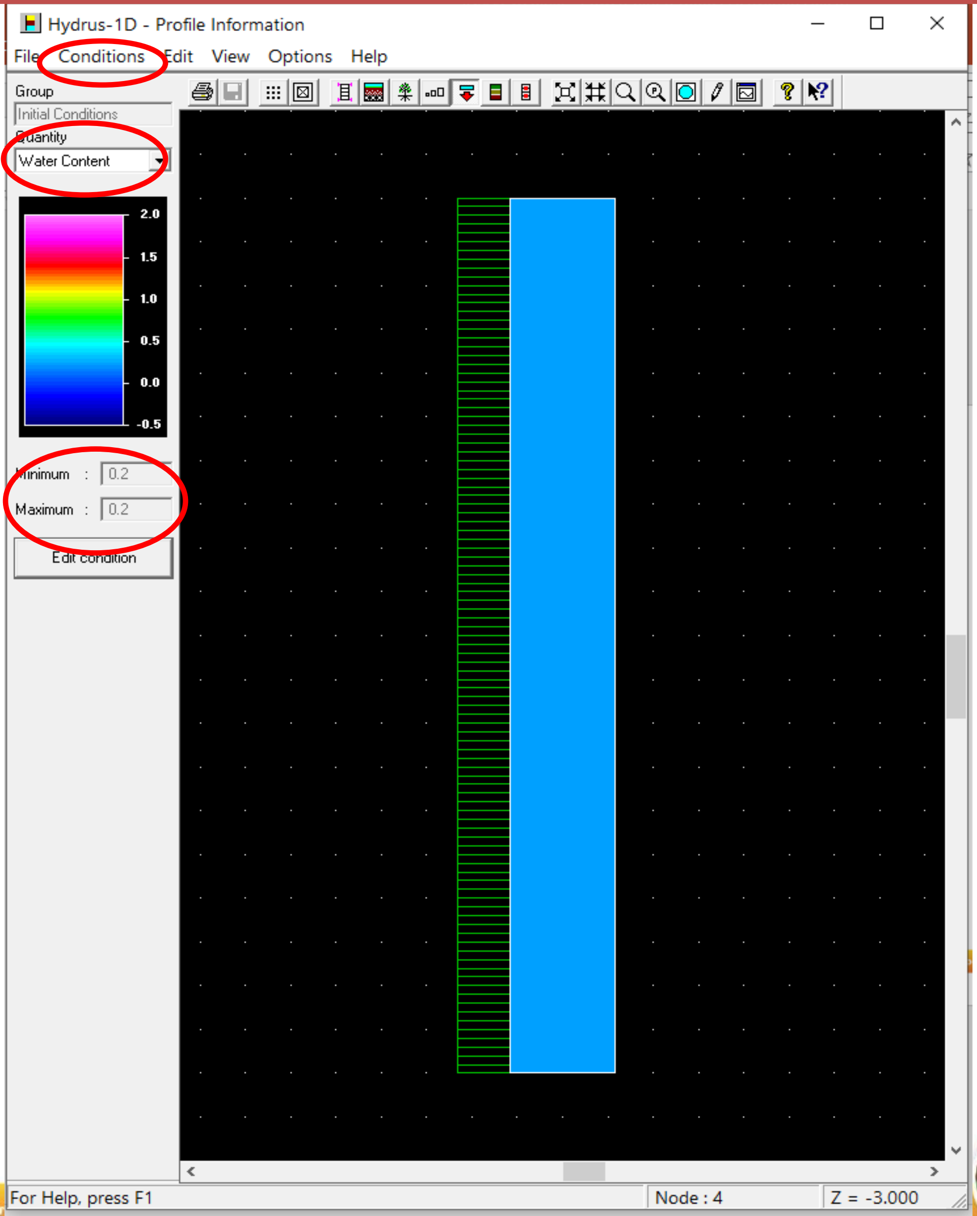

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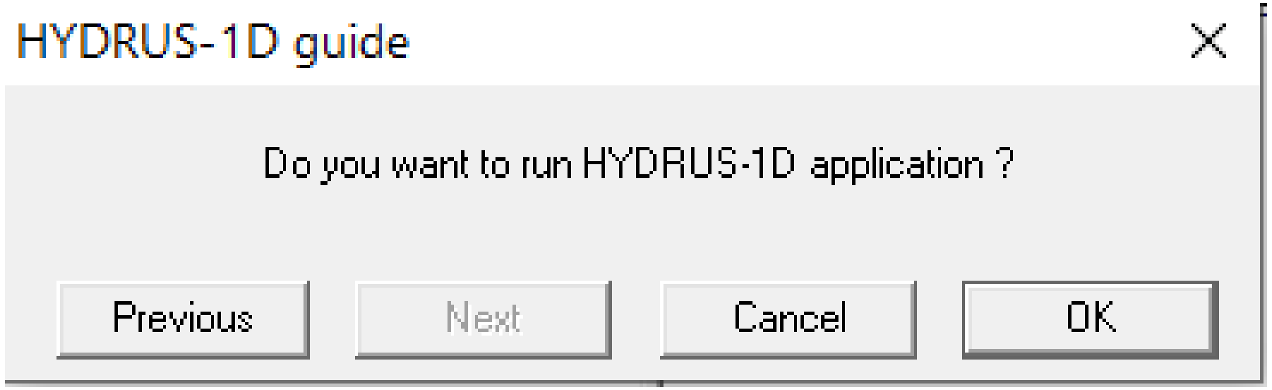

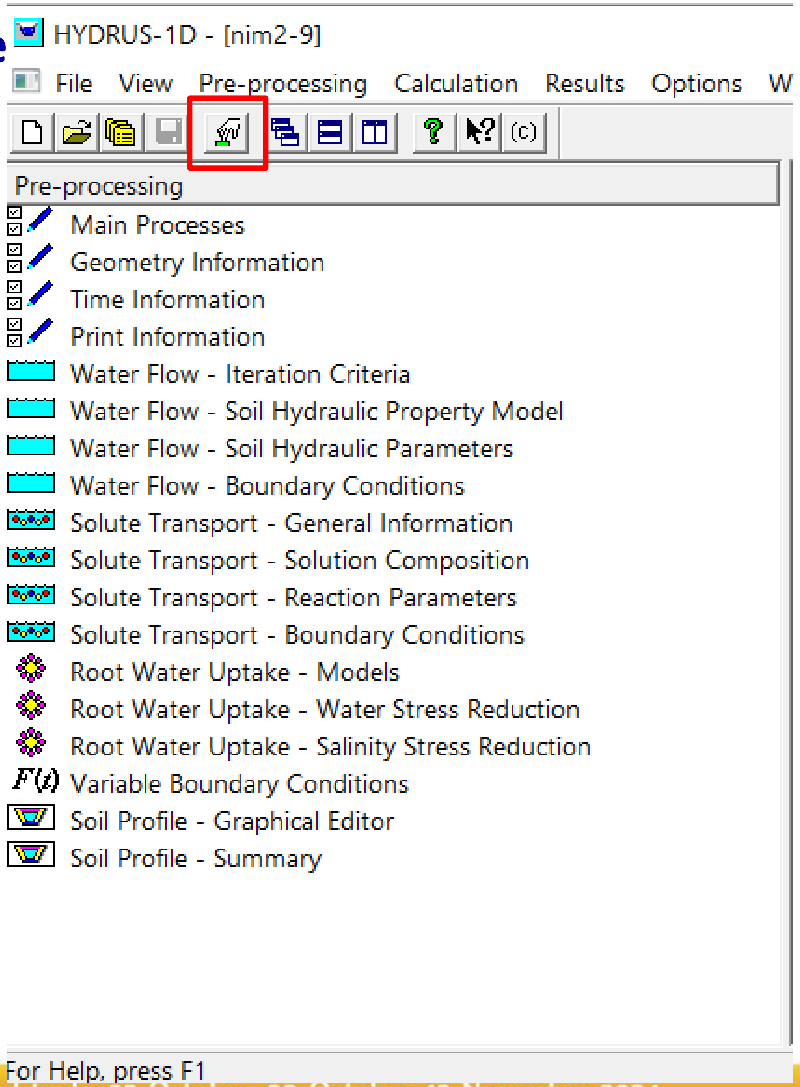

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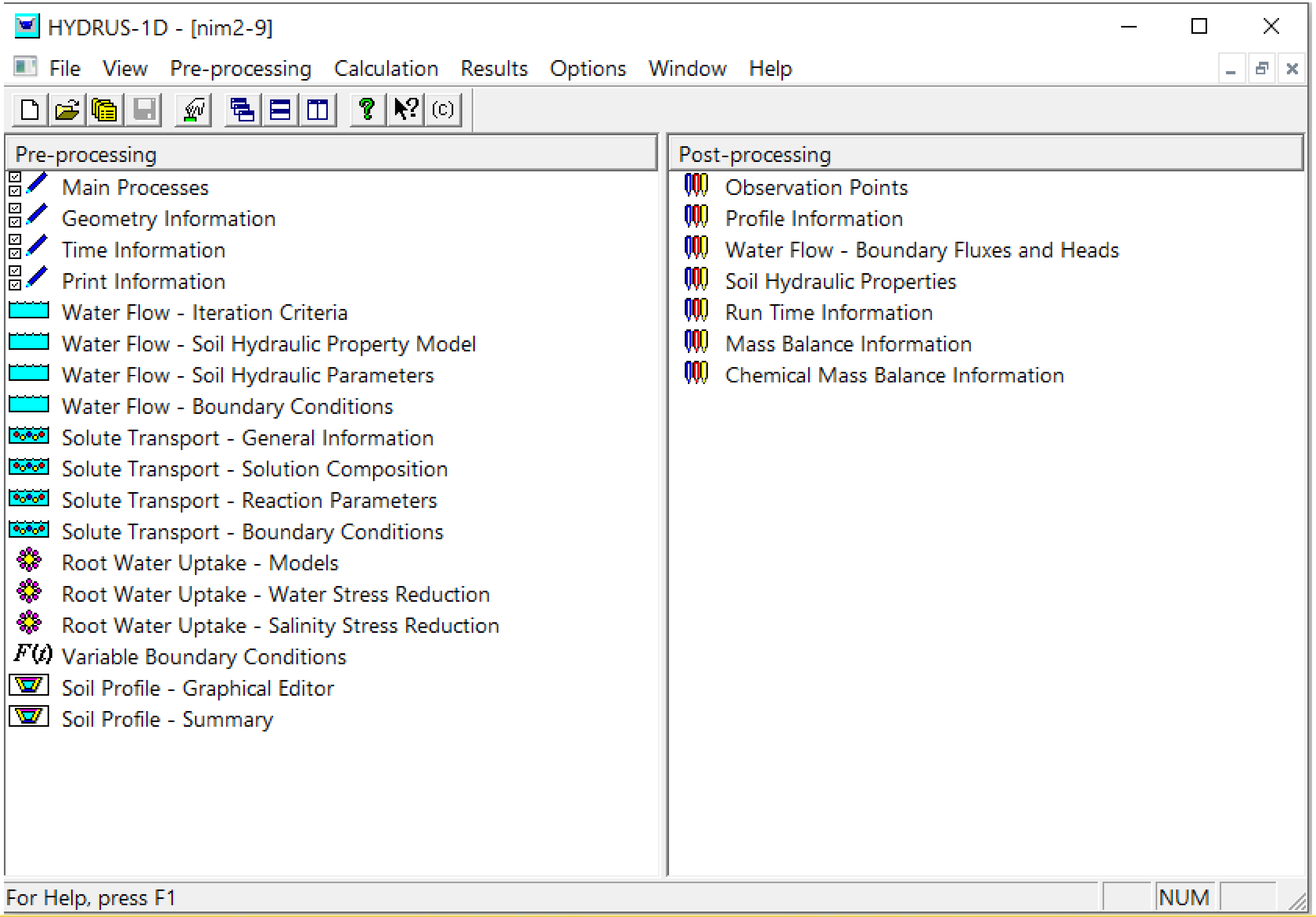

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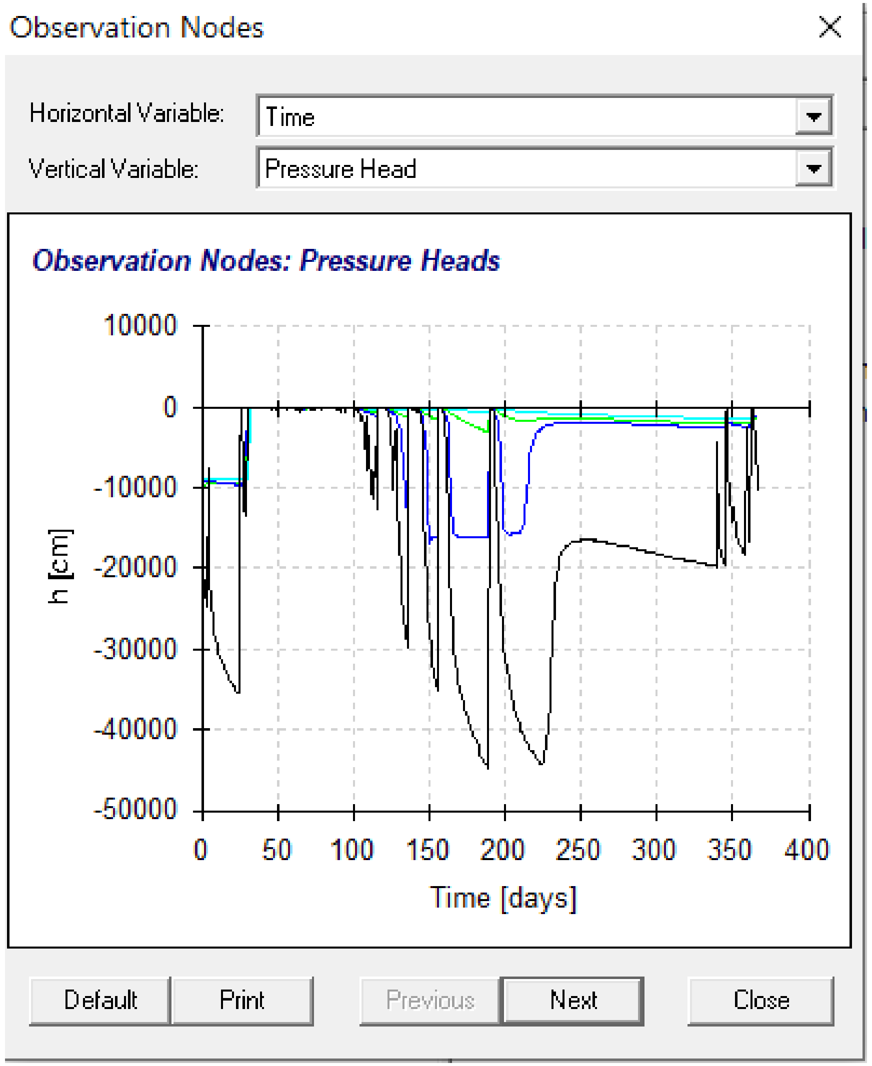

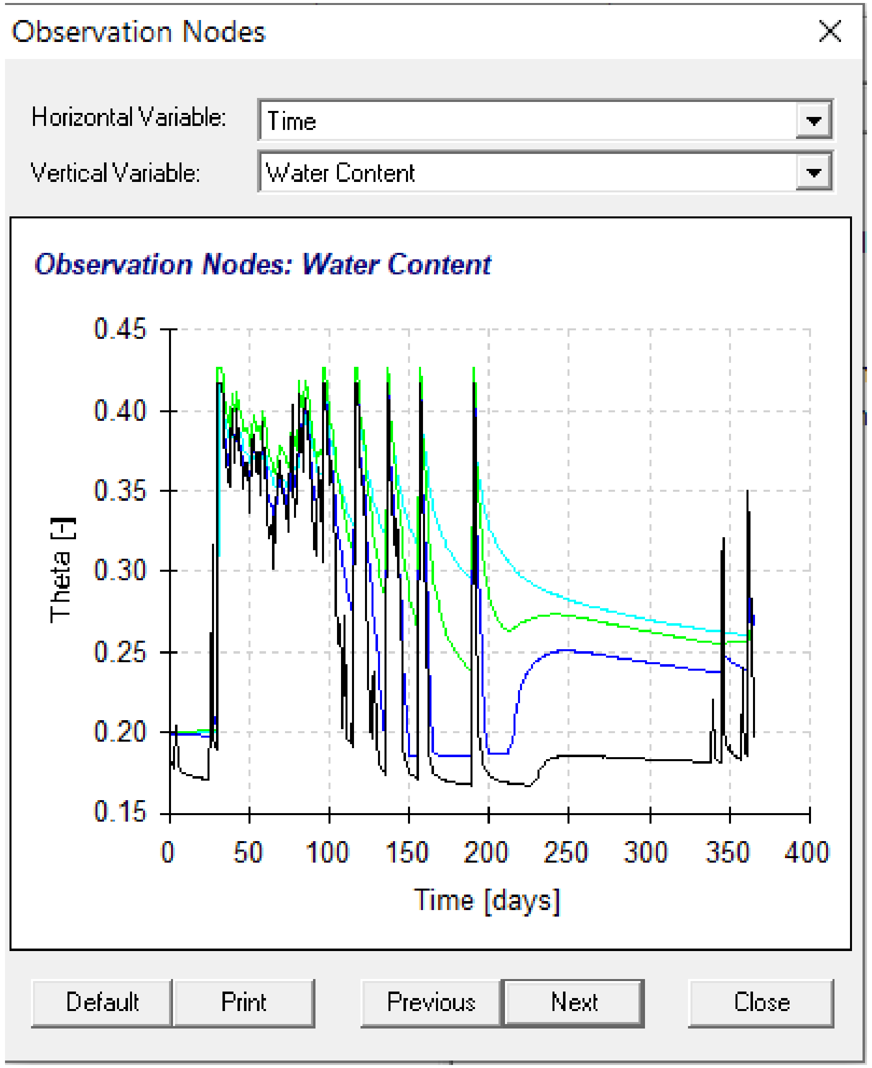

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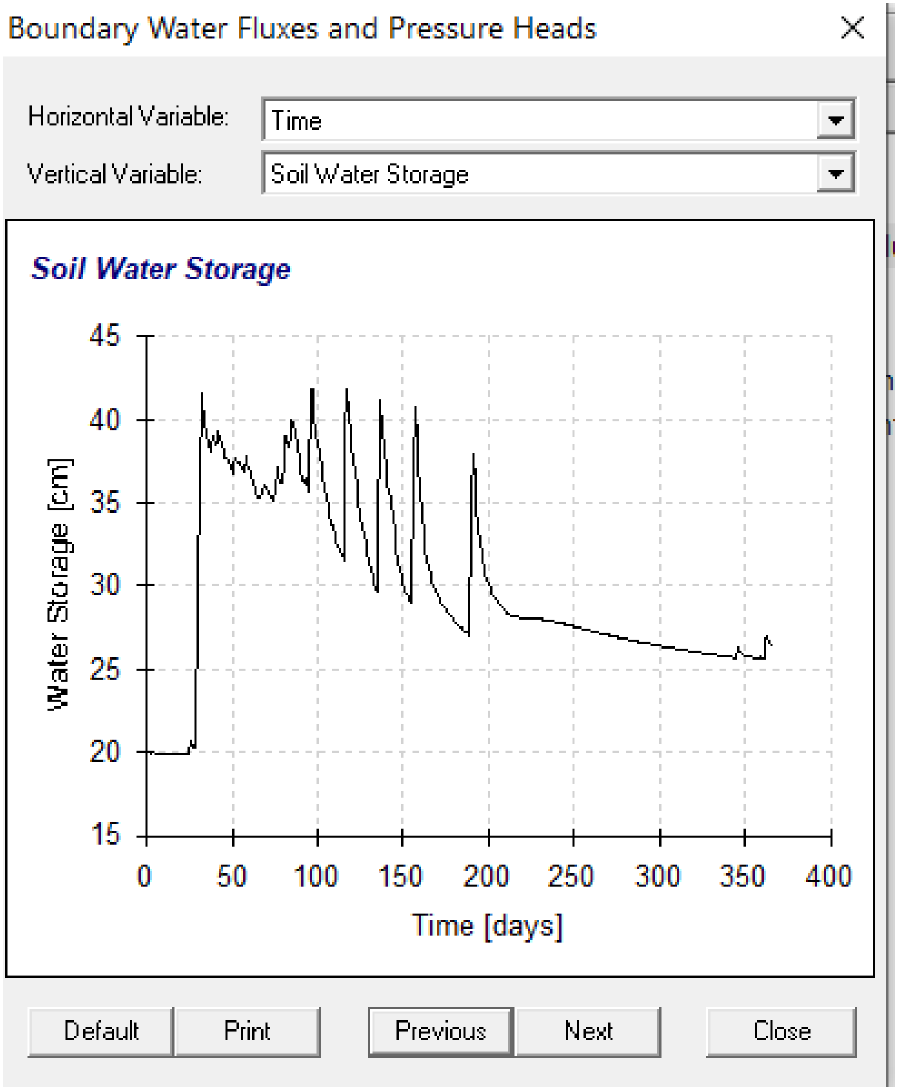

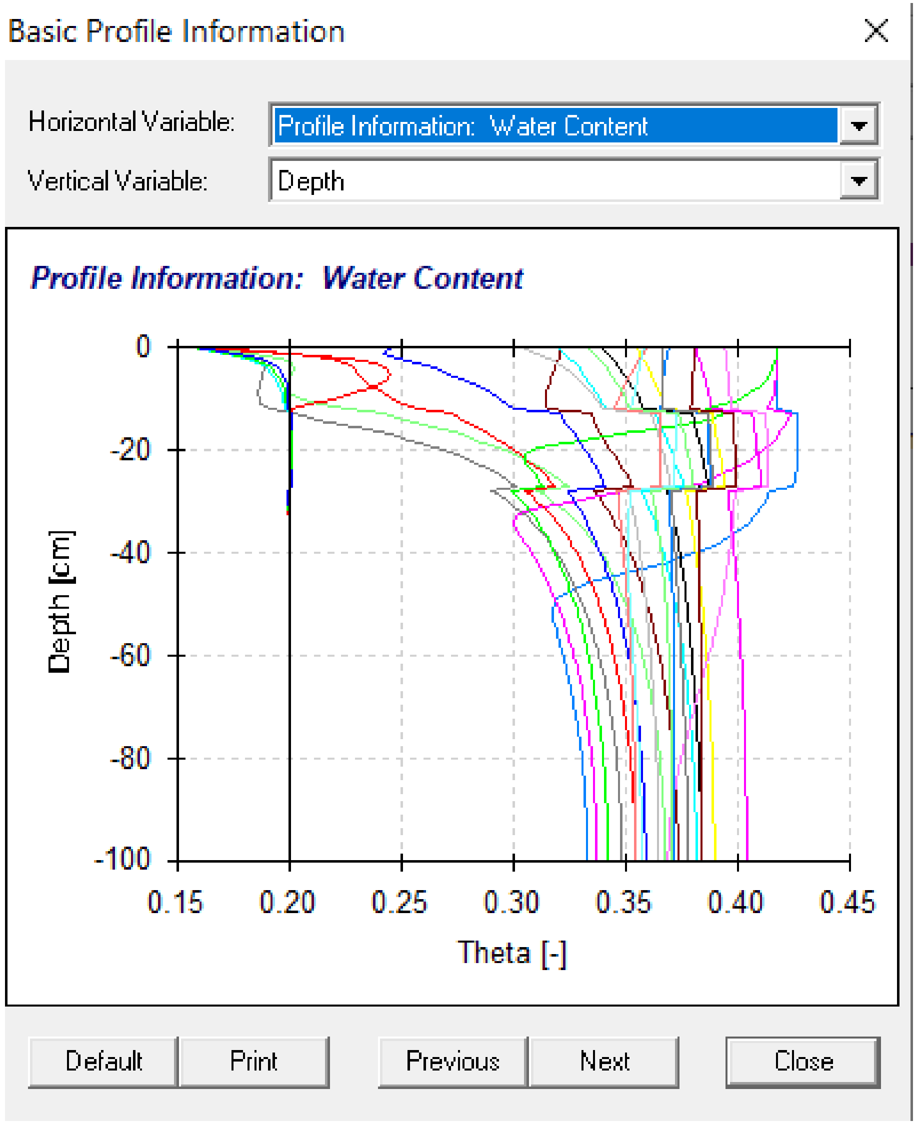

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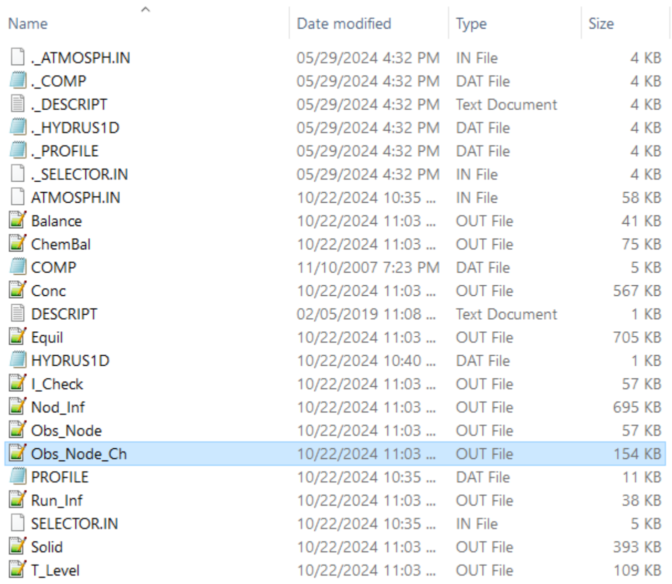

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._COMP	05/29/2024 4:32 PM	DAT File	4 KB
._DESCRIPT	05/29/2024 4:32 PM	Text Document	4 KB
._HYDRUS1D	05/29/2024 4:32 PM	DAT File	4 KB
._PROFILE	05/29/2024 4:32 PM	DAT File	4 KB
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DESCRIPT	02/05/2019 11:08 ...	Text Document	1 KB
Equil	10/22/2024 11:03 ...	OUT File	705 KB
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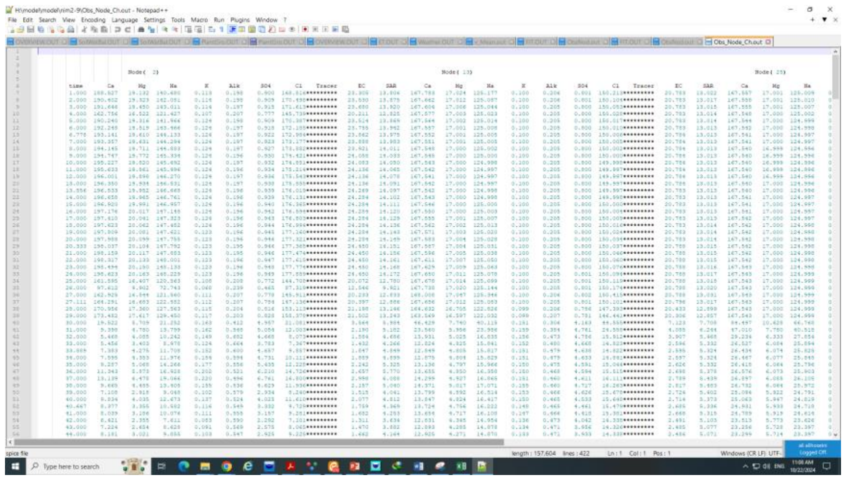
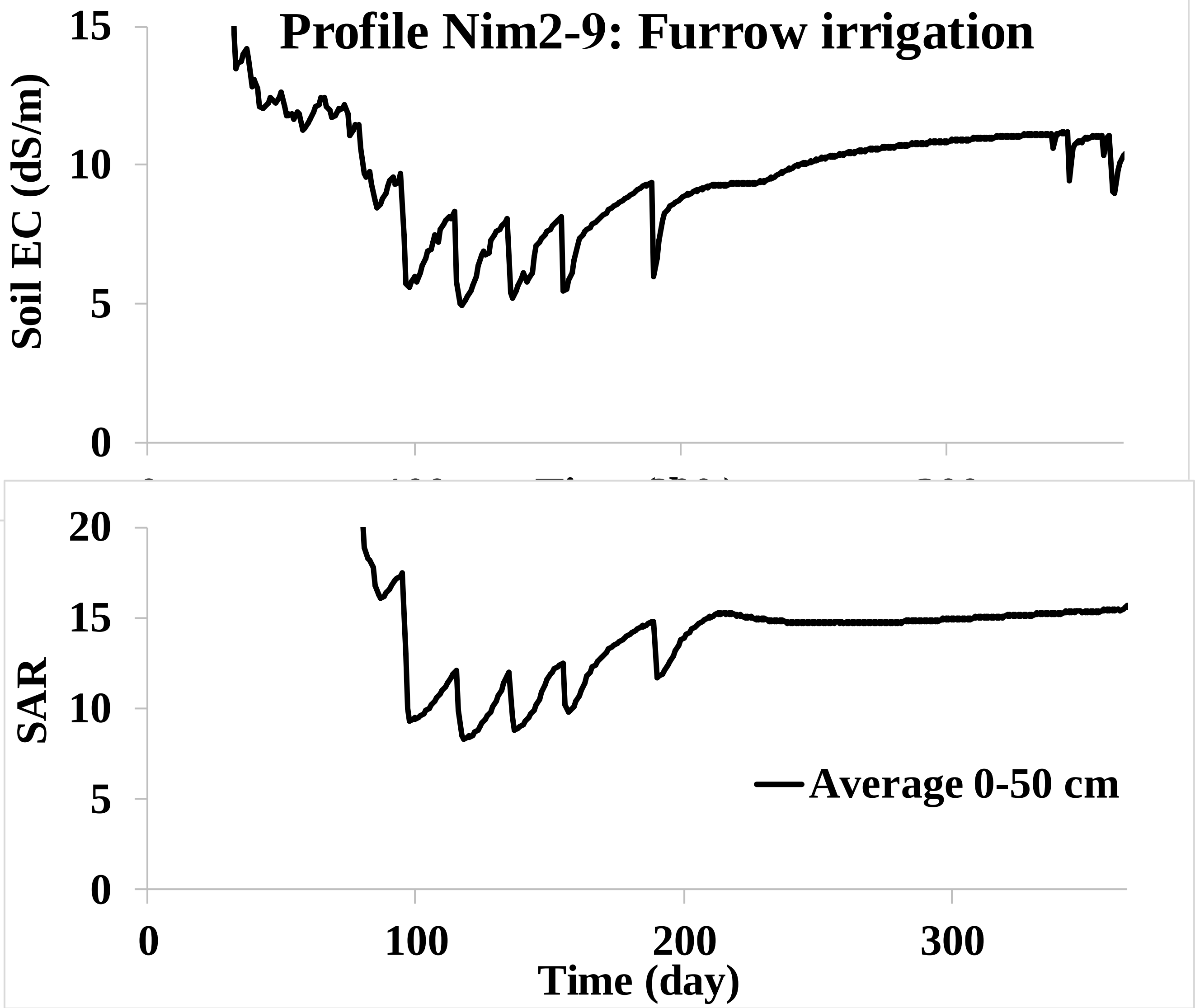
Obs_Node	10/22/2024 11:03 ...	OUT File	57 KB
Obs_Node_Ch	10/22/2024 11:03 ...	OUT File	154 KB
PROFILE	10/22/2024 10:35 ...	DAT File	11 KB
Run_Inf	10/22/2024 11:03 ...	OUT File	38 KB
SELECTOR.IN	10/22/2024 10:35 ...	IN File	5 KB
Solid	10/22/2024 11:03 ...	OUT File	393 KB
T_Level	10/22/2024 11:03 ...	OUT File	109 KB





Food and Agriculture Organization of the United Nations

Thank you for your attention

International Network of Salt-Affected Soils

Optimization of crop irrigation under the risk of salinization using agrohydrological tools

22 October – 29 October – 12 November 2024

GLOBAL SOIL PARTNERSHIP

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