Numerical Modeling of Vadose Zone Processes

(with focus on HYDRUS Software Packages)

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(with contributions from)

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Outline

- **Modeling**
  - -> Scientific Modeling
    - -> Mathematical Modeling
      - -> Numerical Modeling
        - -> Modeling of Vadose Zone Processes

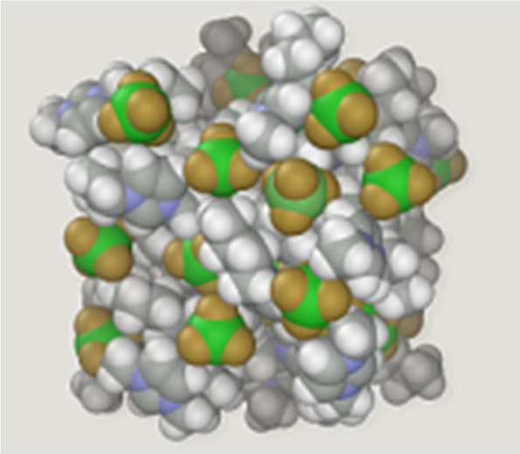
- **HYDRUS** Family of Models and Modules:

- HP1/HP2	- general biogeochemical module
- UnsatChem	- transport of major ions
- Wetland	- C and N processes
- DualPerm	- preferential flow and transport
- Fumigants	- transport of fumigants
- C-Ride	- colloid-facilitated solute transport

Modeling

The process of creating abstract or conceptual models

- **Sculpting** - to create a form from a substance such as clay
- **Fashion Modeling** - to display objects (clothing) for others to see
- **Molecular Modeling** - to mimic the behavior of molecules
- **Modeling Psychology** - a type of behavior learned through observation of others demonstrating the same behavior
- **Physical Models** - to make a miniature model of an technical artifact
- **Scientific Modeling** - the process of creating abstract or conceptual models and their use in the creation of predictive statements.

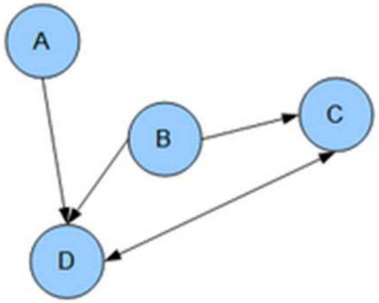


Scientific Modeling

Scientific Modeling is the process of generating various **abstract**, **physical**, **graphical**, **conceptual**, and/or **mathematical** models.

A **Scientific Model** is a **simplified** abstract view of a complex reality, in which empirical objects, phenomena, and physical processes are represented in a logical way by graphical objects, abstract ideas, or mathematical equations.

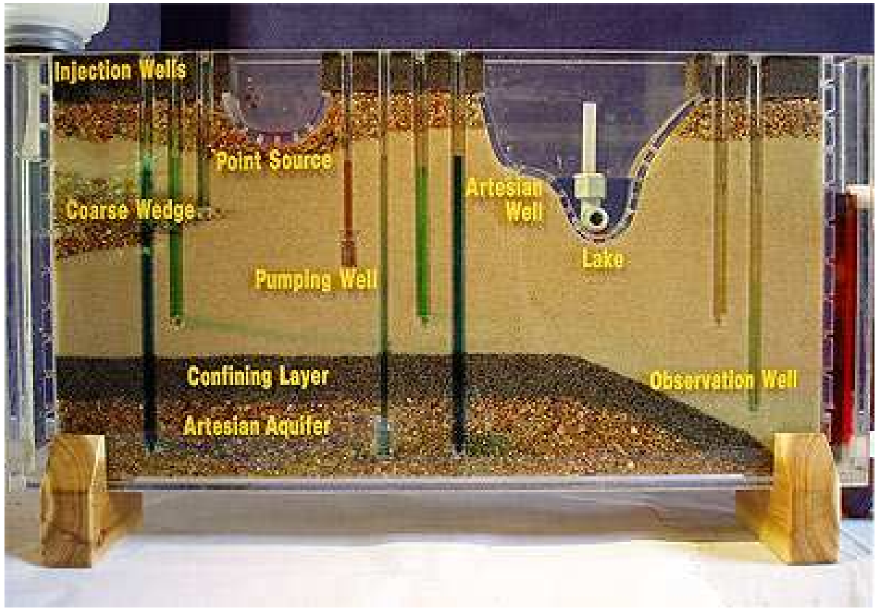
A **Graphical Model** is a probabilistic model, in which a graph denotes the conditional dependence structure between random variables.



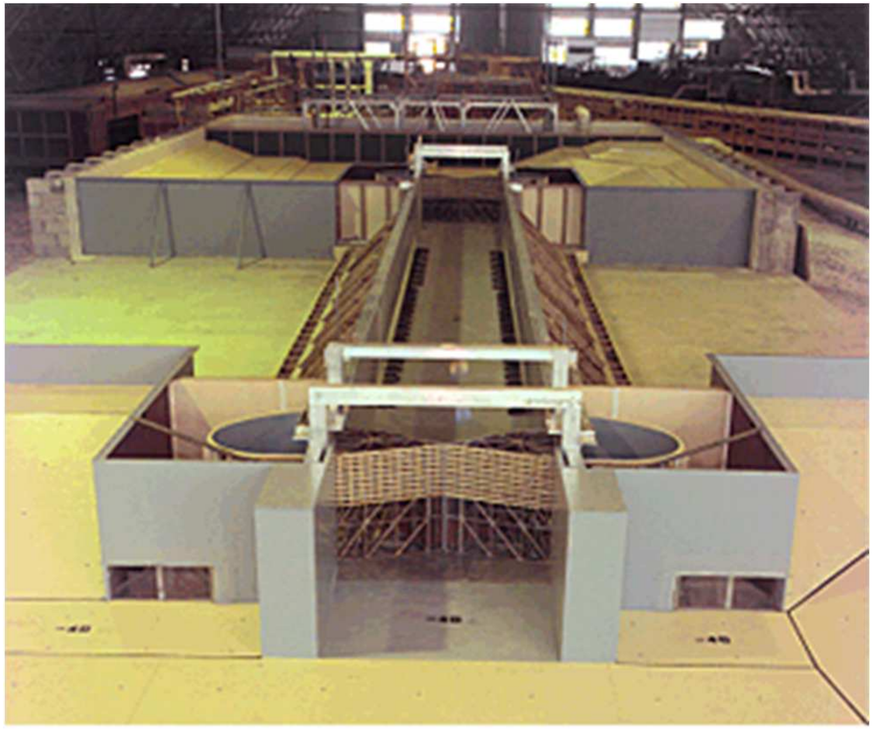
An example of a graphical model

Physical Models in Hydrology

Mostly used before the development and wide use of numerical hydrological models.



Example of a Physical Groundwater Model
Photo Credit: West Virginia Conservation Agency



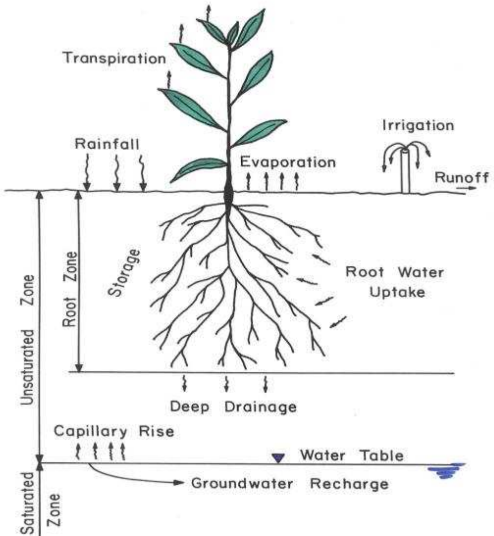
Dry bed view of Type 1 physical model
looking from lakeside to riverside.

Conceptual Model

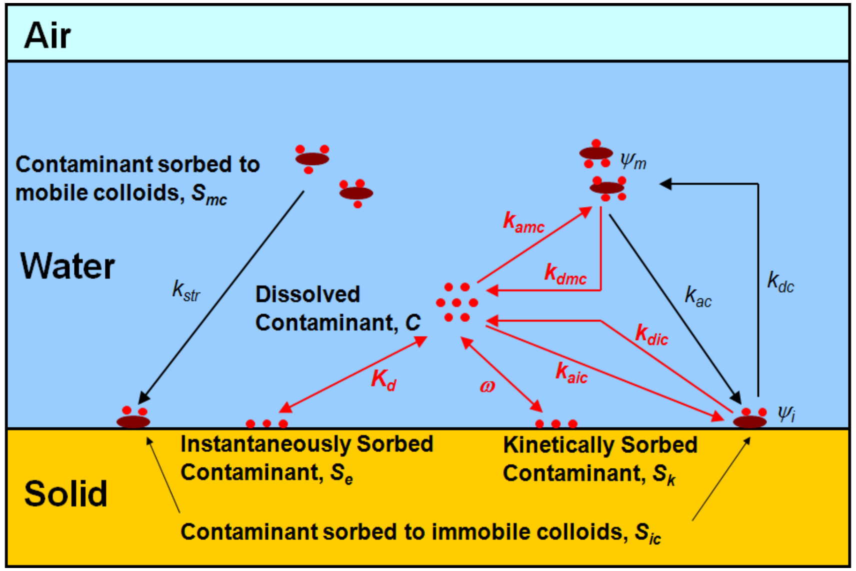
Conceptual Model - formed after a conceptualization process in the mind.

Conceptual Model - used to help us know and understand the subject matter they represent.

Conceptual Modeling is the **activity** of formally describing some aspects of the physical and social world around us for the purposes of understanding and communication.



Water flow in the plant-soil-atmosphere system



A colloid-facilitated solute transport

Mathematical Modeling

A Mathematical Model is a description of a physical system using mathematical concepts and language.

Flow and transport processes in the vadose zone are usually described using various partial differential equations.

Water flow, and solute and heat transport in the plant-soil-atmosphere system (HYDRUS-1D)

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

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

Colloid-Facilitated Solute Transport (C-Ride Module)

Mass Balance of Total Contaminant:

$$\frac{\partial \theta C}{\partial t} + \rho \frac{\partial S_e}{\partial t} + \rho \frac{\partial S_k}{\partial t} + \frac{\partial \theta_w C_c S_{mc}}{\partial t} + \rho \frac{\partial S_c S_{ic}}{\partial t} =$$

$$= \frac{\partial}{\partial x}\left(\theta D \frac{\partial C}{\partial x} \right) - \frac{\partial qC}{\partial x} + \frac{\partial}{\partial x}\left(\theta_w S_{mc} D_c \frac{\partial C_c}{\partial x} \right) - \frac{\partial q_c C_c S_{mc}}{\partial x} + R$$

Left-hand side sums the Mass of Contaminant:

- in the liquid phase
- sorbed instantaneously and kinetically to the solid phase
- sorbed to mobile and immobile colloids

Right-hand side considers various Mass Fluxes

- dispersive and advective transport of the dissolved contaminant
- dispersive and advective transport of contaminant sorbed to mobile colloids

and Transformation/Reaction (e.g., degradation).

Analytical Models

Analytical Models represent a classical mathematical approach to solve mathematical equations, leading to an exact solution for a particular problem.

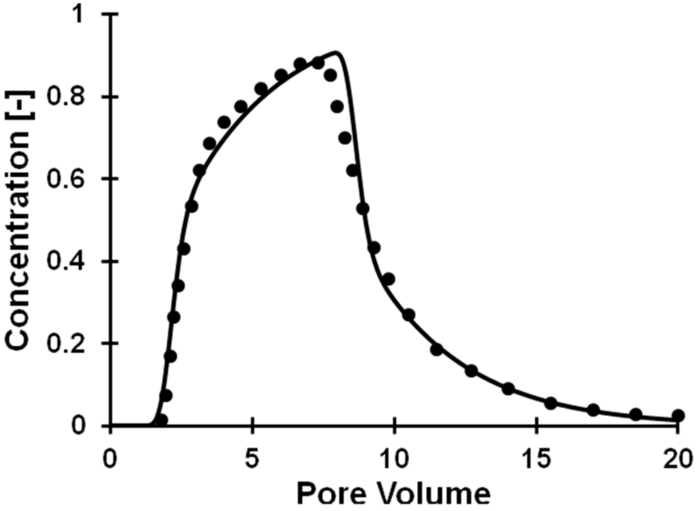
Analytical Models usually result in an explicit equation that states that concentration (or water content or temperature) is equal to a certain value at a particular time and location.

$$c(x,t)=\begin{cases} C_o B(x,t)+C_i A(x,t)+\dfrac{\gamma}{\mu}\left[1-A(x,t)-B(x,t)\right] & 0<t\le t_o \\ C_o\left[B(x,t)-B(x,t-t_o)\right]+C_i A(x,t)+\dfrac{\gamma}{\mu}\left[\left(1-A(x,t)-B(x,t)\right)\right] & t>t_o \end{cases}$$

where

$$A(x,t)=\exp\left(-\frac{\mu t}{R}\right)\left\{1-\frac{1}{2}erfc\left[\frac{Rx-vt}{2\sqrt{DRt}}\right]-\sqrt{\frac{v^2t}{\pi DR}}\exp\left[-\frac{(Rx-vt)^2}{4DRt}\right]\right.$$
$$\left.+\frac{1}{2}\left(1+\frac{vx}{D}+\frac{v^2t}{DR}\right)\exp\left(\frac{vx}{D}\right)erfc\left[\frac{Rx+vt}{2\sqrt{DRt}}\right]\right\}$$

$$B(x,t)=\frac{v}{u+v}\exp\left[\frac{(v-u)x}{2D}\right]erfc\left[\frac{Rx-ut}{2\sqrt{DRt}}\right]-\frac{v}{u-v}\exp\left[\frac{(v+u)x}{2D}\right]erfc\left[\frac{Rx+ut}{2\sqrt{DRt}}\right]$$
$$+\frac{v^2}{2\mu D}\exp\left(\frac{vx}{D}-\frac{\mu t}{R}\right)erfc\left[\frac{Rx+vt}{2\sqrt{DRt}}\right]$$

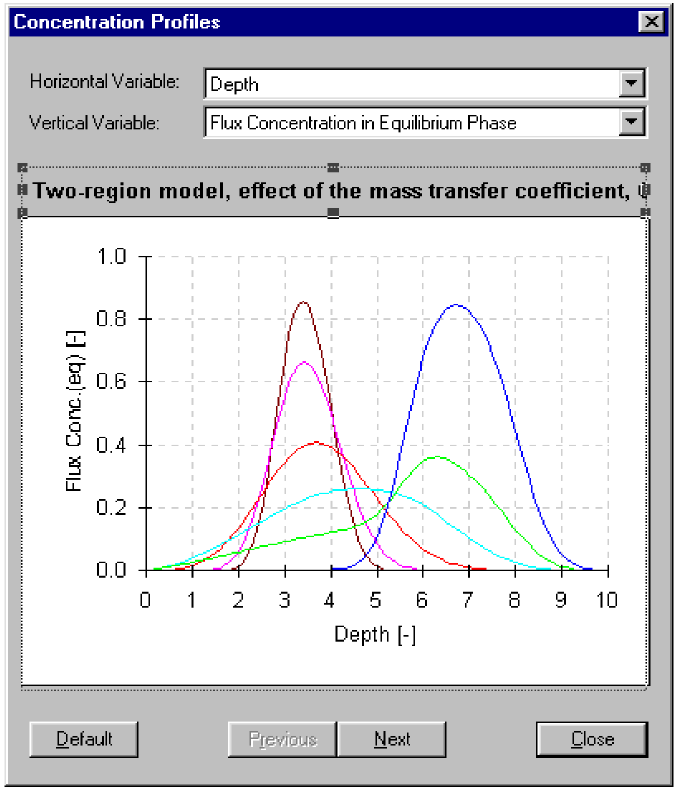


Observed (circles) and fitted (solid line) breakthrough curves for boron transport through a 30 cm long soil column filled with Glendale clay loam (van Genuchten, 1974).

STANMOD

Computer Software for Evaluating Solute Transport in Porous Media Using Analytical Solutions of the Convection-Dispersion Equation

J. Šimůnek, M. Th. van Genuchten, M. Šejna, N. Toride, and F. J. Leij



Horizontal Variable: Depth

Vertical Variable: Flux Concentration in Equilibrium Phase

Two-region model, effect of the mass transfer coefficient,

A powerful and very versatile Windows-based software package.

One-Dimensional Transport Models:

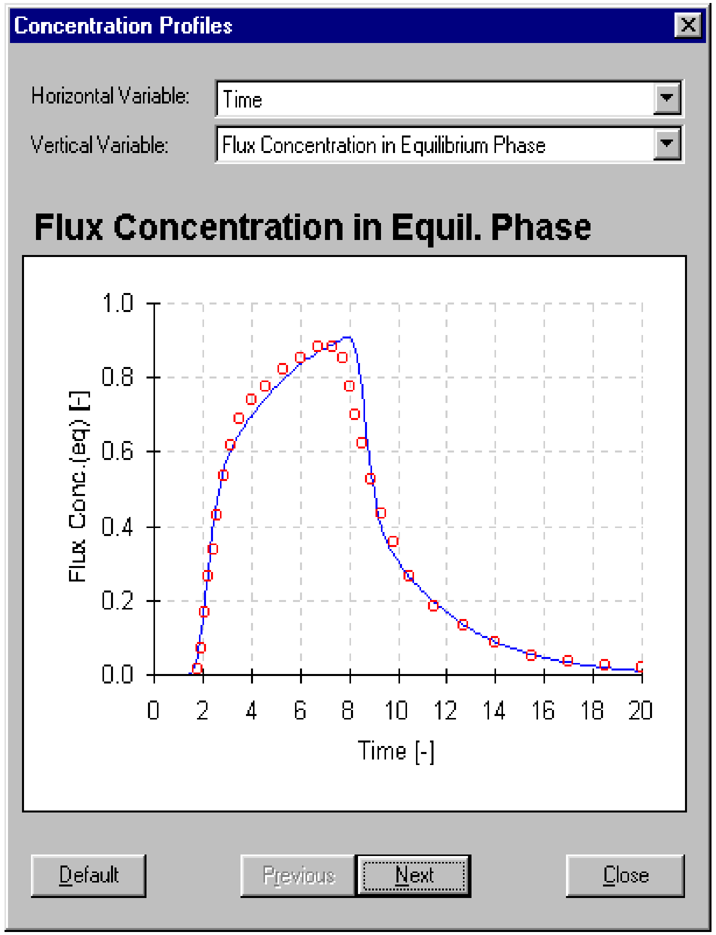
CFITM	**[*van Genuchten*, 1980]**
CFITIM	**[*van Genuchten*, 1981]**
CHAIN	**[*van Genuchten*, 1985]**
CXTFIT2	**[*Toride et al.*, 1995]**
SCREEN	**[*Jury et al.*, 1987]**

Two/Three-Dimensional Transport Models:

3DADE	**[*Leij and Bradford*, 1994]**
N3DADE	**[*Leij and Toride*, 1995]**

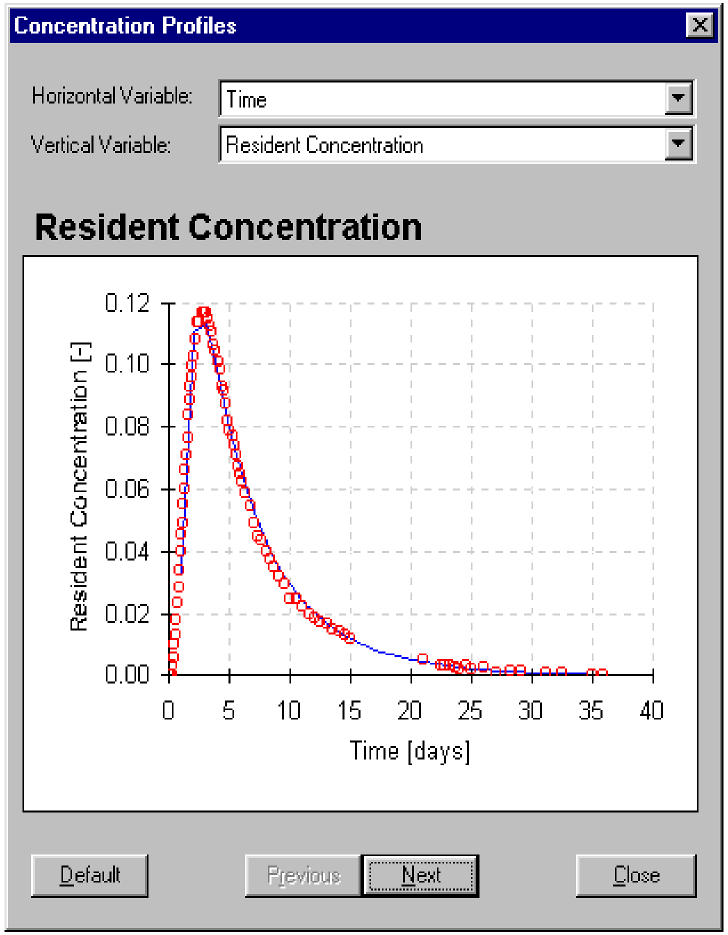
STANMOD (1D Applications)

Inverse Analysis



Horizontal Variable: Time

Vertical Variable: Flux Concentration in Equilibrium Phase



Horizontal Variable: Time

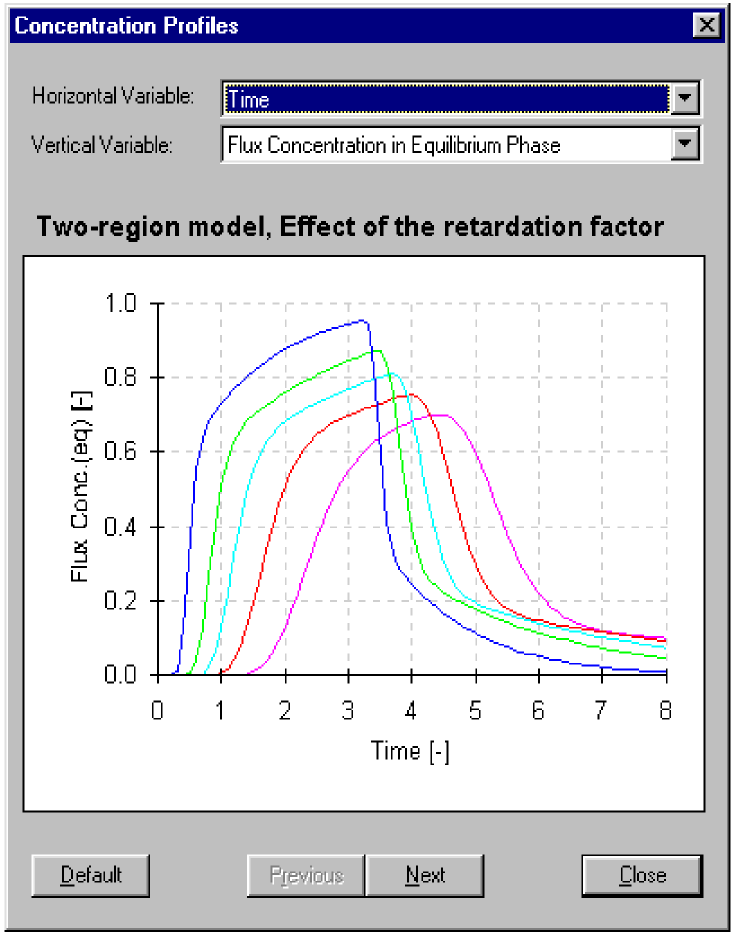
Vertical Variable: Resident Concentration

Deterministic Analysis

Stochastic Analysis

STANMOD (1D Applications)

Direct Analysis



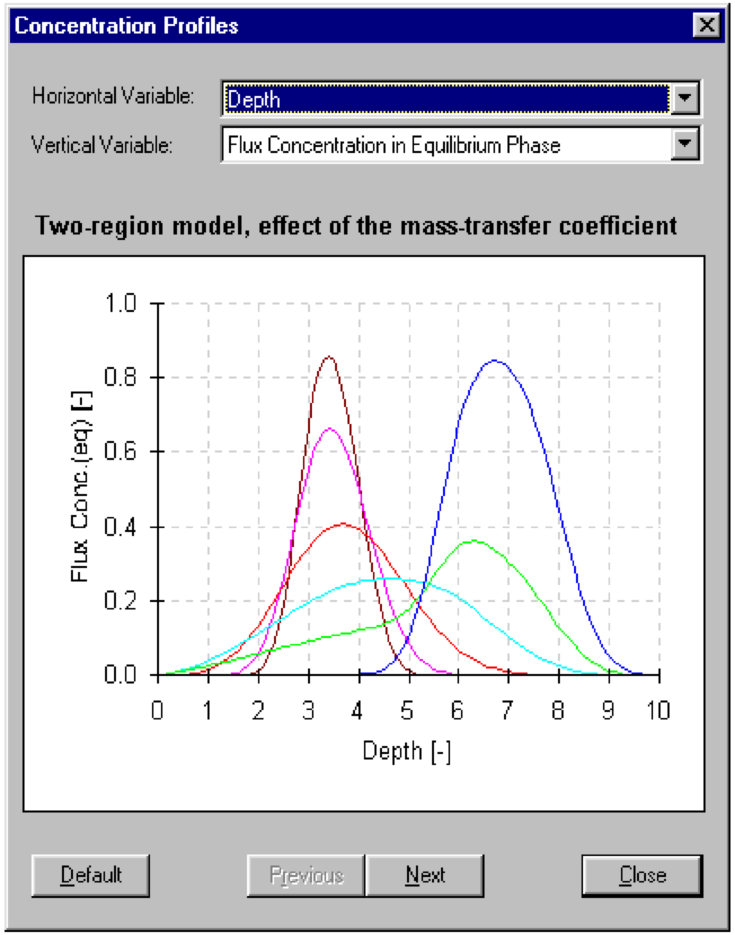
Concentration Profiles

Horizontal Variable: Time

Vertical Variable: Flux Concentration in Equilibrium Phase

Two-region model, Effect of the retardation factor

Retardation Factor



Concentration Profiles

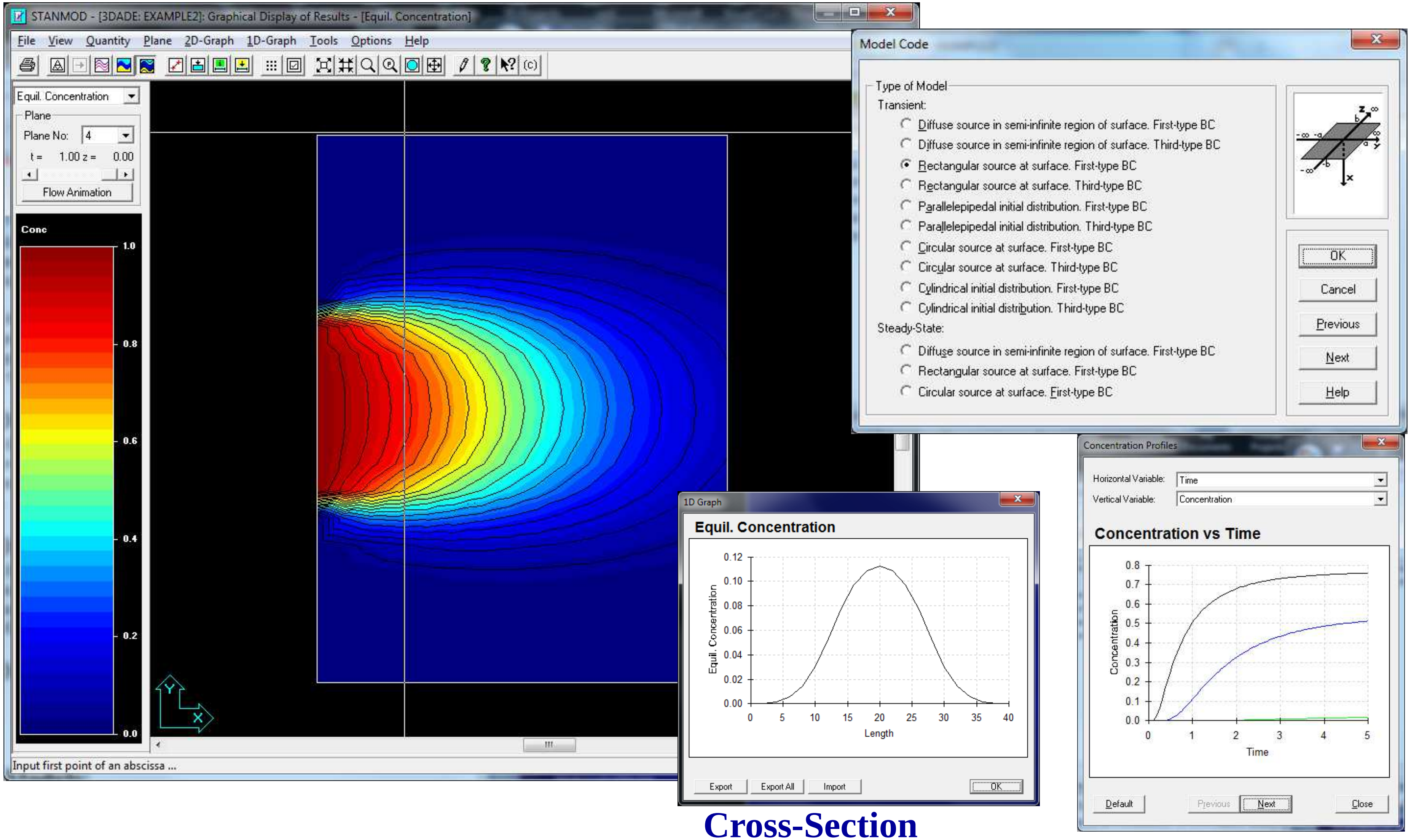
Horizontal Variable: Depth

Vertical Variable: Flux Concentration in Equilibrium Phase

Two-region model, effect of the mass-transfer coefficient

Mass Transfer Coefficient

STANMOD (2D Applications)



Model Code

Type of Model

Transient:

- ○ Diffuse source in semi-infinite region of surface. First-type BC
- ○ Diffuse source in semi-infinite region of surface. Third-type BC
- ● Rectangular source at surface. First-type BC
- ○ Rectangular source at surface. Third-type BC
- ○ Parallelepipedal initial distribution. First-type BC
- ○ Parallelepipedal initial distribution. Third-type BC
- ○ Circular source at surface. First-type BC
- ○ Circular source at surface. Third-type BC
- ○ Cylindrical initial distribution. First-type BC
- ○ Cylindrical initial distribution. Third-type BC

Steady-State:

- ○ Diffuse source in semi-infinite region of surface. First-type BC
- ○ Rectangular source at surface. First-type BC
- ○ Circular source at surface. First-type BC

Plane No: 4

t = 1.00 z = 0.00

Input first point of an abscissa ...

Horizontal Variable: Time

Vertical Variable: Concentration

Cross-Section

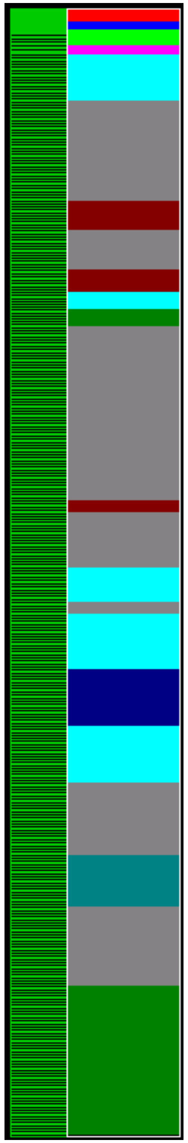
Observation Nodes

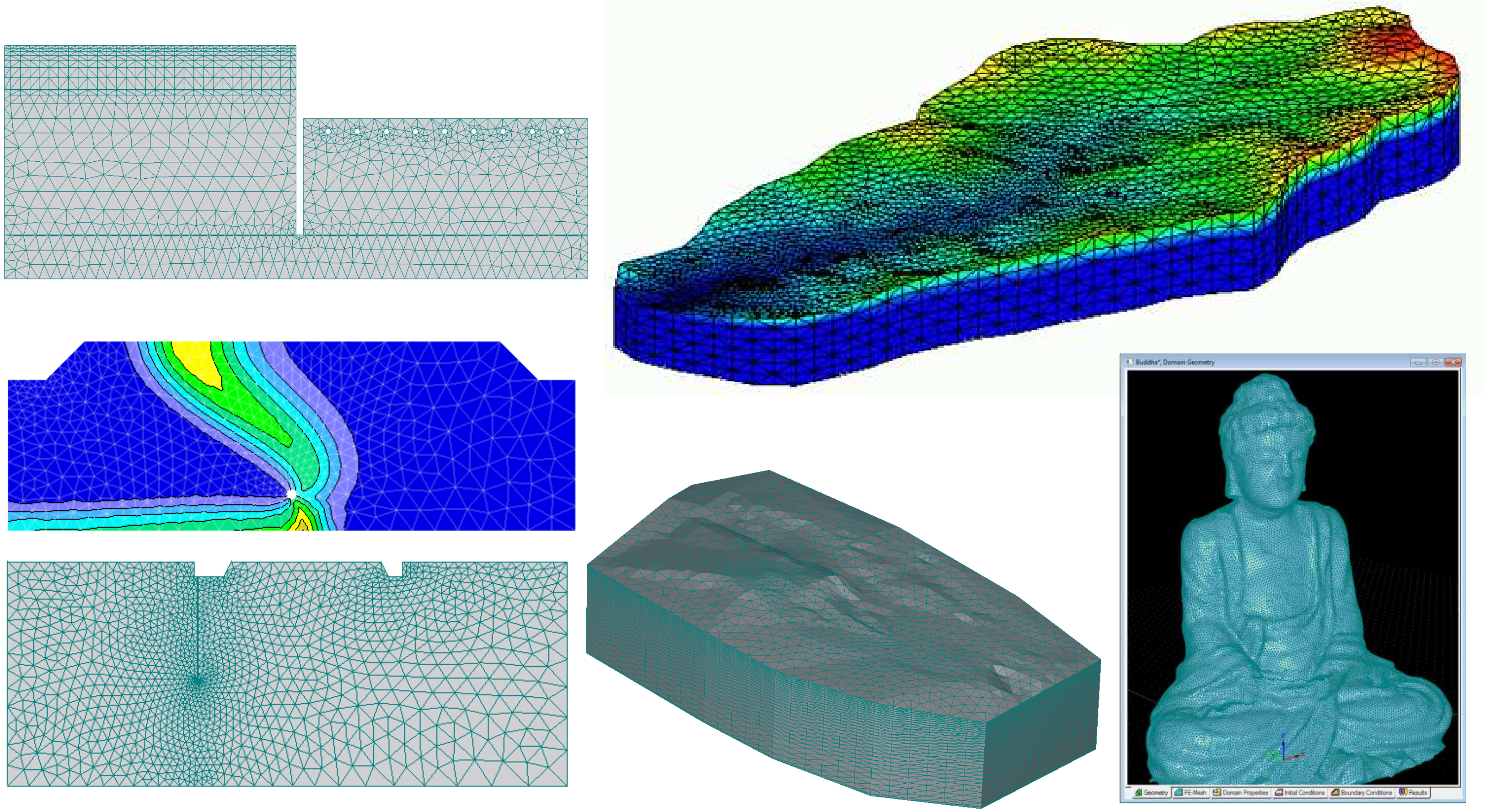
Analytical Models

- **Using Analytical Solutions one can often more easily evaluate interrelationships among parameters and get better insight into how various processes control the basic flow and transport processes.**
- **Analytical Solutions are often used to check the correctness and accuracy of numerical models.**
- **Many Analytical Solutions lead to relatively complicated formulations that include infinite series and/or integrals.**
- **Analytical Solutions can usually be derived only for simplified transport systems involving linearized governing equations, homogeneous soils, simplified geometries of the transport domain, and constant or highly simplified initial and boundary conditions.**
- **For more complex situations, such as for transient water flow or nonequilibrium solute transport with nonlinear reactions, Analytical Solutions are generally not available and/or cannot be derived, in which case Numerical Models must be employed.**

Numerical Modeling

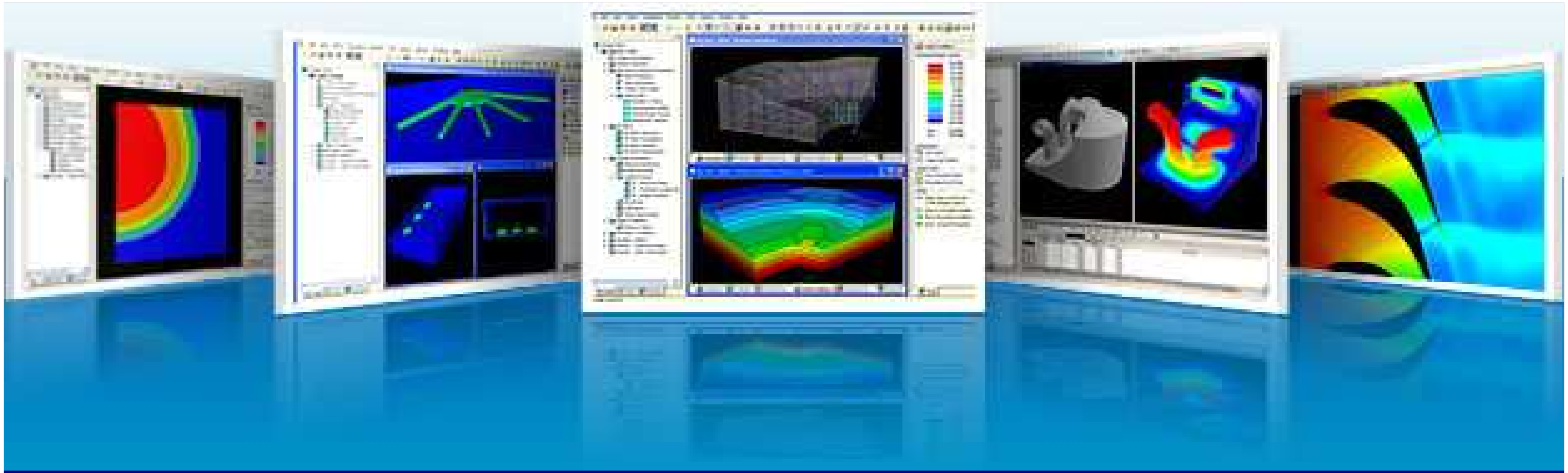
Time and space is divided into small pieces (e.g., finite differences, finite elements, finite volumes) and the governing equations are integrated over these pieces.





Numerical Models

- **Numerical Methods** are superior to **Analytical Methods** in terms of being able to solve practical problems.
- **Numerical Methods** allow users
  - to design complicated geometries that reflect complex natural geologic and hydrologic conditions,
  - to control parameters in space and time,
  - to prescribe realistic initial and boundary conditions, and
  - to implement nonlinear constitutive relationships.
- **Numerical Methods** usually
  - subdivide the time and spatial coordinates into smaller pieces, such as finite differences, finite elements, or finite volumes, and
  - reformulate the continuous form of governing partial differential equations in terms of a system of algebraic eqs.
- In order to obtain solutions at certain times, **Numerical Methods** generally require intermediate simulations (time-stepping) between the initial condition and the points in time for which the solution is needed.

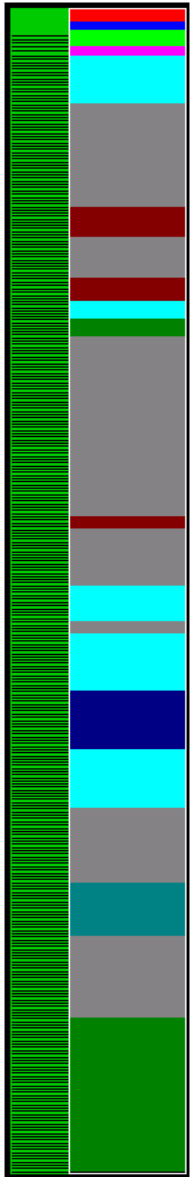


HYDRUS (1D/2D/3D)

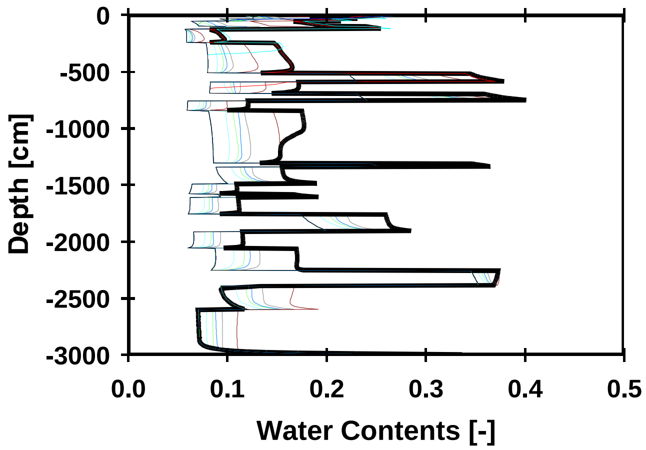
Software for Simulating Water Flow and Solute Transport in One/Two/Three - Dimensional Variably-Saturated Soils Using Numerical Solutions

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

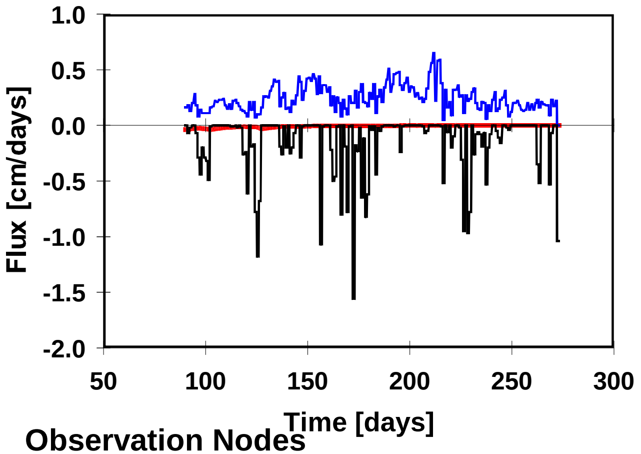
HYDRUS-1D



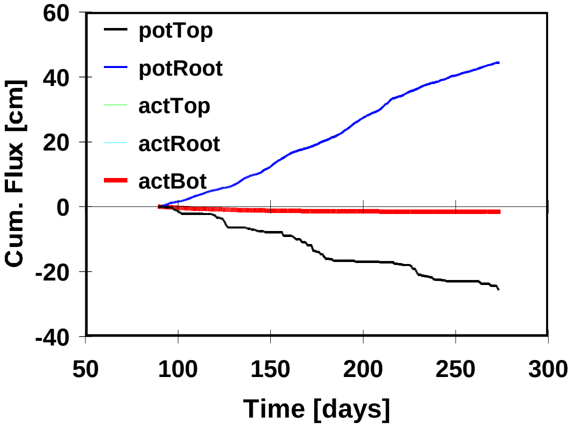
Profile Information



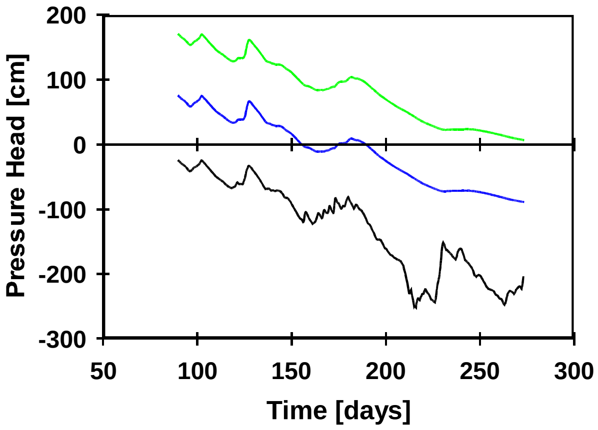
All Fluxes



Cumulative Fluxes



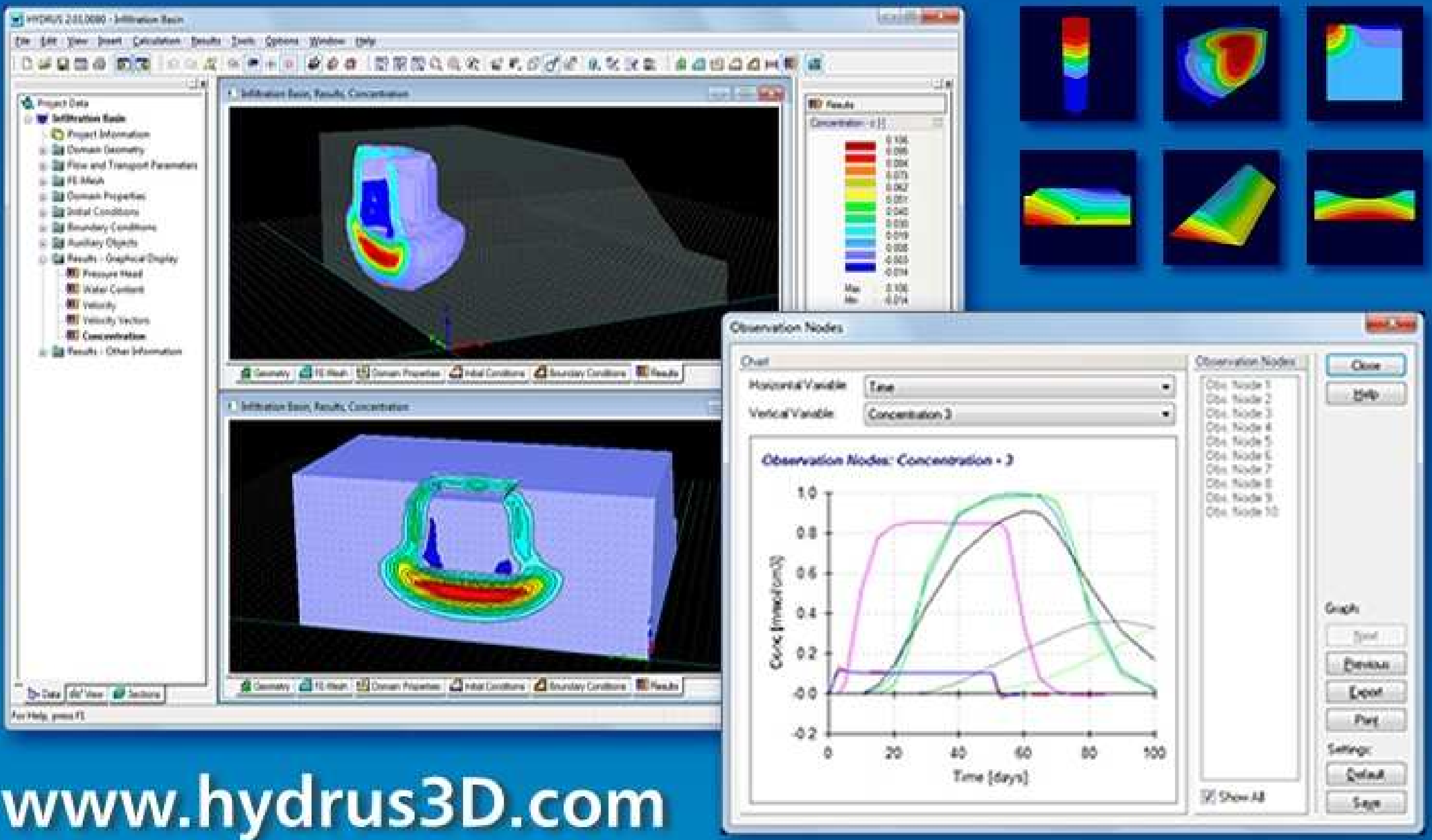
Observation Nodes



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

HYDRUS

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

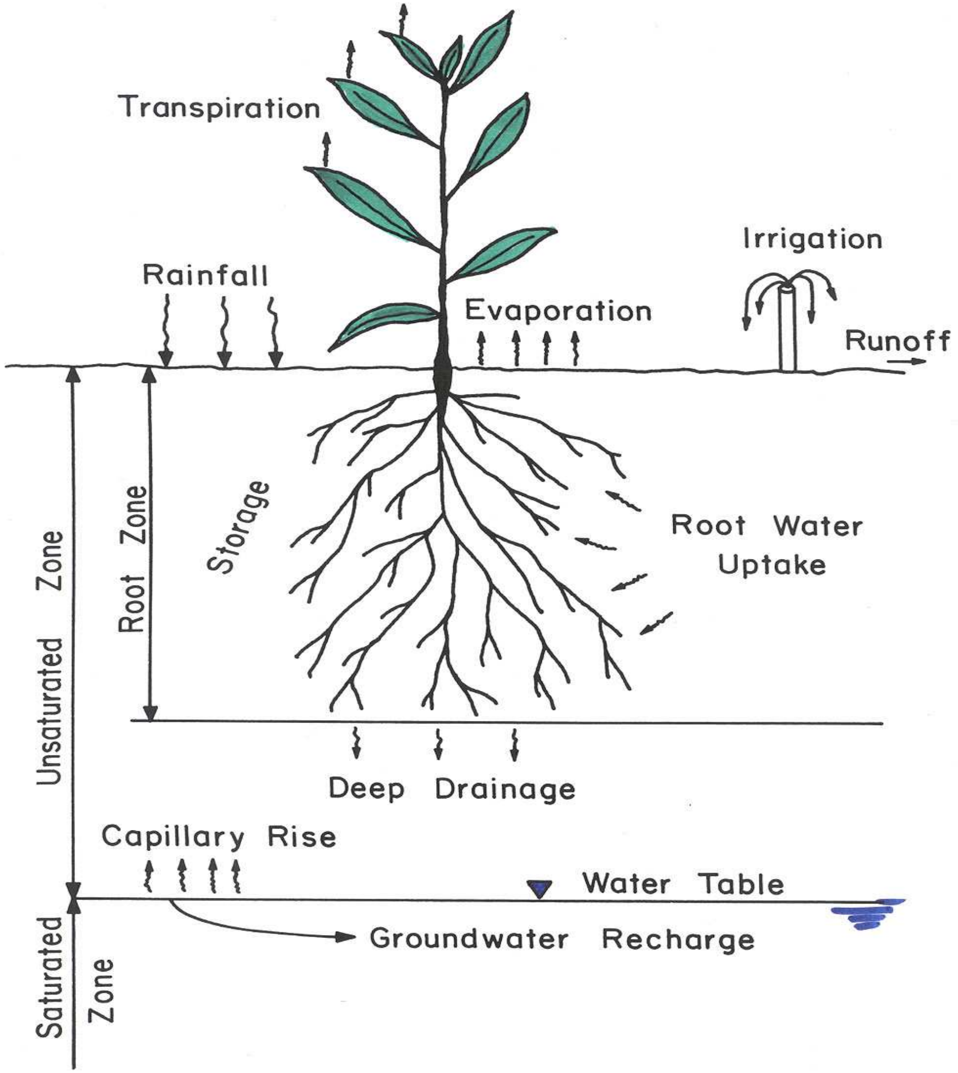


www.hydrus3D.com

Agricultural Applications

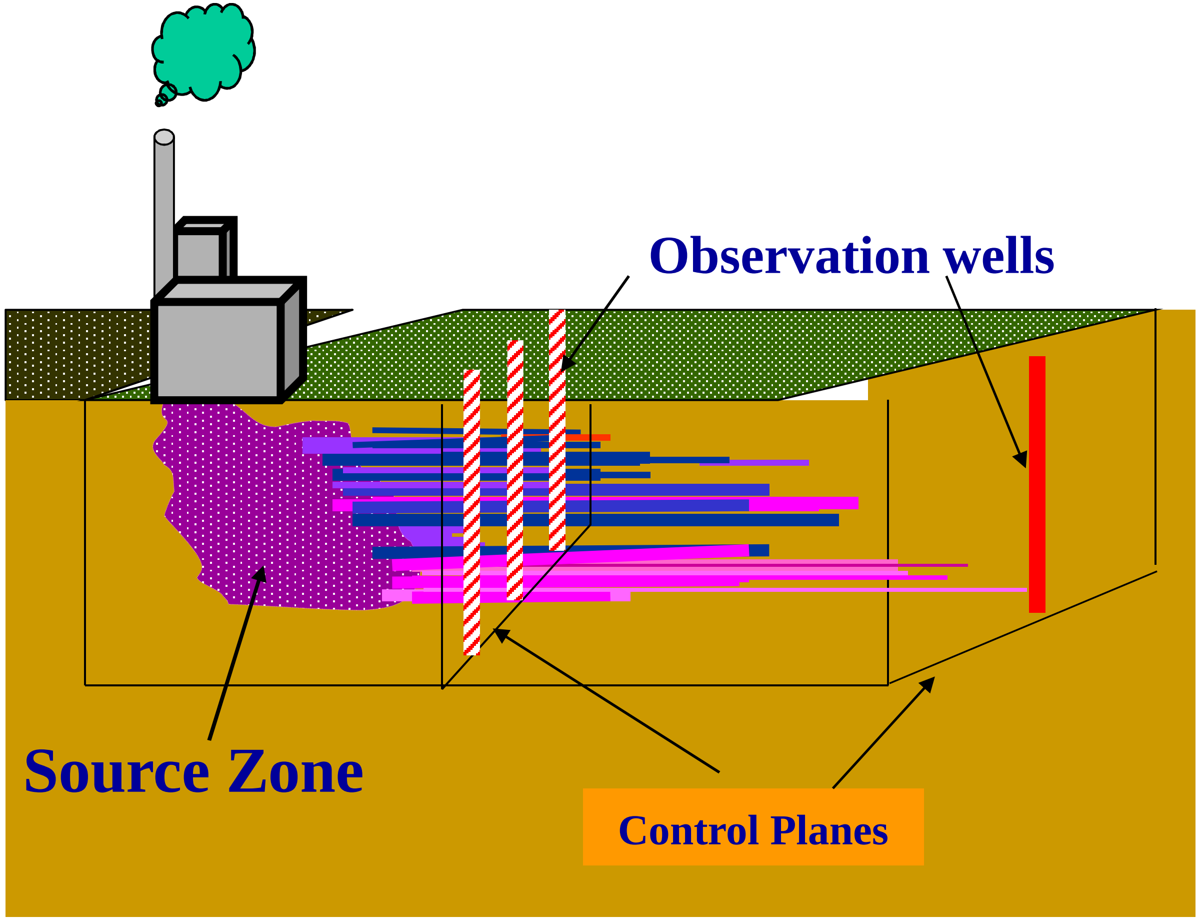
- **Precipitation**
- **Irrigation**
- **Runoff**
- **Evaporation**
- **Transpiration**
- **Root Water Uptake**
- **Capillary Rise**
- **Deep Drainage**

- **Fertilizers**
- **Pesticides**
- **Fumigants**
- **Emerging Pollutants (steroids and hormones, pharmaceuticals)**
- **Colloids**
- **Pathogens**
- **Nanoparticles**



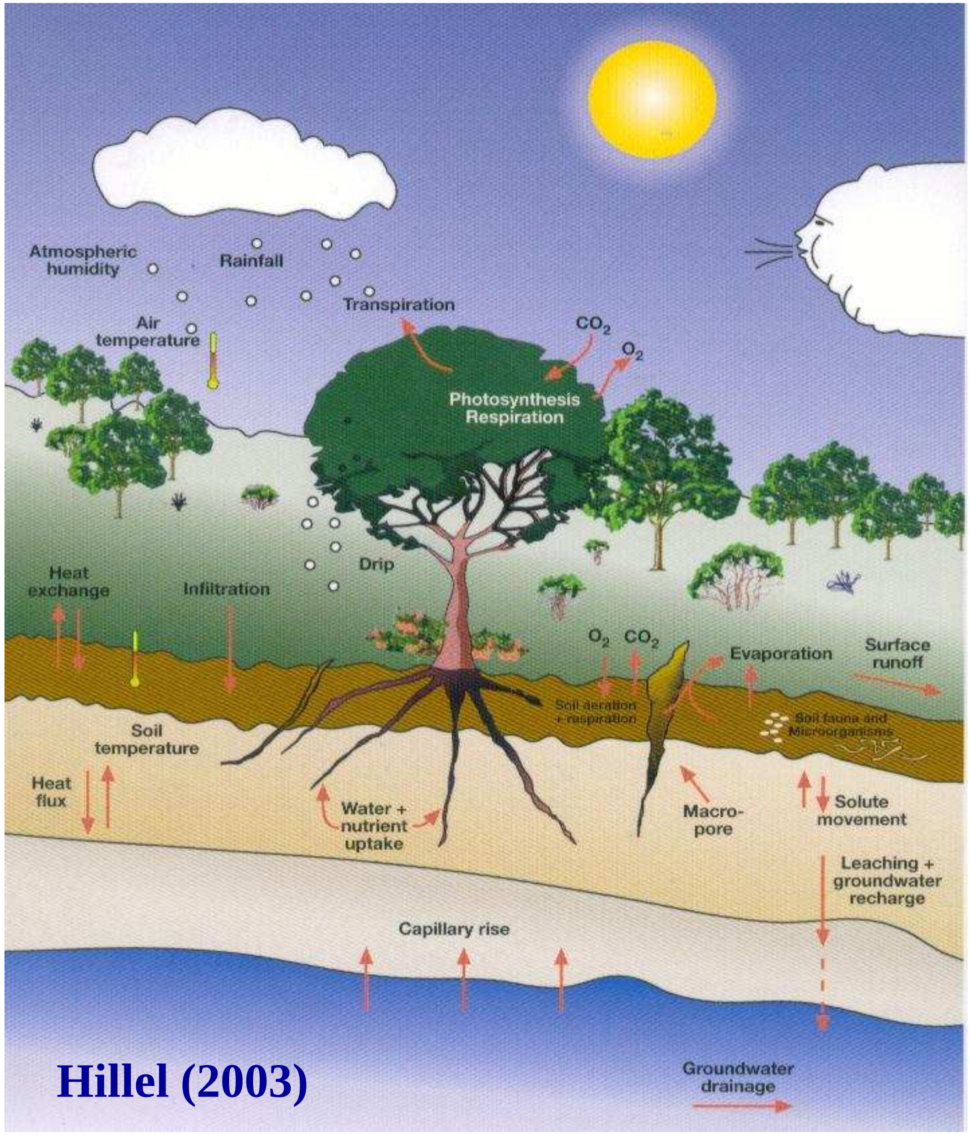
Industrial Applications

- **Industrial Pollution**
- **Municipal Pollution**
- **Landfill Covers**
- **Waste Repositories**
- **Radioactive Waste Disposal Sites**
- **Remediation**
- **Brine Releases**
- **Contaminant Plumes**
- **Seepage of Wastewater from Land Treatment Systems**
- **Emerging Pollutants (gasoline additives, industrial additives, personal hygiene products, flame retardants, explosives, surfactants)**



Environmental Applications

- **Ecological Apps**
- **Heat Exchange and Fluxes (including the Surface Energy Balance)**
- **Carbon Storage and Fluxes**
- **Nutrient Transport**
- **Soil Respiration**
- **Microbiological Processes**
- **Effects of Climate Change**
- **Riparian Systems**
- **Stream-Aquifer Interactions**



Hillel (2003)

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)

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

Heat Movement (Conduction-Dispersion Equation)

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

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)
- **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 interactions 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)**

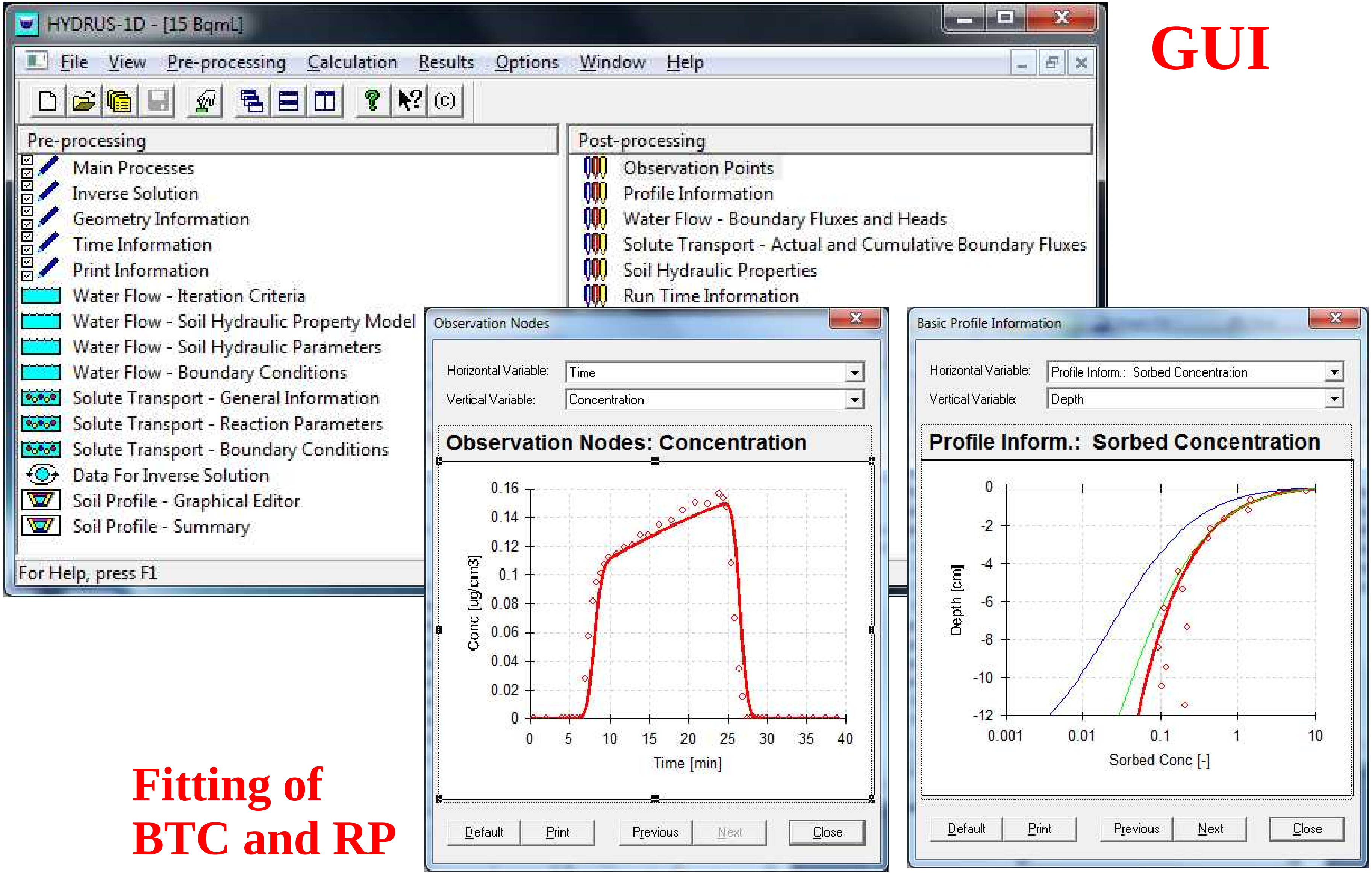
Inverse Optimization **(of flow, transport, and reaction parameters)**

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:** $(NH_2)_2CO$ -> NH_4^+ -> NO_2^- -> 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 HP1/2/3 module)**
- **Processes in Wetlands (the CW2D and CWM1 modules)**
- **Colloid-Facilitated Solute Transport (the C-Ride module)**

HYDRUS-1D
Graphical User Interface

GUI

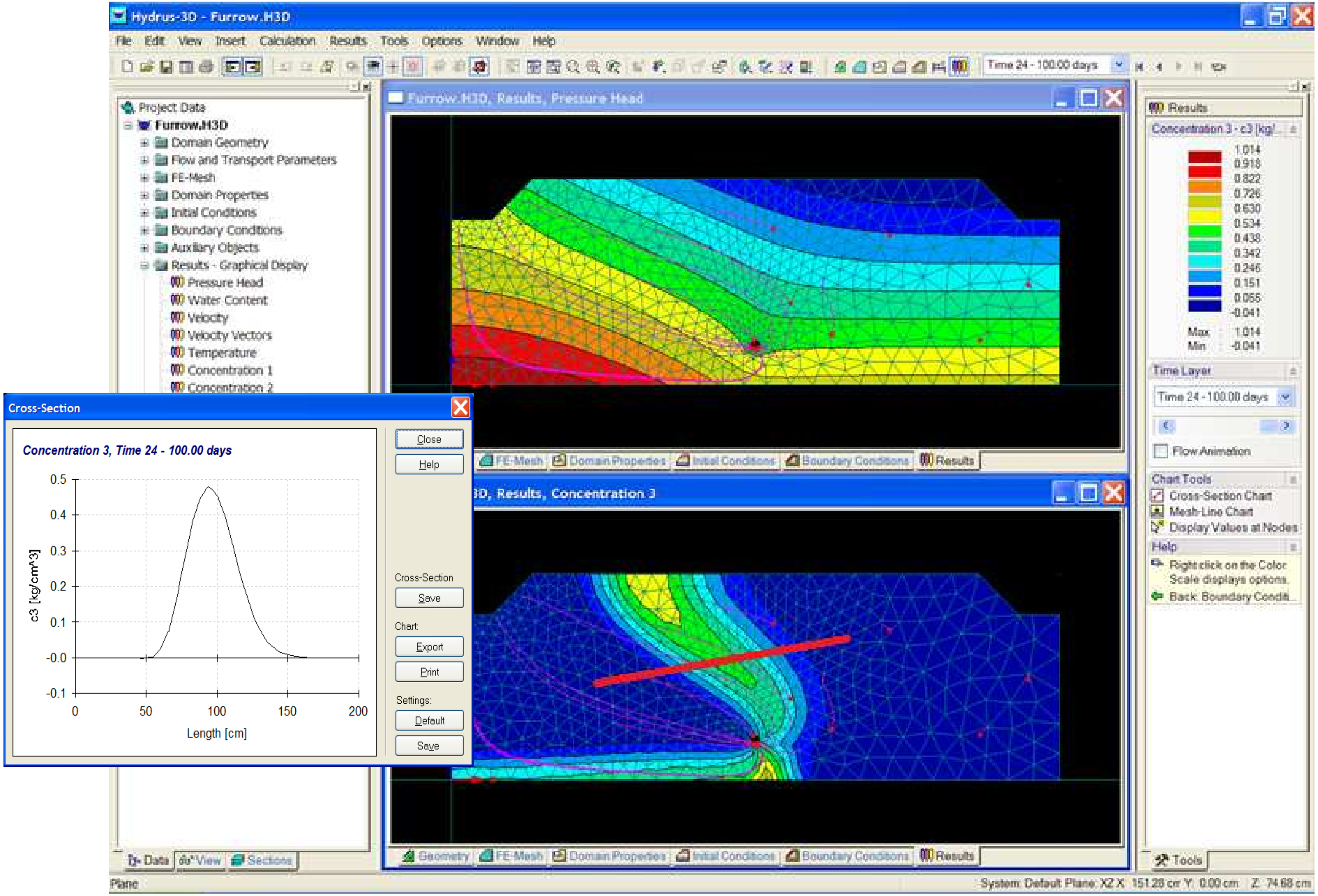


Horizontal Variable: Time
Vertical Variable: Concentration

Horizontal Variable: Profile Inform.: Sorbed Concentration
Vertical Variable: Depth

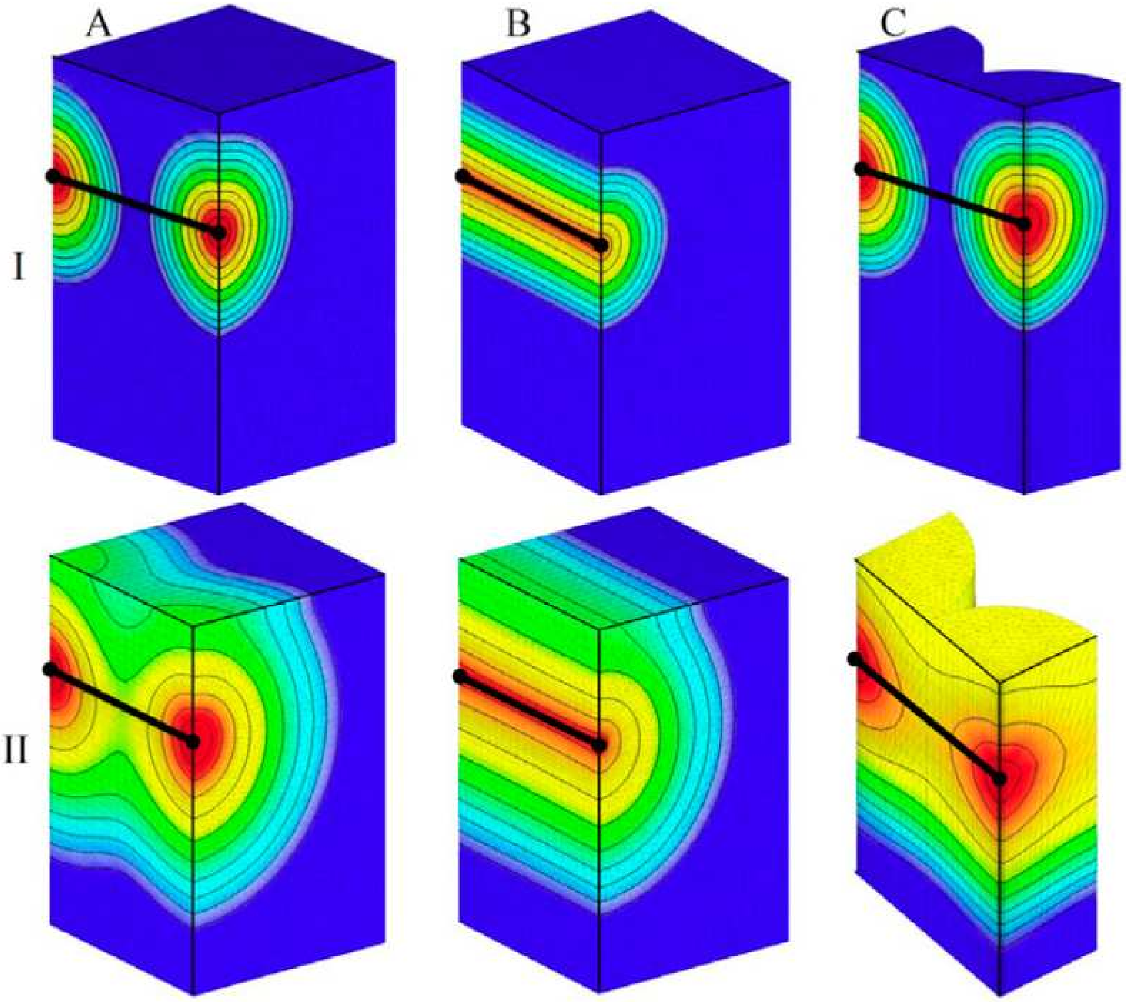
Fitting of BTC and RP

HYDRUS (2D/3D)
Graphical User Interface



System: Default Plane: X2 X: 151.28 cm Y: 0.00 cm Z: 74.68 cm

HYDRUS (2D/3D) - Applications



Subsurface Drip Irrigation System

Soil water content simulated as:

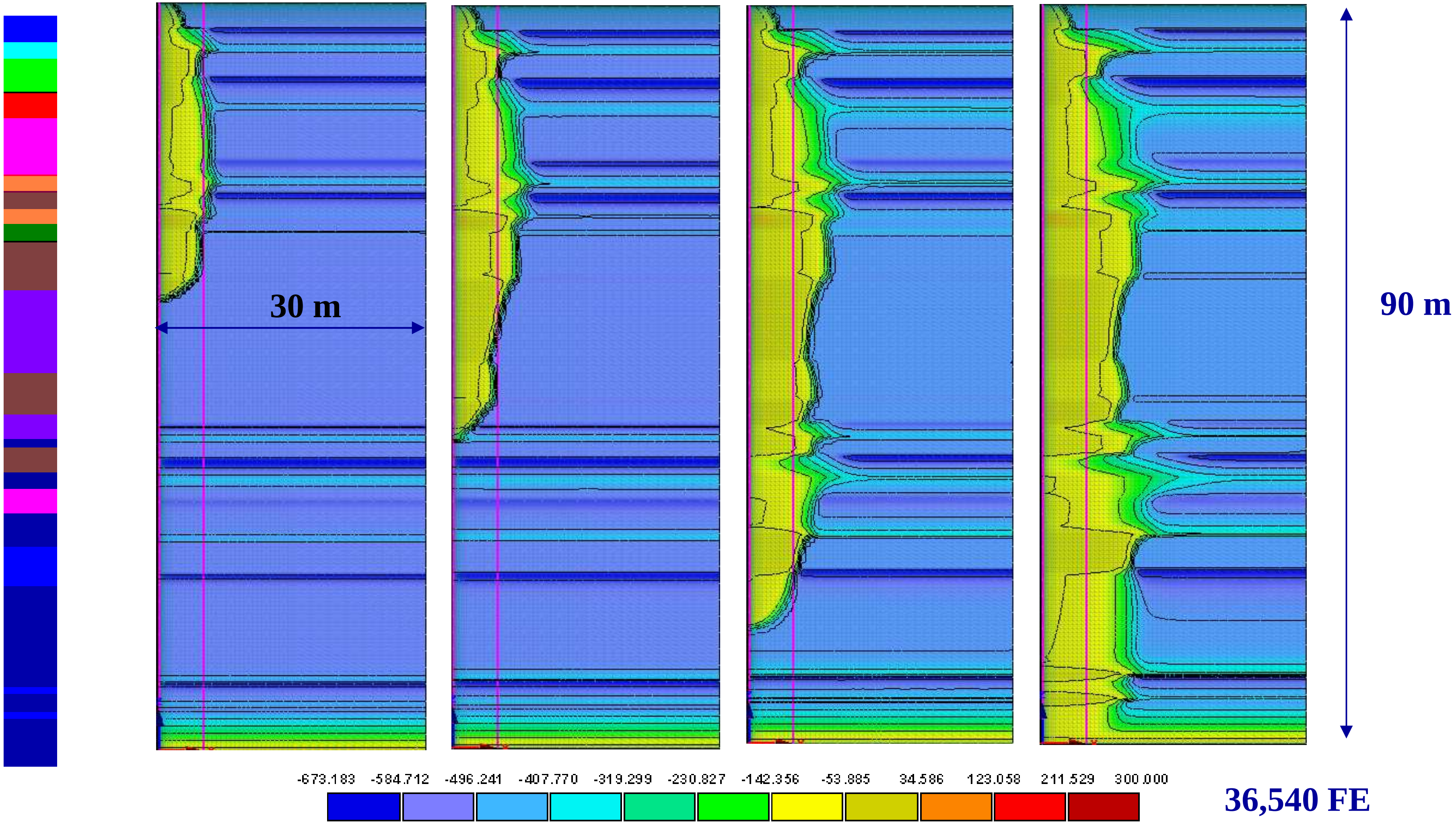
A. **a Three-Dimensional system with multiple point sources**

B. **a Two-Dimensional system with a line source**

C. **An Axisymmetrical two-dimensional system with a point source**

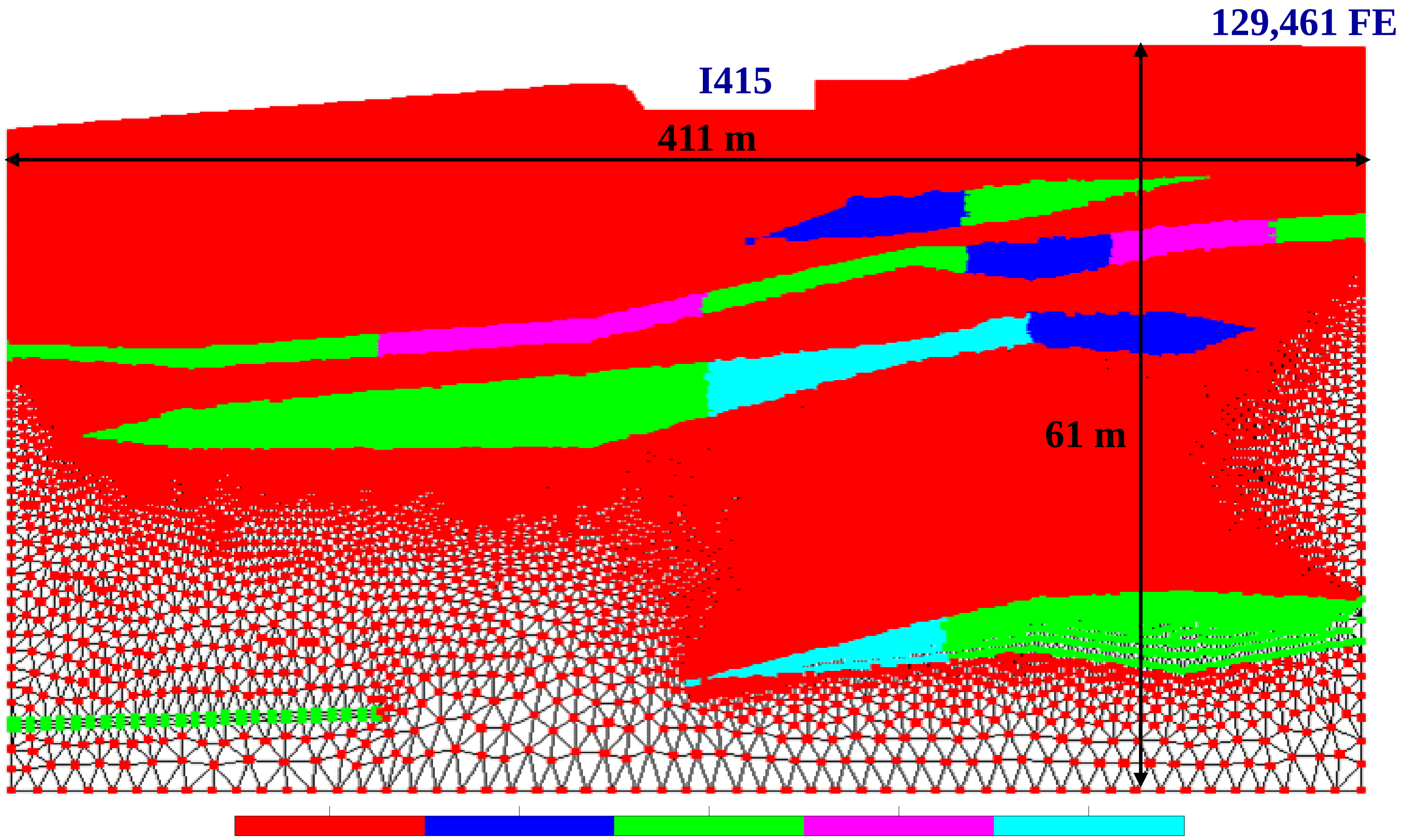
Kandelous, M. M., J. Šimůnek, M. Th. van Genuchten, and K. Malek, Soil water content distributions between two emitters of a subsurface drip irrigation system, *Soil Science Society of America Journal*, *75*(2), 488-497, 2011.

HYDRUS (2D/3D) - Applications



Pressure head profiles after 10, 25, 50, and 100 years.
Leak (2 mm diameter) at the bottom of the Palmdale Reservoir.

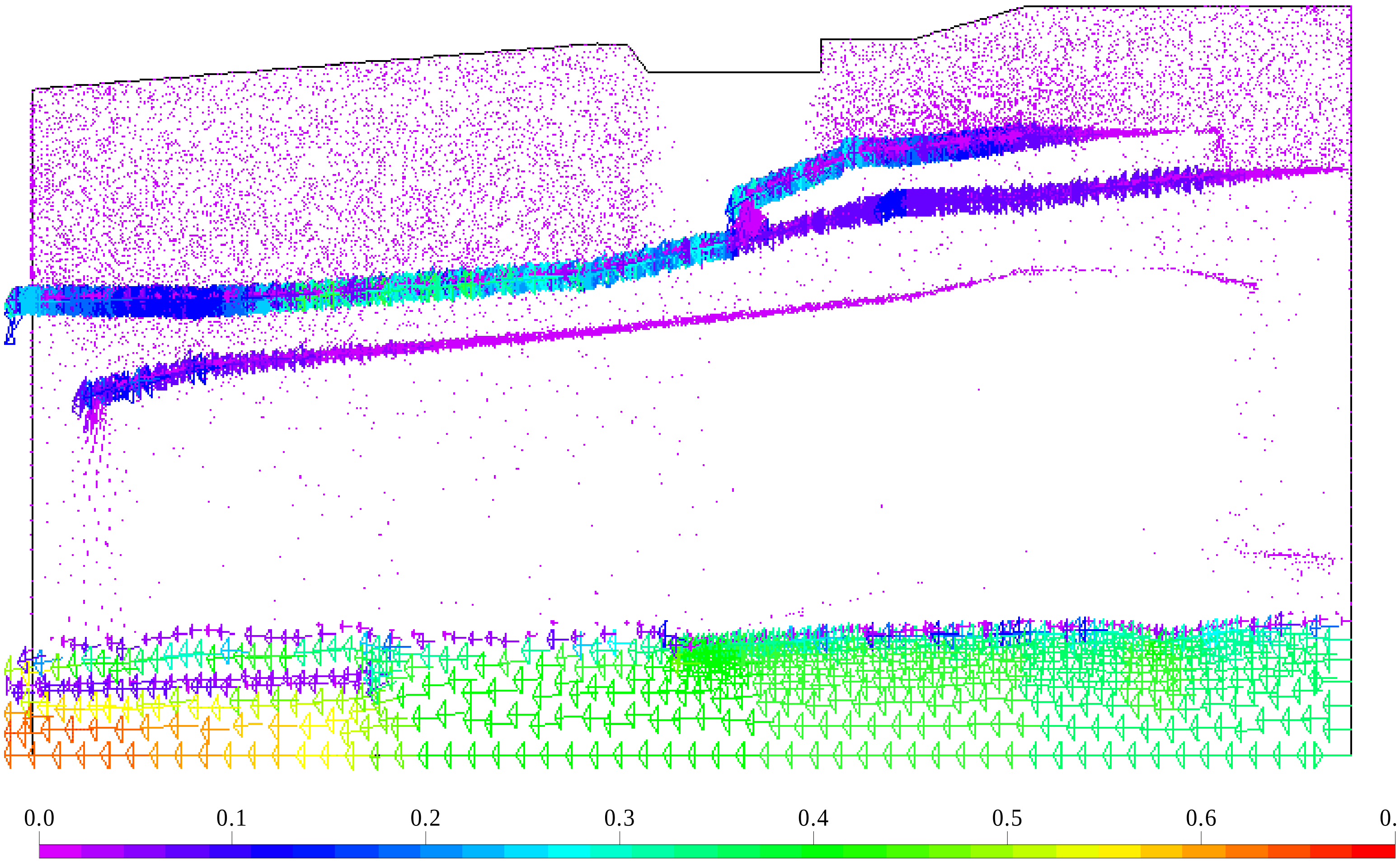
HYDRUS (2D/3D) - Applications



Finite Element Mesh and Material Distribution

A two-dimensional transect, 411 m wide and 61 m deep, with a freeway in the middle

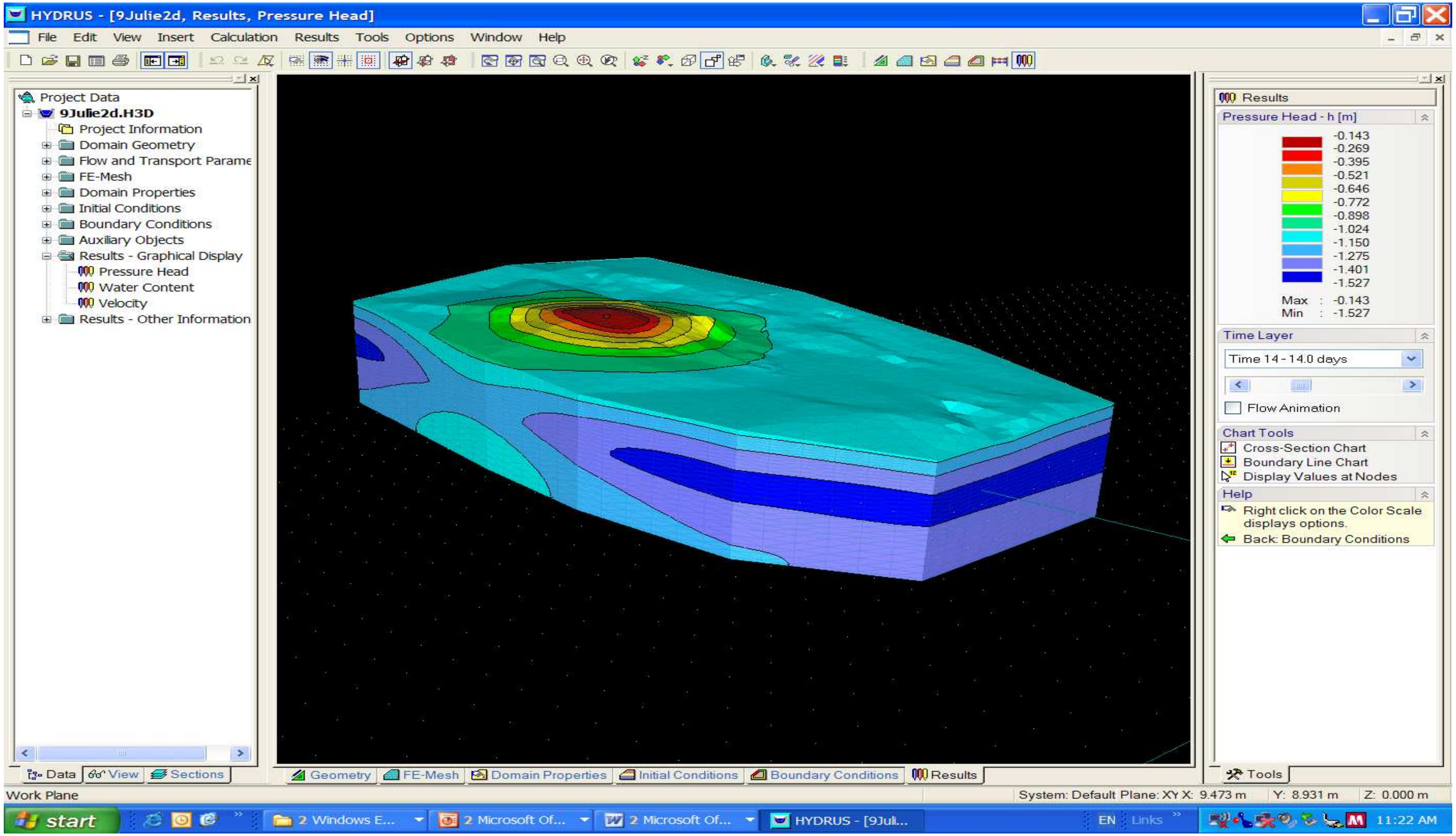
HYDRUS (2D/3D) - Applications



Velocity Vectors

A two-dimensional transect, 411 m wide and 61 m deep, with a freeway in the middle

HYDRUS (2D/3D) - Applications



Pressure Head - h [m]

Max : -0.143
Min : -1.527

Time Layer: Time 14 - 14.0 days

Right click on the Color Scale displays options.

System: Default Plane: XY X: 9.473 m Y: 8.931 m Z: 0.000 m

Pressure Head Distribution
in a Three-Dimensional Transport Domain

HYDRUS (2D/3D) – Transport Domains

HYDRUS Geometries:

A. 2D – Simple

B. 2D – General

C. 3D – Simple

D. 3D – Layered

E. 3D – General

HYDRUS Levels:

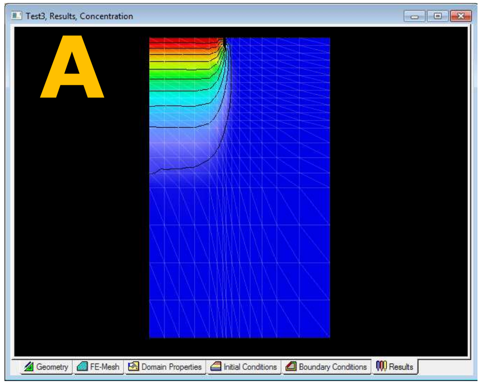
2D – Lite (A)

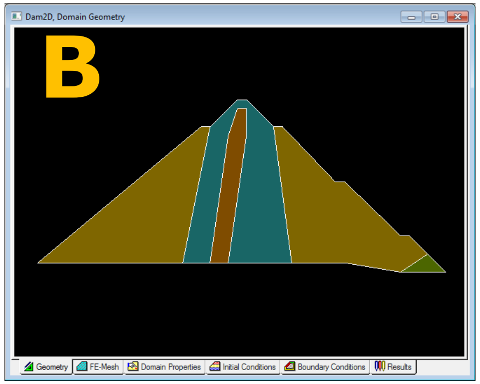
2D – Standard (A+B)

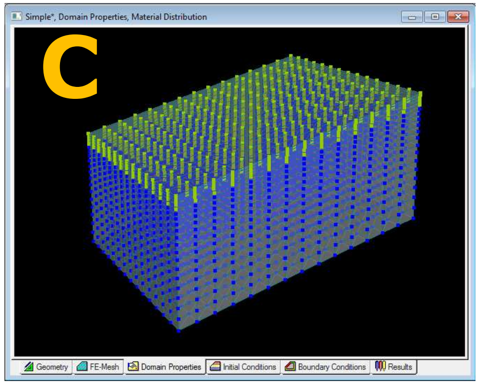
3D – Lite (A+C)

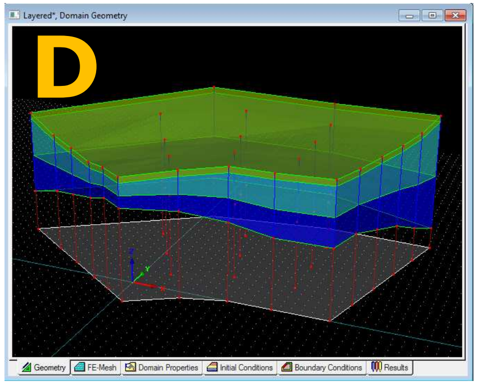
3D – Standard (A+B+C+D)

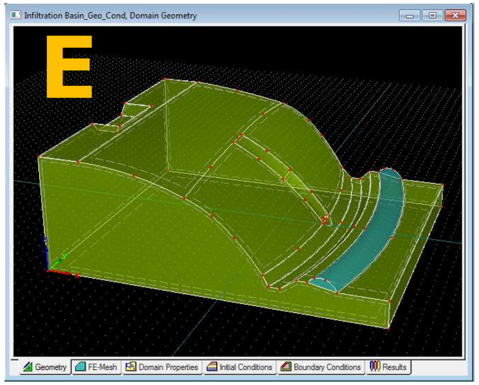
3D – Professional (All)

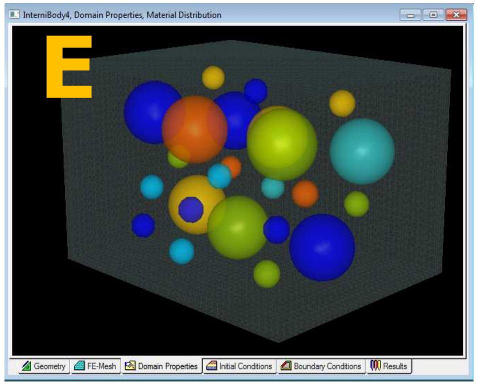






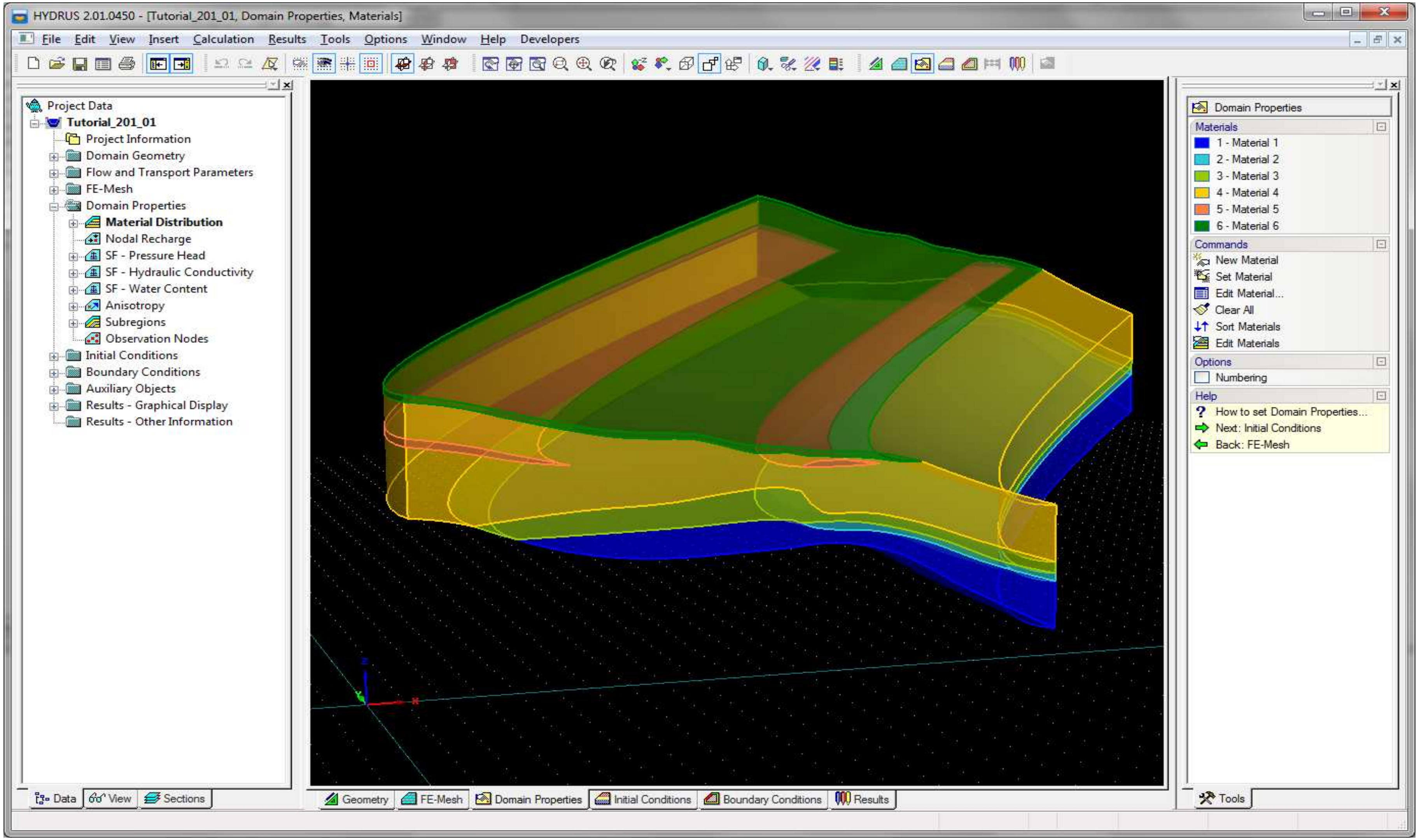






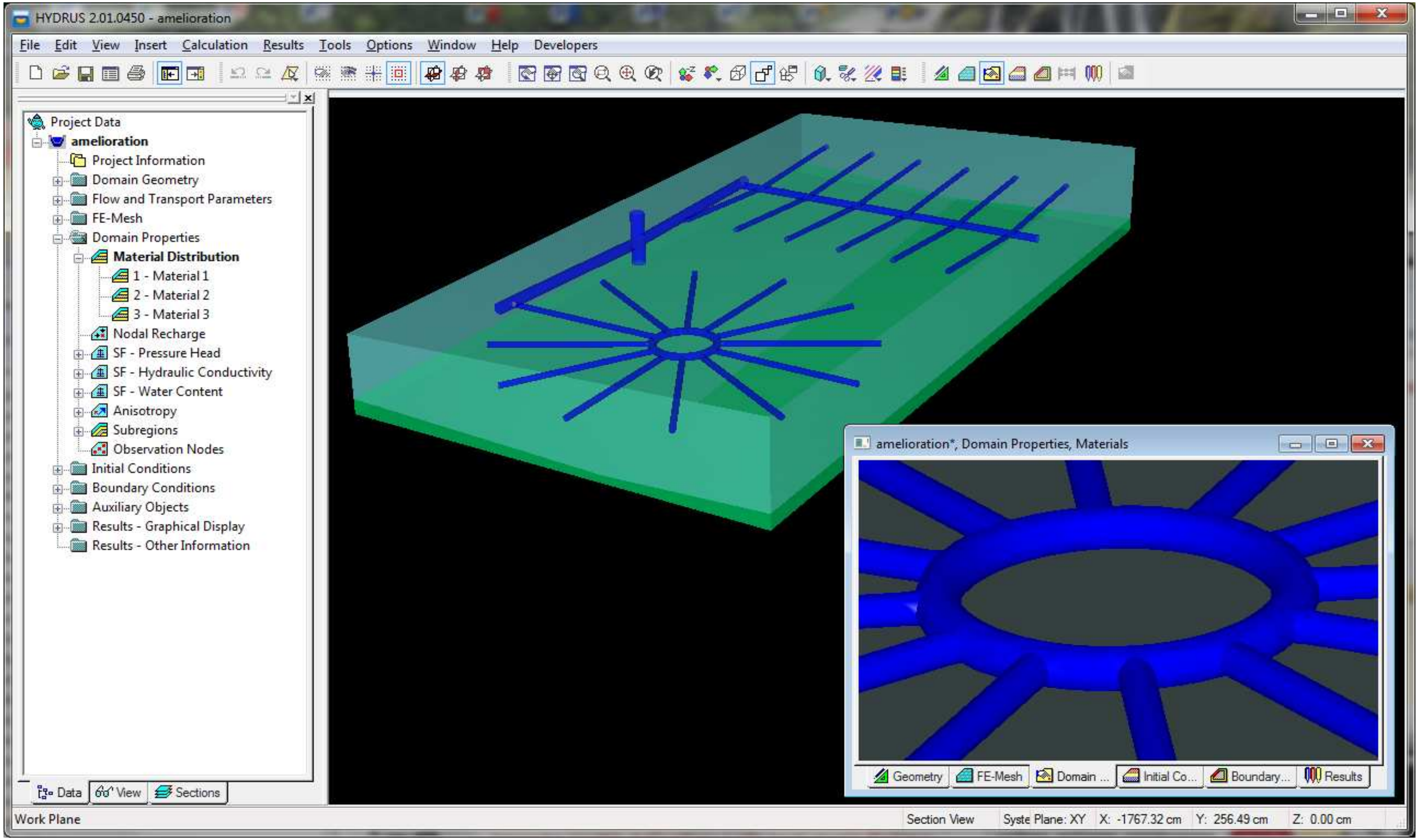
HYDRUS (2D/3D) - Geometries

Discontinuous 3D Layers



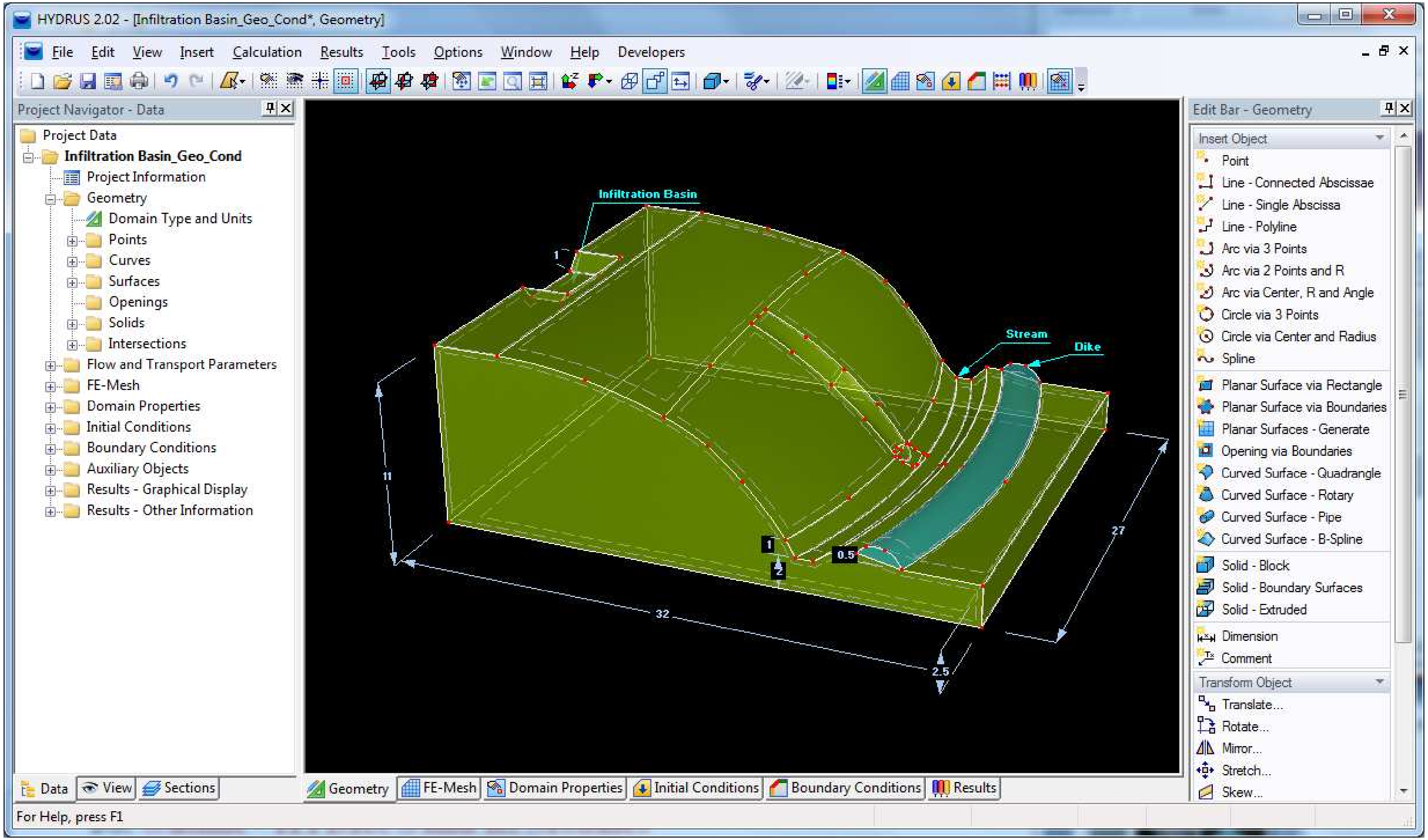
HYDRUS (2D/3D) - Geometries

Complex Drainage System



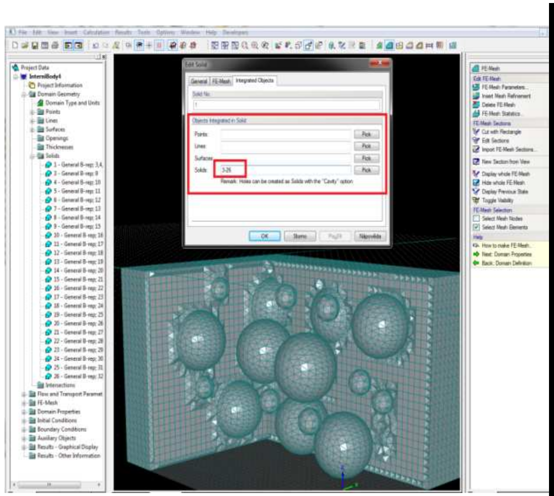
HYDRUS: 3D-Professional

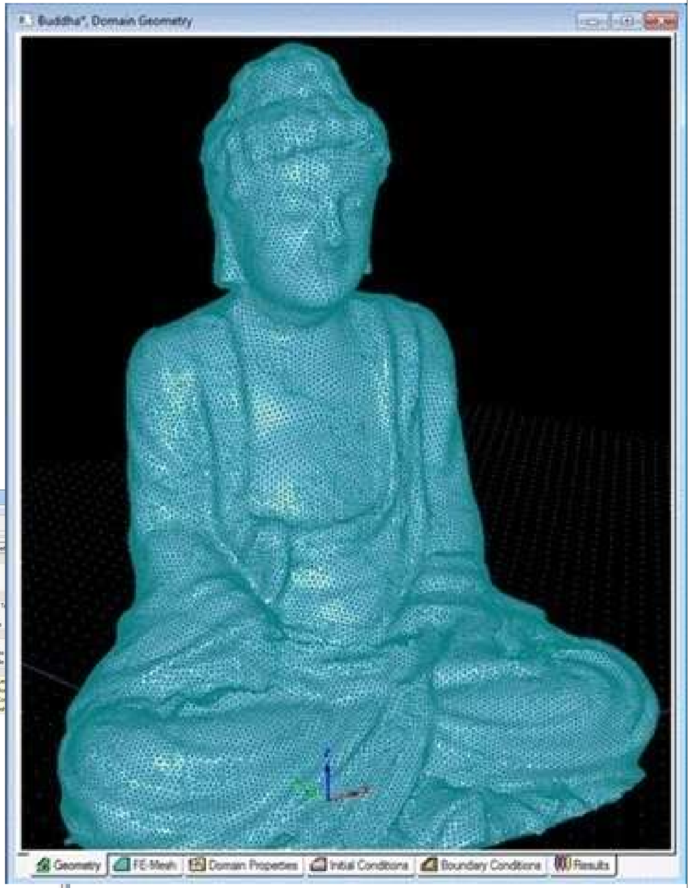
Infiltration Basin and Stream

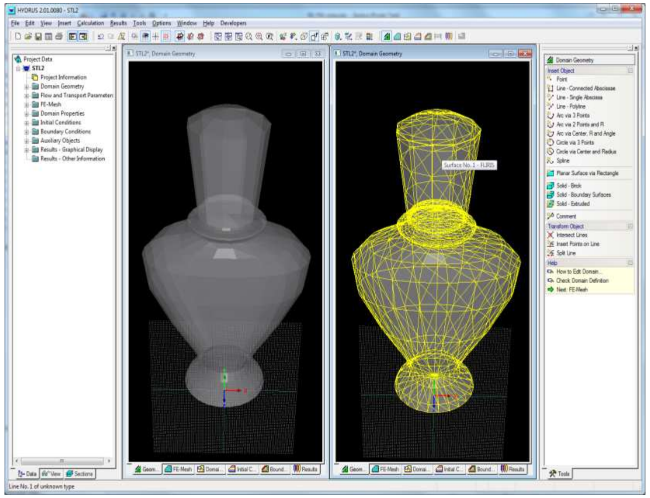


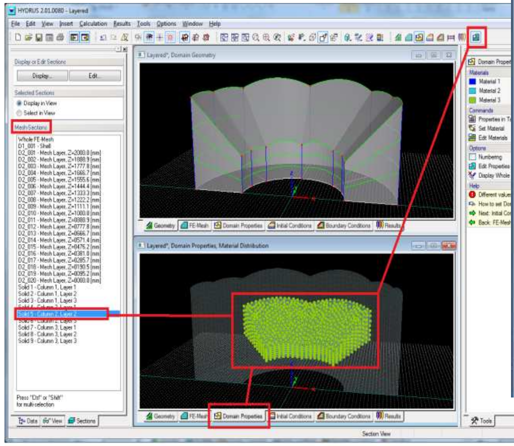
HYDRUS (2D/3D) - Geometries

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





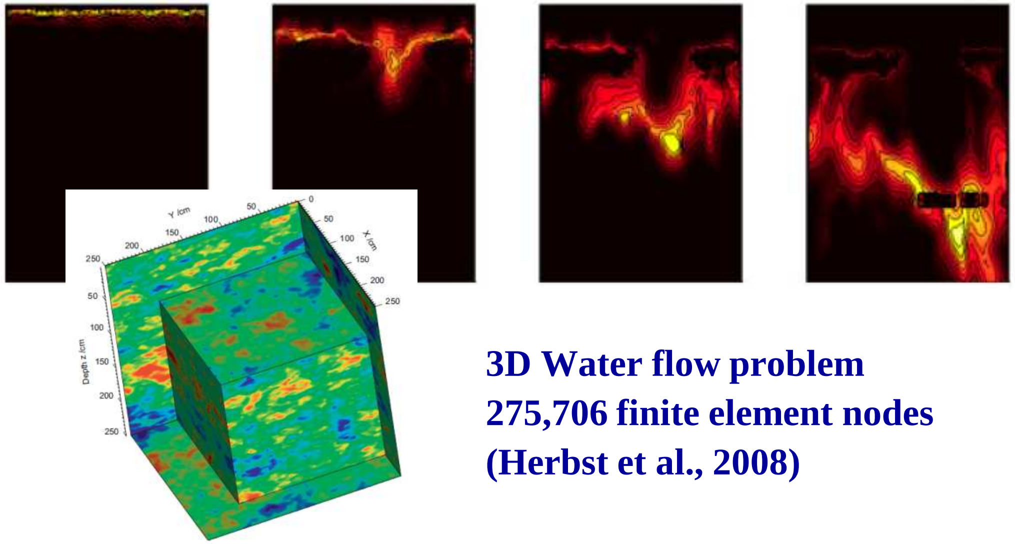




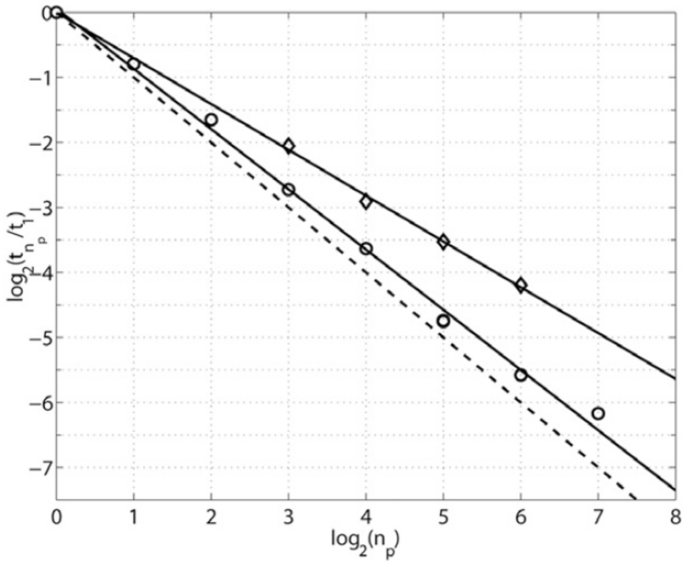
ParSWMS – Parallelized Version of HYDRUS

- **ParSWMS (**Hardelauf et al., 2007) **- Parallelized version of SWMS_3D**, an earlier and simpler version of HYDRUS-3D**.**
- **Developed by the *Forschungszentrum in Jülich, Germany*.**
- **MPI (Message-Passing Interface)**. LINUX or UNIX OSs.
- **Test** - Supercomputer with 41 SMP nodes with 32 processors each (total 1312 processors)

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)



HYDRUS and its Modules

- **HYDRUS + PHREEQC = HP1/2/3**
  (hydrological + biogeochemical processes)
- **HYDRUS + C-Ride**
  (particle and particle-facilitated solute transport)
- **HYDRUS + DualPerm**
  (preferential water flow and solute transport)
- **HYDRUS + UNSATCHEM**
  (hydrological + CO_2 + major ion processes)
- **HYDRUS + Wetland (CW2D/CWM1)**
  (biogeochemical processes in constructed wetlands)
- **HYDRUS + Fumigant**
  (fate and transport of fumigants)

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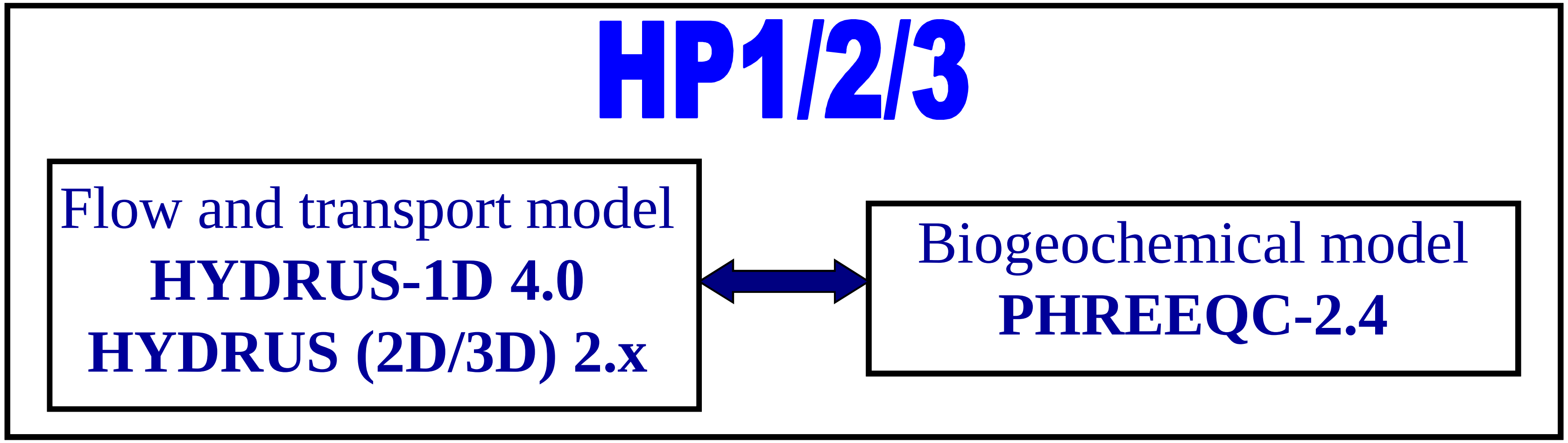
HP1/2/3 (HYDRUS+PHREEQC)

Simulating water flow, transport and bio-geochemical reactions in environmental soil quality problems

HPx

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



HP1/2/3

Flow and transport model
HYDRUS-1D 4.0
HYDRUS (2D/3D) 2.x

Biogeochemical model
PHREEQC-2.4

HP1/2/3 (HYDRUS+PHREEQC)

HYDRUS-1D or HYDRUS (2D/3D):

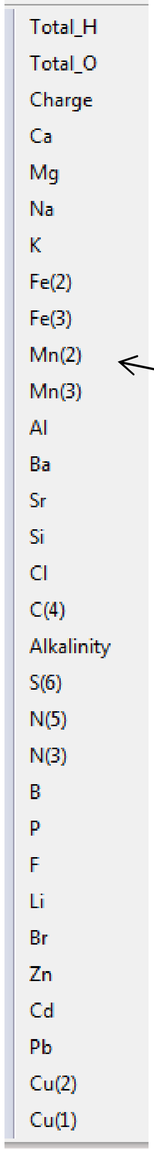
- Variably-Saturated Water Flow
- Solute Transport
- Heat Transport
- Gas Transport
- Root Water Uptake

PHREEQC [Parkhurst and Appelo, 1999]:

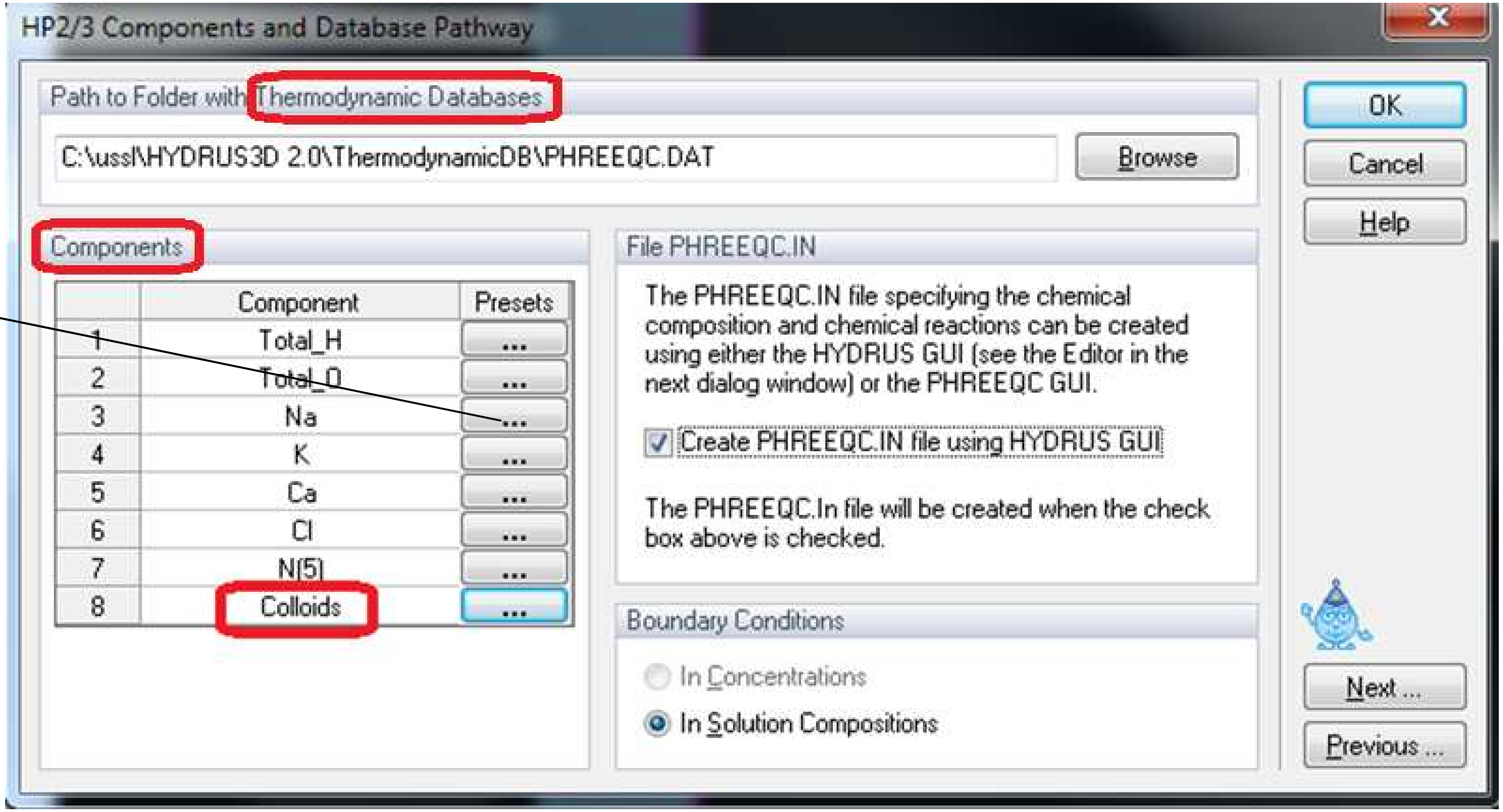
Available Chemical Reactions:

- Aqueous Complexation
- Redox Reactions
- Ion Exchange (Gains-Thomas)
- Surface Complexation (diffuse double-layer model and non-electrostatic surface complexation model)
- Precipitation/Dissolution
- Chemical Kinetics
- Biological Reactions

HYDRUS GUI for HP1/2/3



Total_H
Total_O
Charge
Ca
Mg
Na
K
Fe(2)
Fe(3)
Mn(2)
Mn(3)
Al
Ba
Sr
Si
Cl
C(4)
Alkalinity
S(6)
N(5)
N(3)
B
P
F
Li
Br
Zn
Cd
Pb
Cu(2)
Cu(1)



HP2/3 Components and Database Pathway

Path to Folder with Thermodynamic Databases

C:\ussl\HYDRUS3D 2.0\ThermodynamicDB\PHREEQC.DAT

Components

	Component	Presets
1	Total_H	...
2	Total_O	...
3	Na	...
4	K	...
5	Ca	...
6	Cl	...
7	N(5)	...
8	Colloids	...

File PHREEQC.IN

The PHREEQC.IN file specifying the chemical composition and chemical reactions can be created using either the HYDRUS GUI (see the Editor in the next dialog window) or the PHREEQC GUI.

☑ Create PHREEQC.IN file using HYDRUS GUI

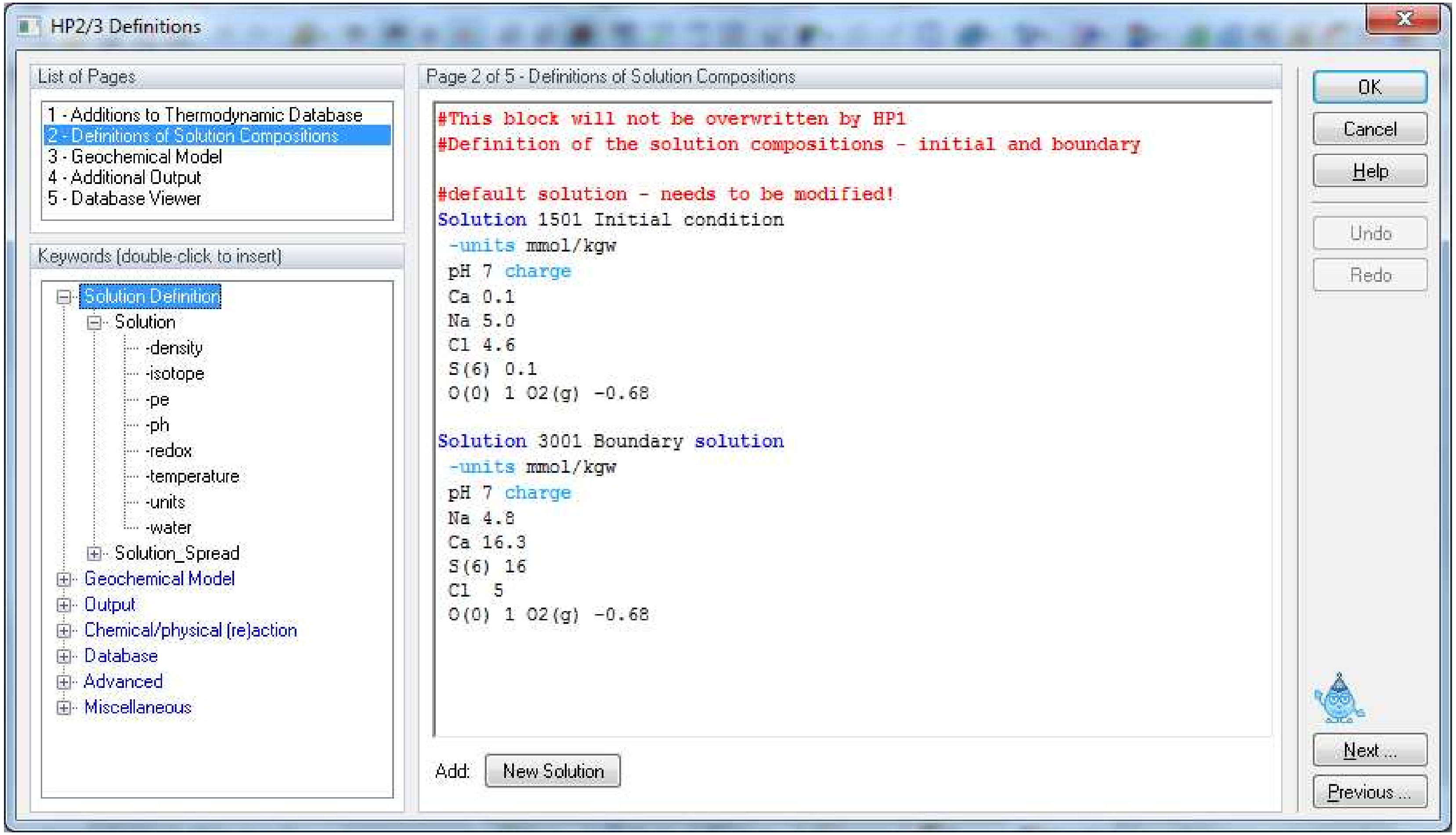
The PHREEQC.In file will be created when the check box above is checked.

Boundary Conditions

○ In Concentrations
● In Solution Compositions

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.

HYDRUS (2D/3D) GUI for HP2/3

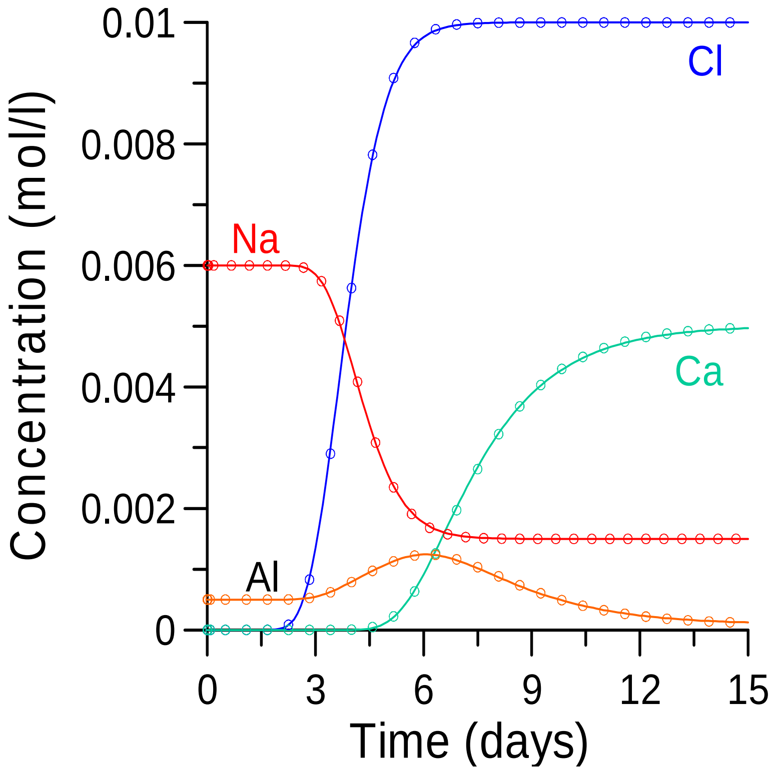


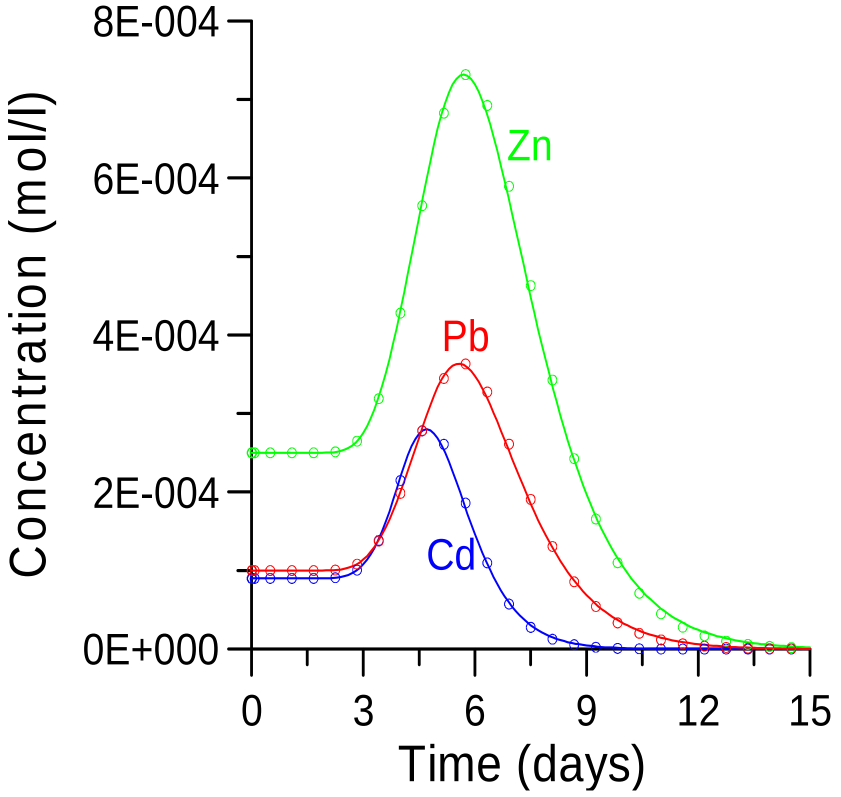
```
#This block will not be overwritten by HP1
#Definition of the solution compositions - initial and boundary

#default solution - needs to be modified!
Solution 1501 Initial condition
 -units mmol/kgw
 pH 7 charge
 Ca 0.1
 Na 5.0
 Cl 4.6
 S(6) 0.1
 O(0) 1 O2(g) -0.68

Solution 3001 Boundary solution
 -units mmol/kgw
 pH 7 charge
 Na 4.8
 Ca 16.3
 S(6) 16
 Cl  5
 O(0) 1 O2(g) -0.68
```

Four text editors to define the geochemical model, required output, and solution compositions are fully incorporated into the GUI.

Transport and Cation Exchange Heavy Metals

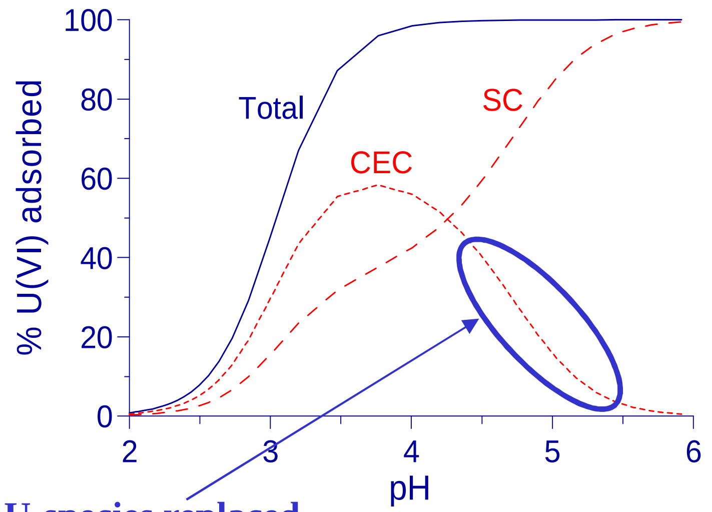
Major ions (Ca, Na, Al, Cl) and Heavy Metals (Zn, Pb, Cd)





A (8-cm) soil column is initially contaminated with heavy metals (in equilibrium with the cation exchanger). The column is then flushed with a $CaCl_2$ solution without heavy metals.

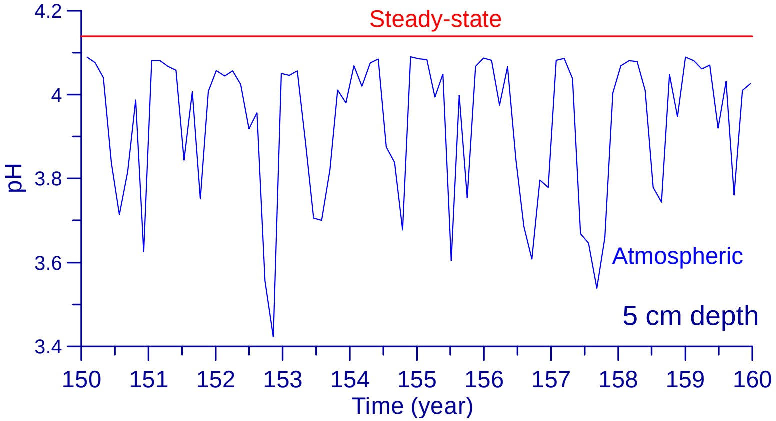
U-Transport in Agricultural Field Soils



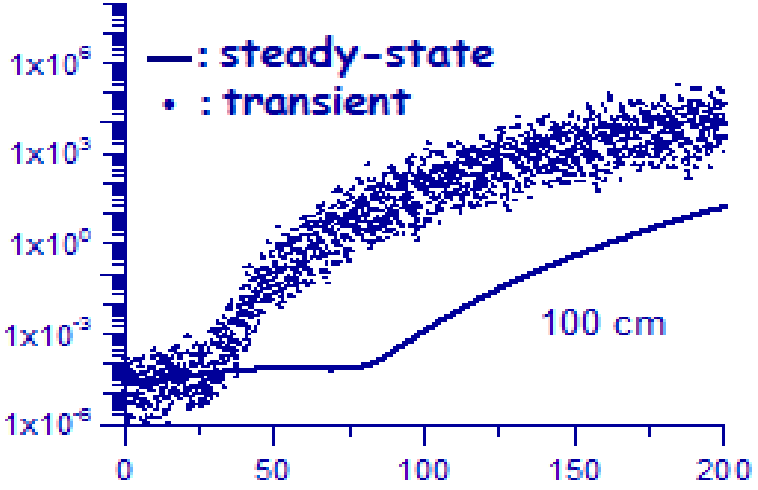
U-species replaced by other cations

Increased deprotonation

Increased U-sorption



- ◆ **Water content variations induce pH variations (dry soil => low pH)**
- ◆ **pH variations => variations in sorption potential (low pH => low sorption – higher mobility)**



- ◆ **Aqueous speciation reactions**

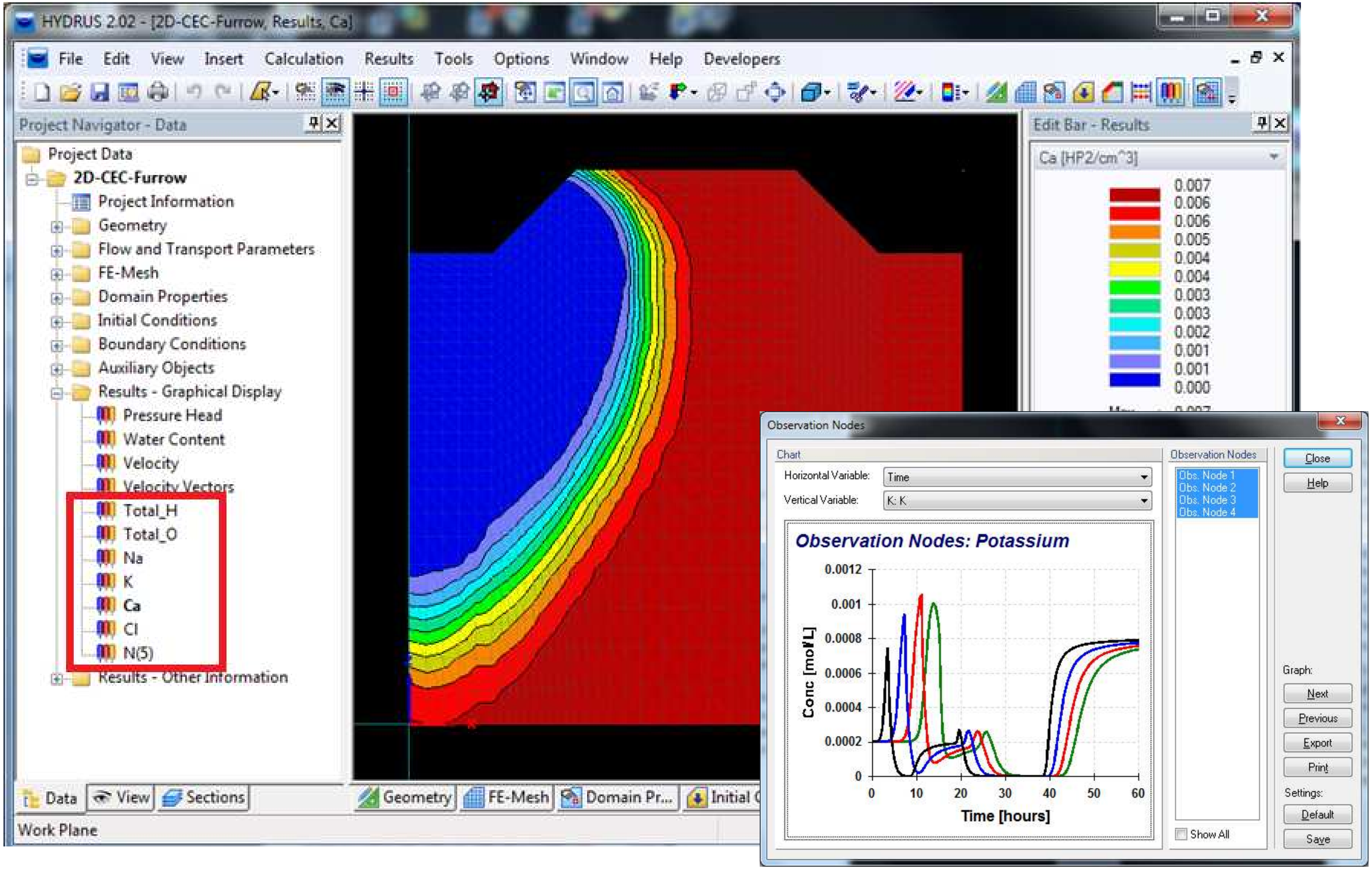
  C, Ca, Cl, F, H, K, Mg, N(5), Na, O(0), O(-2), P, S(6), U(6)

- ◆ **Multi-site cation exchange reactions**
  - **Related to amount of organic matter**
  - **Increases with increasing pH**
  - **UO_2^{2+} adsorbs**

- ◆ **Surface complexation reactions**
  - **Specific binding to charged surfaces (≡FeOH)**
  - **Related to amount of Fe-oxides**

Jacques et al., VZJ, 2008.

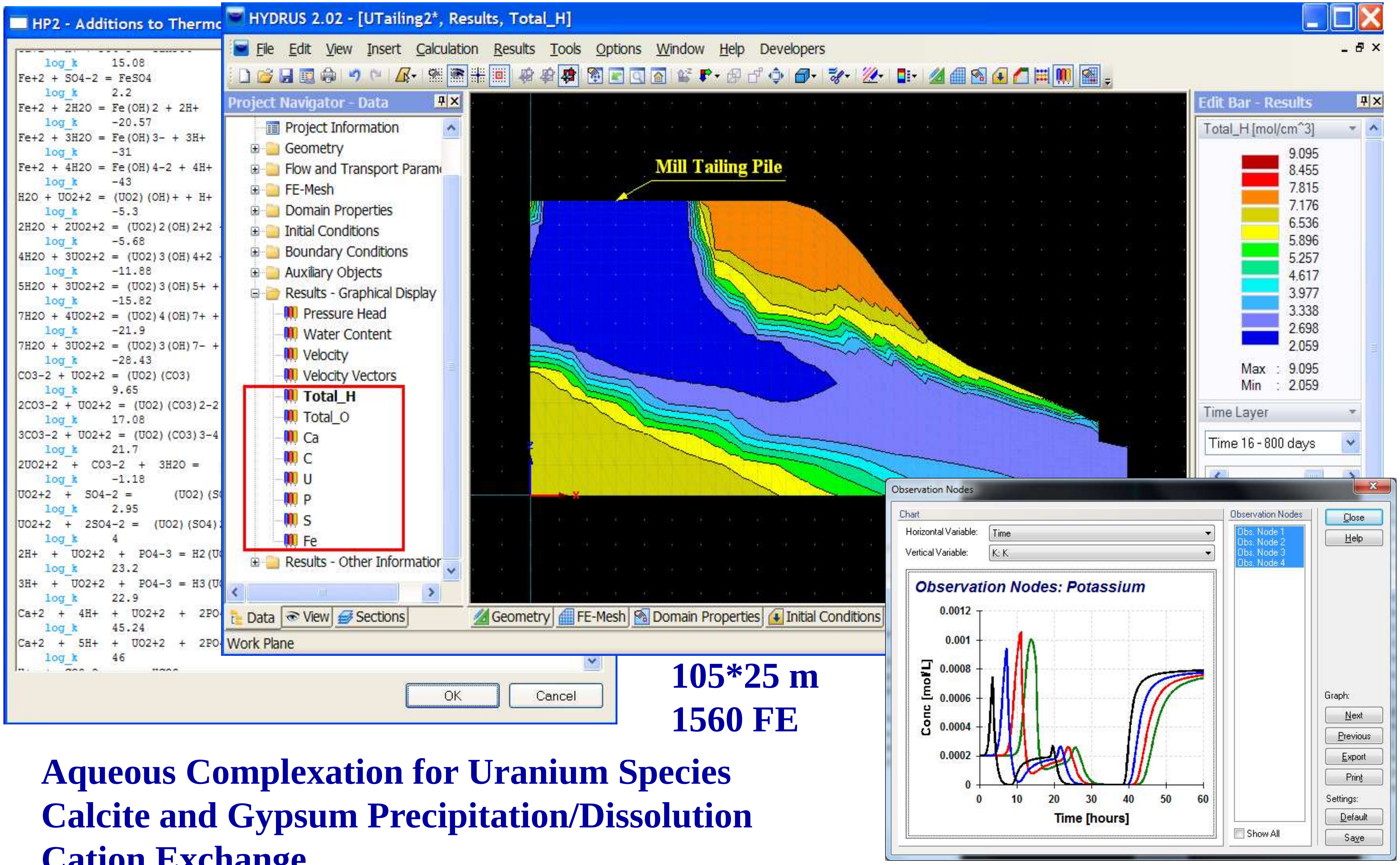
HP2 – Reclamation of a Sodic Soil



Horizontal Variable: Time

Vertical Variable: K: K

Uranium Transport from a Mill Tailing Pile



HP2 - Additions to Thermo

```
    log_k       15.08
Fe+2 + SO4-2 = FeSO4
    log_k       2.2
Fe+2 + 2H2O = Fe(OH)2 + 2H+
    log_k       -20.57
Fe+2 + 3H2O = Fe(OH)3- + 3H+
    log_k       -31
Fe+2 + 4H2O = Fe(OH)4-2 + 4H+
    log_k       -43
H2O + UO2+2 = (UO2)(OH)+ + H+
    log_k       -5.3
2H2O + 2UO2+2 = (UO2)2(OH)2+2
    log_k       -5.68
4H2O + 3UO2+2 = (UO2)3(OH)4+2
    log_k       -11.88
5H2O + 3UO2+2 = (UO2)3(OH)5+ +
    log_k       -15.82
7H2O + 4UO2+2 = (UO2)4(OH)7+ +
    log_k       -21.9
7H2O + 3UO2+2 = (UO2)3(OH)7- +
    log_k       -28.43
CO3-2 + UO2+2 = (UO2)(CO3)
    log_k       9.65
2CO3-2 + UO2+2 = (UO2)(CO3)2-2
    log_k       17.08
3CO3-2 + UO2+2 = (UO2)(CO3)3-4
    log_k       21.7
2UO2+2  +  CO3-2  +  3H2O =
    log_k       -1.18
UO2+2  +  SO4-2 =       (UO2)(S
    log_k       2.95
UO2+2  +  2SO4-2 =  (UO2)(SO4)
    log_k       4
2H+  +  UO2+2  +  PO4-3 = H2(U
    log_k       23.2
3H+  +  UO2+2  +  PO4-3 = H3(U
    log_k       22.9
Ca+2  +  4H+  +  UO2+2  +  2PO
    log_k       45.24
Ca+2  +  5H+  +  UO2+2  +  2PO
    log_k       46
```

HYDRUS 2.02 - [UTailing2*, Results, Total_H]

Edit Bar - Results: Total_H [mol/cm^3]

Max : 9.095
Min : 2.059

Time Layer: Time 16 - 800 days

Observation Nodes

Horizontal Variable: Time
Vertical Variable: K: K

105*25 m
1560 FE

Aqueous Complexation for Uranium Species
Calcite and Gypsum Precipitation/Dissolution
Cation Exchange

HP1 Examples

- Transport of Heavy Metals (Zn^{2+}, Pb^{2+}, and Cd^{2+}) subject to a multiple pH-dependent Cation Exchange
- Transport and mineral dissolution of Amorphous SiO_2 and Gibbsite
- 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 reactions

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- HYDRUS + Fumigant
  (fate and transport of fumigants)

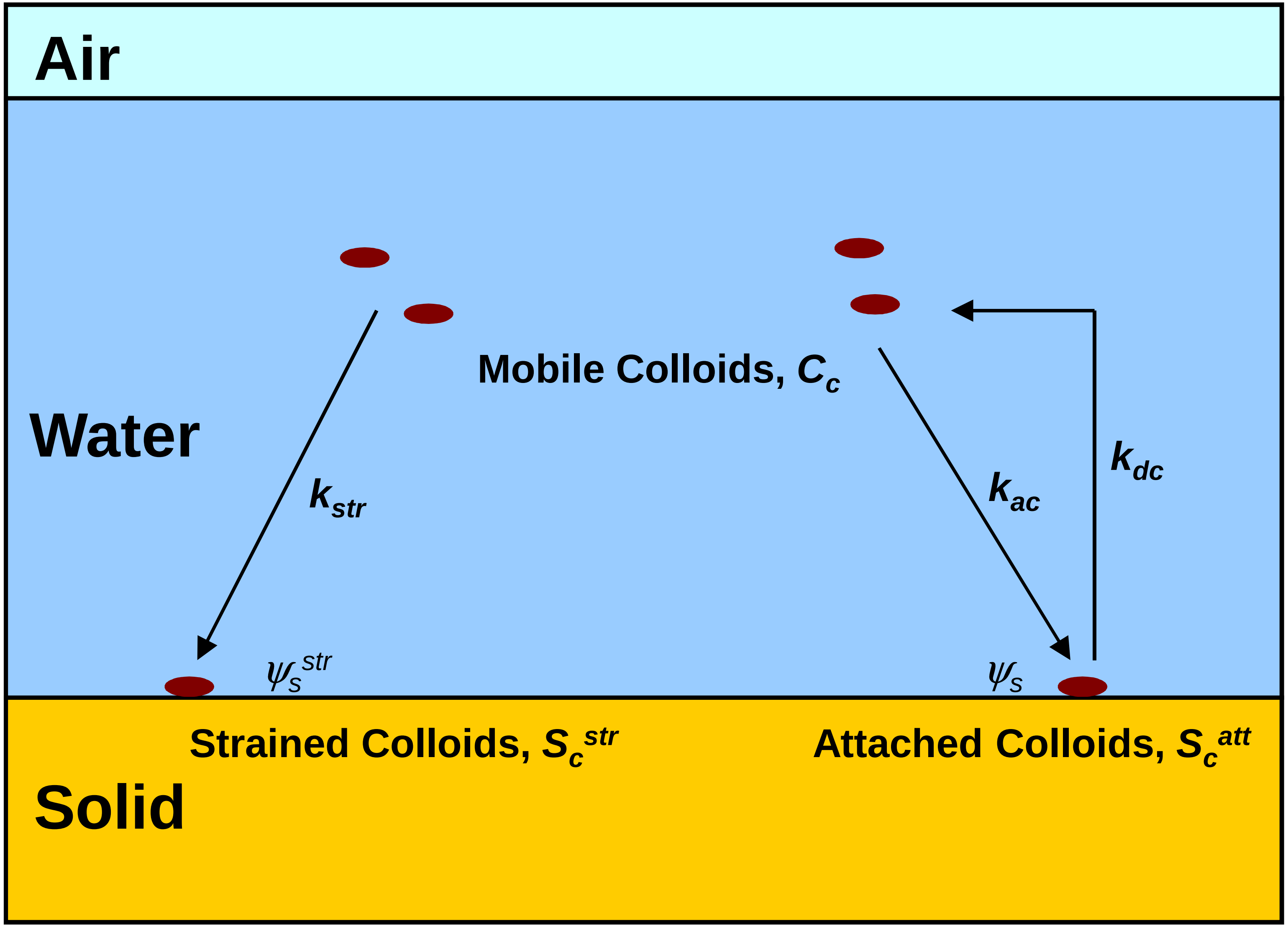
Colloid-Facilitated Solute Transport

- Many contaminants should be relatively immobile in the subsurface since under normal conditions they are strongly sorbed to soil
- They can also sorb to colloids, which often move at rates similar or faster as non-sorbing tracers
- Experimental evidence exists that many contaminants are transported not only in a dissolved state by water, but also sorbed to moving colloids
- Examples: heavy metals, radionuclides, pesticides, viruses, pharmaceuticals, hormones, and other contaminants

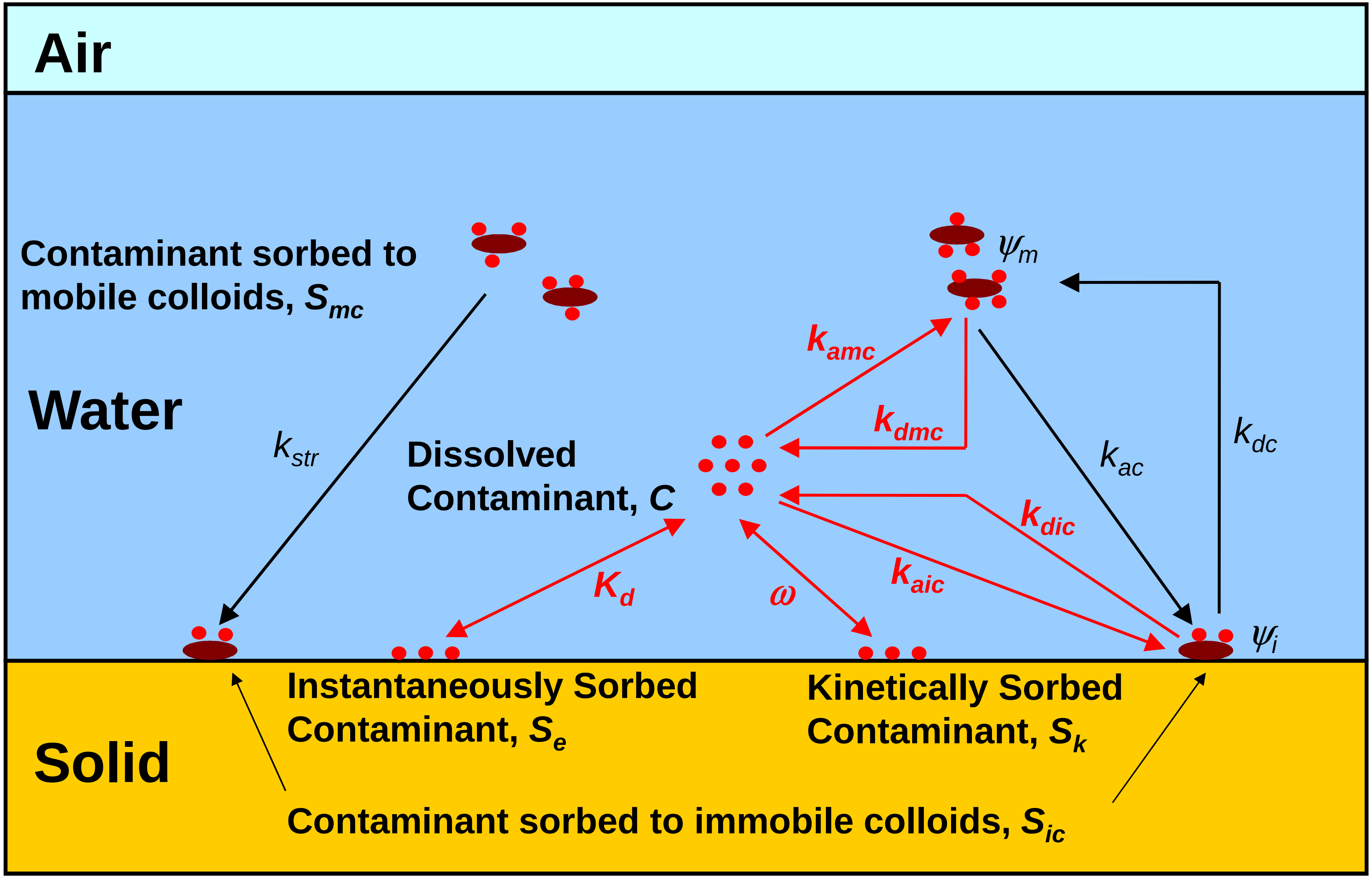
HYDRUS + C-Ride Module

- **HYDRUS-1D and HYDRUS (2D/3D)**
  - Variably-Saturated Water Flow
  - Solute Transport
  - Heat Transport
  - Root Water Uptake
- **C-Ride** (Šimůnek et al., 2006)
  - Particle Transport
    - colloids, bacteria, viruses, nanoparticles
    - attachment/detachment, straining, blocking
  - Particle-Facilitated Solute Transport
    - transport of solutes attached to particles

Colloid, Virus, and Bacteria Transport



Colloid-Facilitated Solute Transport



Air

Water

Solid

Contaminant sorbed to mobile colloids, S_{mc}

Dissolved Contaminant, C

Instantaneously Sorbed Contaminant, S_e

Kinetically Sorbed Contaminant, S_k

Contaminant sorbed to immobile colloids, S_{ic}

ψ_m

ψ_i

k_{str}

k_{amc}

k_{dmc}

k_{ac}

k_{dc}

k_{dic}

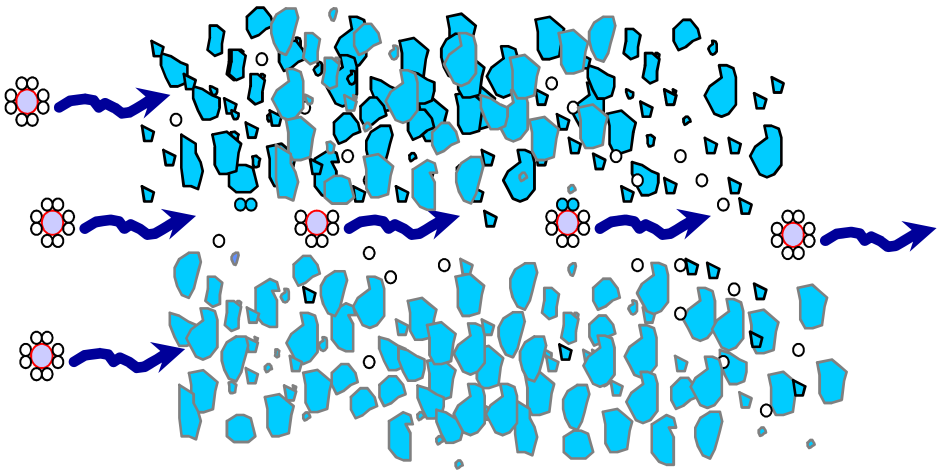
k_{aic}

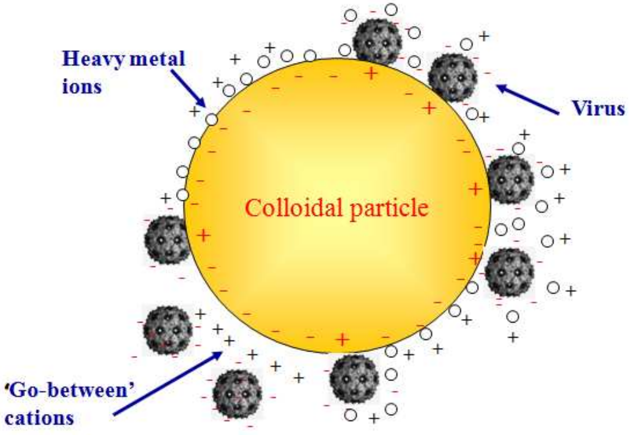
K_d

ω

Particle-Facilitated Solute Transport

Pang et al. [2005]: Bacteria act as carriers for heavy metals in gravel aquifers



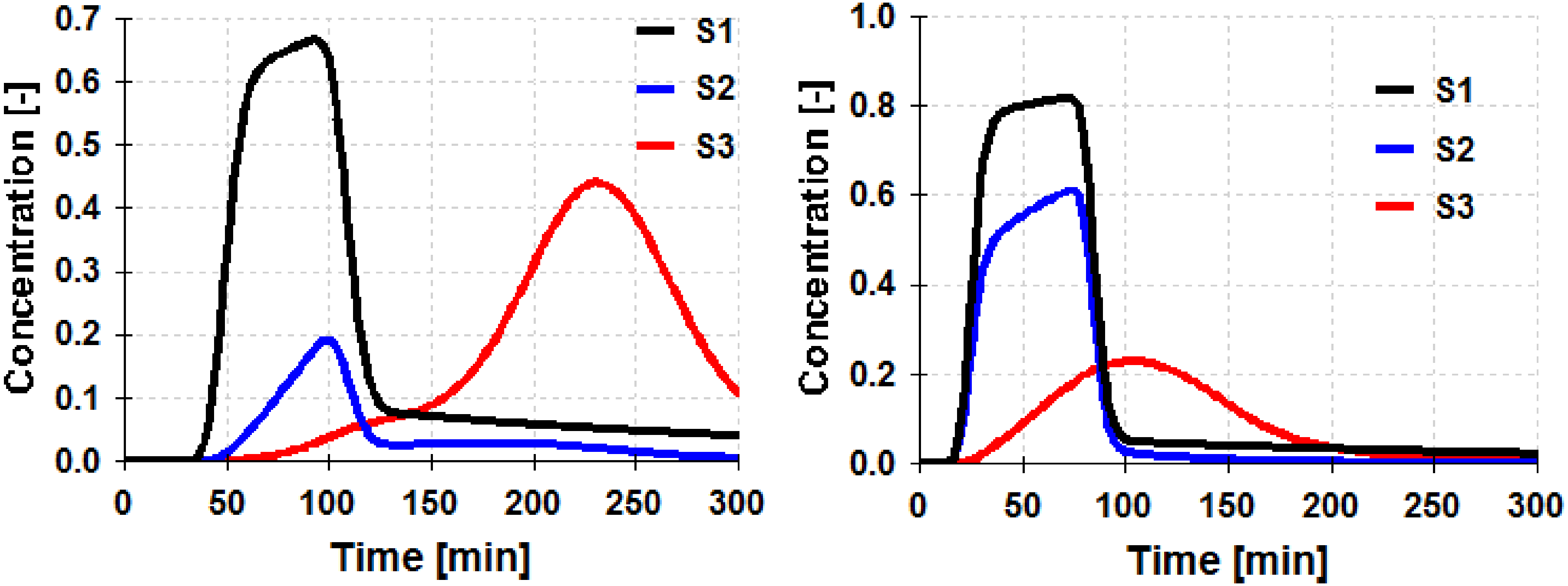


Since bacteria may be excluded from small pores, they move through interconnected larger pores and cracks where water moves quicker.

Since contaminants can sorb to these bacteria, they provide a vehicle for rapid transport of less mobile contaminants.

Colloid-Facilitated Solute Transport

C-Ride Module



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

Left: **solute and colloids are applied independently**

Right: **solute is initially attached to colloids**

The Retardation Factor for colloids is equal to 1 and for solute to 4

Unit input concentrations.

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Preferential Flow and Transport

Fractured Rock

Heterogeneous Sediments

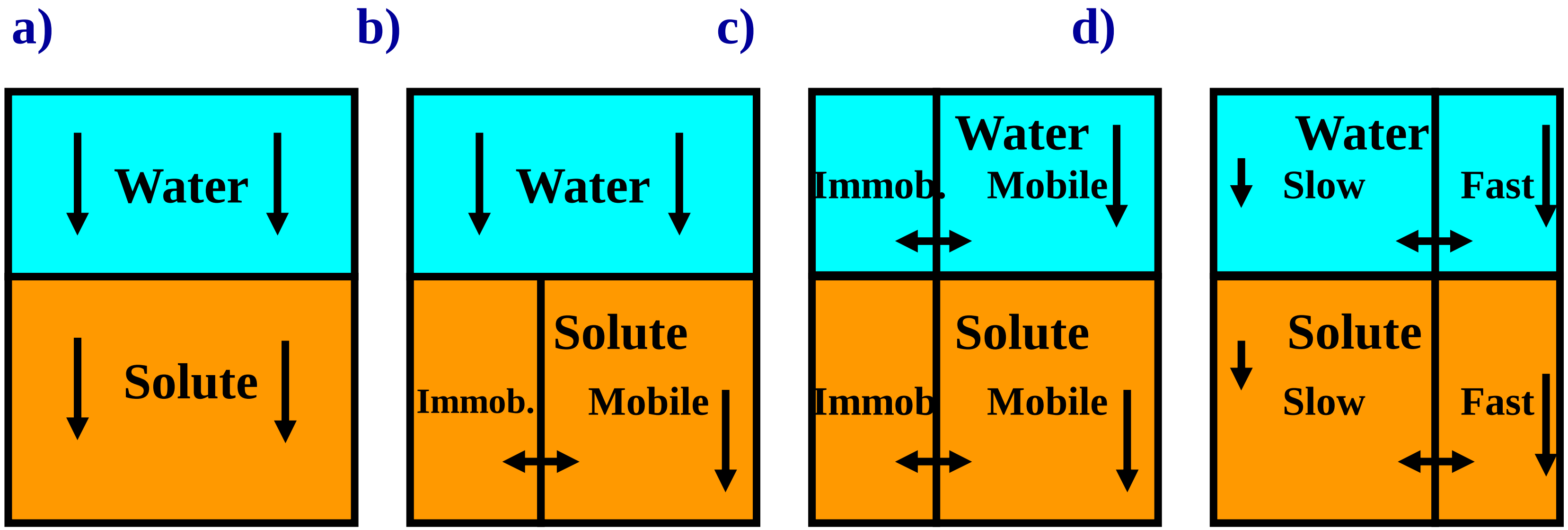
Macroporous Soil

The DualPerm Module

Physical Nonequilibrium

Solute Transport Models

Šimůnek and van Genuchten (2008):



θ $\qquad$ $\theta = \theta_{im} + \theta_{mo}$ $\qquad$ $\theta = \theta_{im} + \theta_{mo}$ $\qquad$ $\theta = \theta_M + \theta_F$

a) Uniform Flow

b) Mobile-Immobile Water

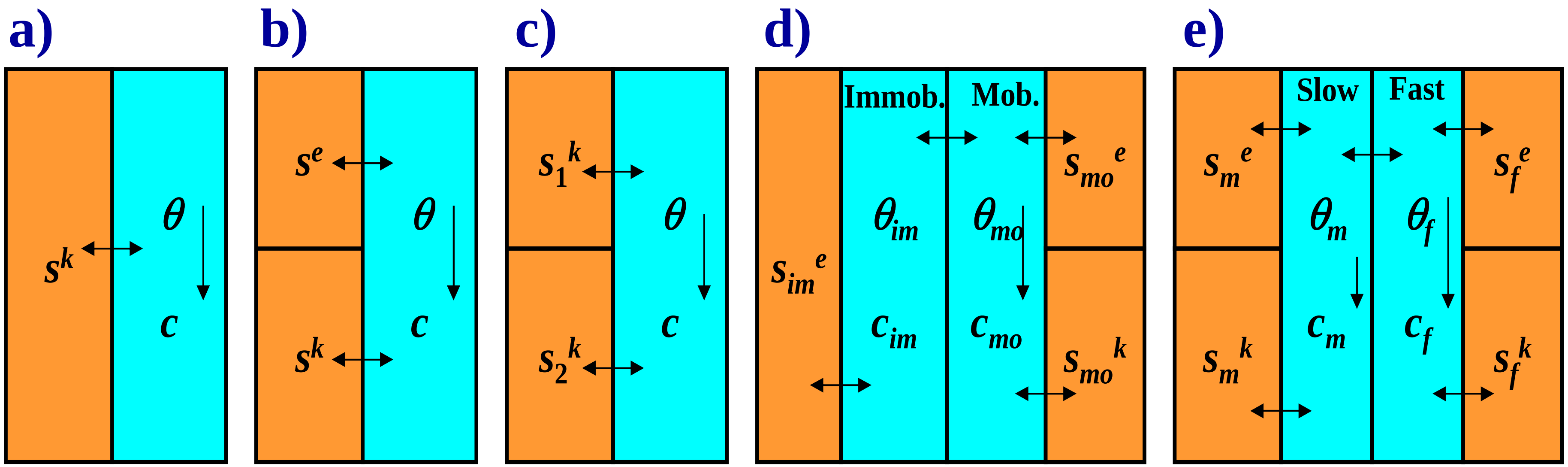
c) Dual-Porosity (Šimůnek et al., 2003)

d) Dual-Permeability (Gerke and van Genuchten, 1993)

Chemical Nonequilibrium

Solute Transport Models

Šimůnek and van Genuchten (2008):

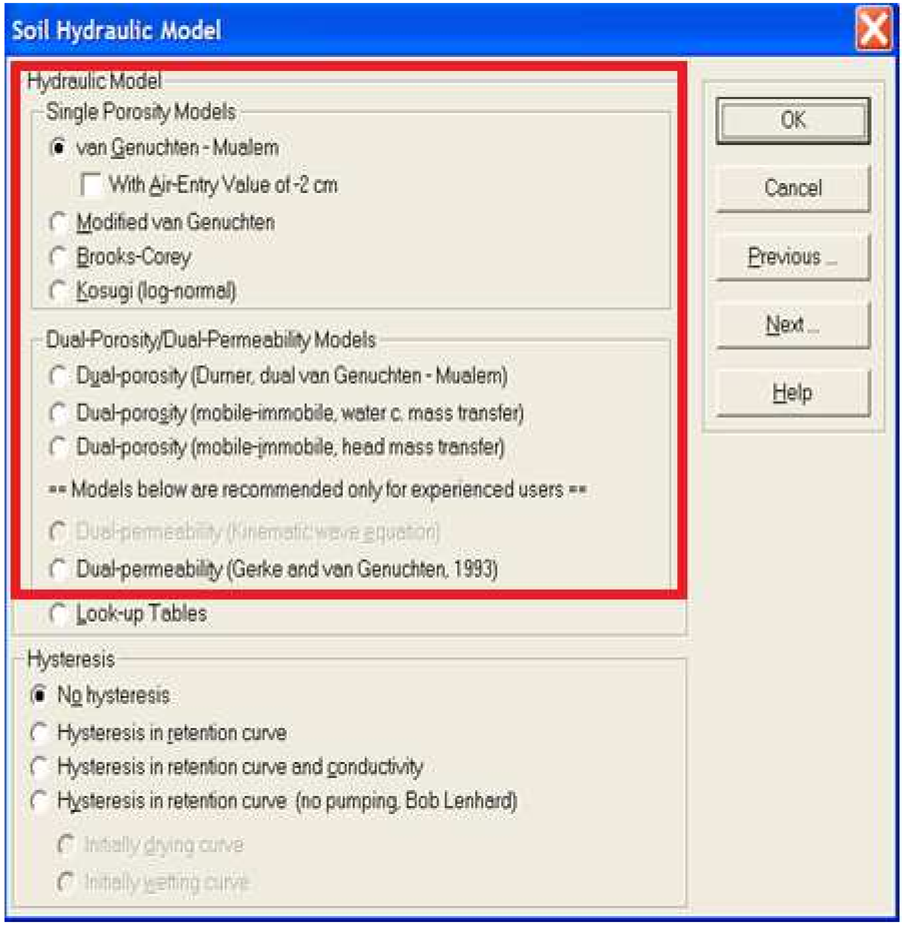


- a) **One-Site Kinetic Model**
- b) **Two-Site Model (kinetic and instantaneous sorption)**
- c) **Two Kinetic Sites Model**
  (particle transport, e.g. colloids, viruses, bacteria)
- d) **Dual-Porosity with One Kinetic Site Model**
- e) **Dual-permeability with Two-Site Model**

Nonequilibrium Models

in the HYDRUS GUI

Variably-Saturated Water Flow



Hydraulic Model

Single Porosity Models

- ● van Genuchten - Mualem
  - ☐ With Air-Entry Value of -2 cm
- ○ Modified van Genuchten
- ○ Brooks-Corey
- ○ Kosugi (log-normal)

Dual-Porosity/Dual-Permeability Models

- ○ Dual-porosity (Durner, dual van Genuchten - Mualem)
- ○ Dual-porosity (mobile-immobile, water c. mass transfer)
- ○ Dual-porosity (mobile-immobile, head mass transfer)

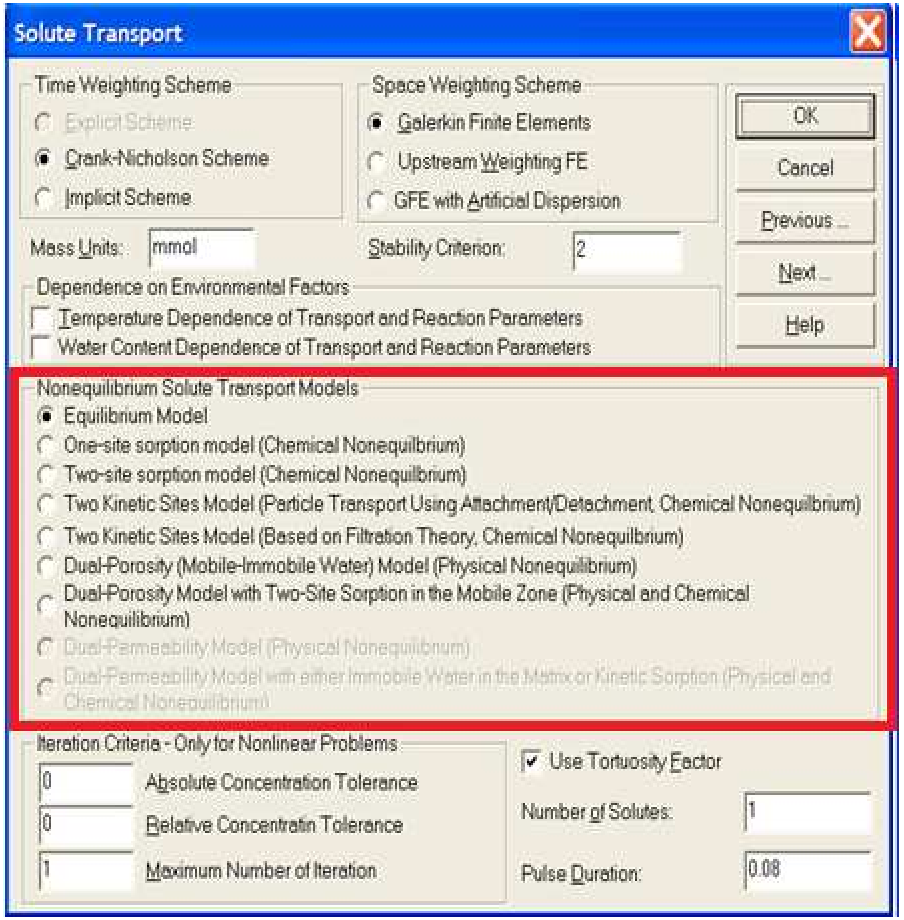
== Models below are recommended only for experienced users ==

- ○ Dual-permeability (Kinematic wave equation)
- ○ Dual-permeability (Gerke and van Genuchten, 1993)
- ○ Look-up Tables

Hysteresis

- ● No hysteresis
- ○ Hysteresis in retention curve
- ○ Hysteresis in retention curve and conductivity
- ○ Hysteresis in retention curve (no pumping, Bob Lenhard)
  - ○ Initially drying curve
  - ○ Initially wetting curve

Solute Transport



Time Weighting Scheme

- ○ Explicit Scheme
- ● Crank-Nicholson Scheme
- ○ Implicit Scheme

Space Weighting Scheme

- ● Galerkin Finite Elements
- ○ Upstream Weighting FE
- ○ GFE with Artificial Dispersion

Mass Units: mmol

Stability Criterion: 2

Dependence on Environmental Factors

- ☐ Temperature Dependence of Transport and Reaction Parameters
- ☐ Water Content Dependence of Transport and Reaction Parameters

Nonequilibrium Solute Transport Models

- ● Equilibrium Model
- ○ One-site sorption model (Chemical Nonequilbrium)
- ○ Two-site sorption model (Chemical Nonequilbrium)
- ○ Two Kinetic Sites Model (Particle Transport Using Attachment/Detachment, Chemical Nonequilbrium)
- ○ Two Kinetic Sites Model (Based on Filtration Theory, Chemical Nonequilbrium)
- ○ Dual-Porosity (Mobile-Immobile Water) Model (Physical Nonequilibrium)
- ○ Dual-Porosity Model with Two-Site Sorption in the Mobile Zone (Physical and Chemical Nonequilibrium)
- ○ Dual-Permeability Model (Physical Nonequilibrium)
- ○ Dual-Permeability Model with either Immobile Water in the Matrix or Kinetic Sorption (Physical and Chemical Nonequilibrium)

Iteration Criteria - Only for Nonlinear Problems

0 Absolute Concentration Tolerance

0 Relative Concentratin Tolerance

1 Maximum Number of Iteration

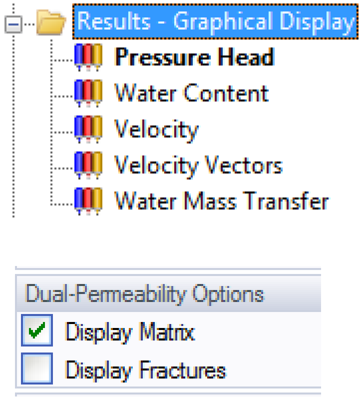
☑ Use Tortuosity Factor

Number of Solutes: 1

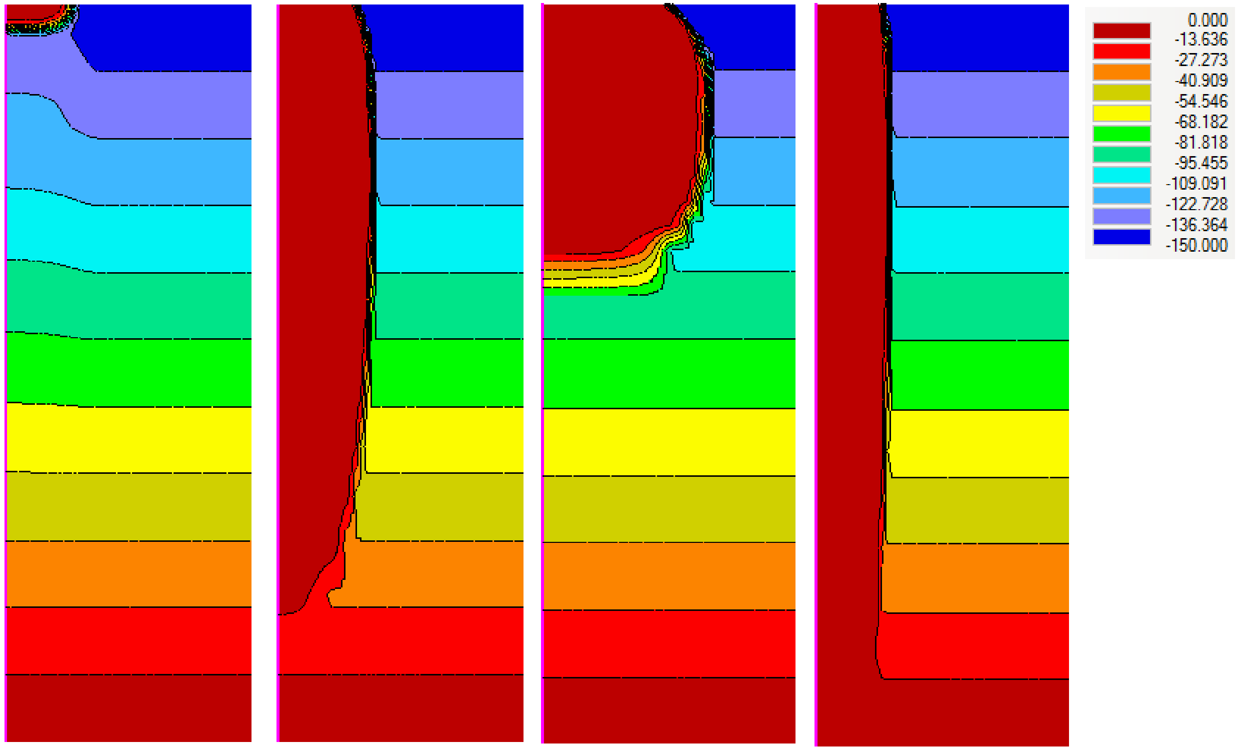
Pulse Duration: 0.08

The DualPerm Module – An Application

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



☑ Display Matrix
☐ Display Fractures



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 and its Modules

- HYDRUS + PHREEQC = HP1/2/3
  (hydrological + biogeochemical processes)
- HYDRUS + C-Ride
  (particle and particle-facilitated solute transport)
- HYDRUS + DualPerm
  (preferential water flow and solute transport)
- **HYDRUS + UNSATCHEM**
  (hydrological + CO_2 + geochemical processes)
- HYDRUS + Wetland (CW2D/CWM1)
  (biogeochemical processes in constructed wetlands)
- HYDRUS + Fumigant
  (fate and transport of fumigants)

HYDRUS + UNSATCHEM

- **HYDRUS-1D and HYDRUS (2D/3D)**
  - Variably-Saturated Water Flow
  - Solute Transport
  - Heat Transport
  - Root Water Uptake
- **UNSATCHEM** (Šimůnek et al., 1996)
  - Carbon Dioxide Transport and Production
  - Major Ion Chemistry
    - Cation Exchange
    - Precipitation-Dissolution (instantaneous and kinetic)
    - Aqueous Complexation

UNSATCHEM Module

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	$CaCO_3$, $CaSO_4 \cdot 2H_2O$, $CaMg(CO_3)_2$, $MgCO_3 \cdot 3H_2O$, $Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O$, $Mg_2Si_3O_{7.5}(OH) \cdot 3H_2O$
4	Sorbed Species (exchangeable)	4	XCa, XMg, XNa, XK
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

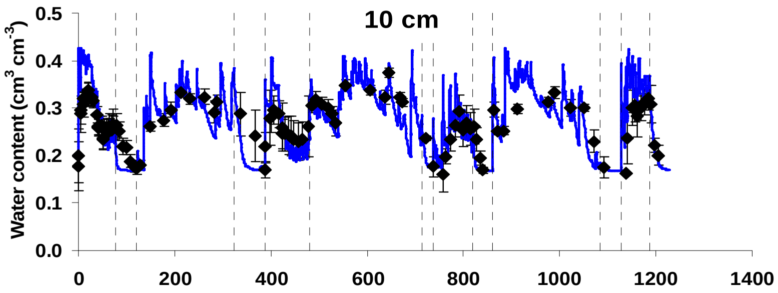
Activity coefficients: extended Debye-Hückel equations, Pitzer expressions

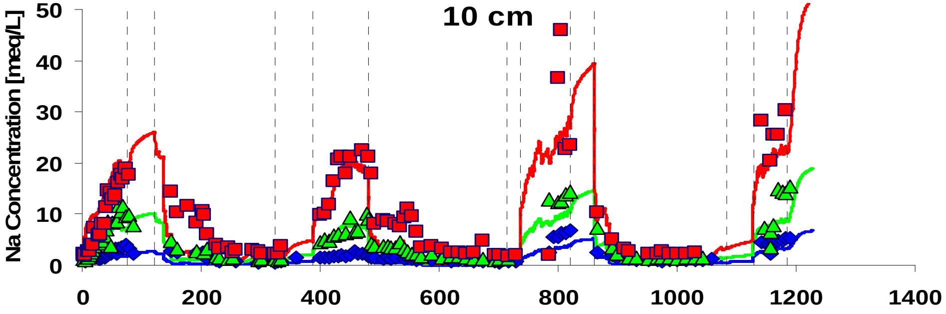
UNSATCHEM - Lysimeter Study

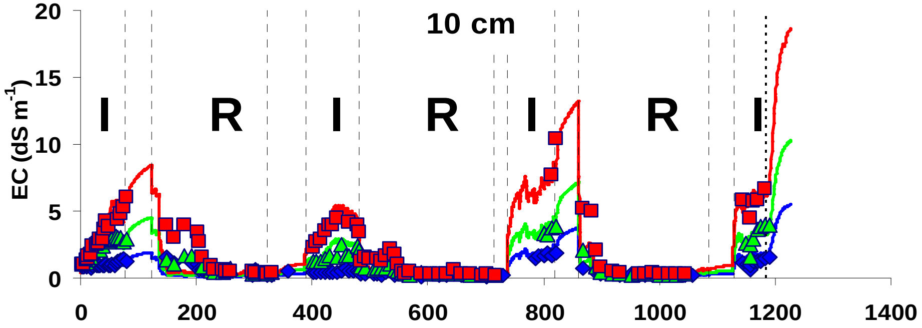
To evaluate the effectiveness of HYDRUS to predict:

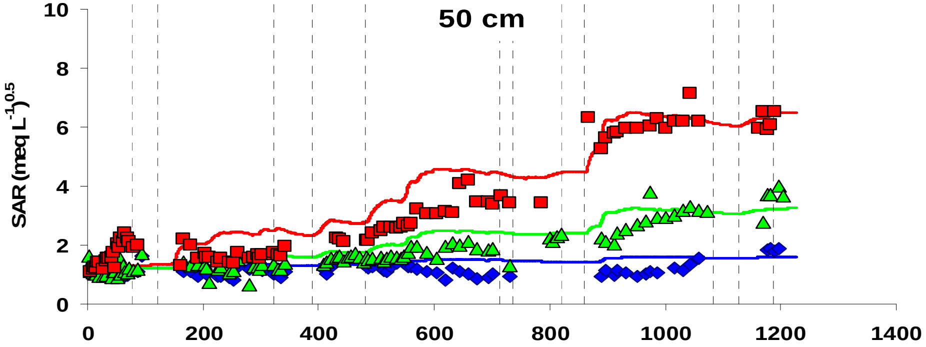
- **Water content and fluxes**
- **Concentration of individual cations (e.g., Ca^{2+}, Mg^{2+})**
- **Overall salinity (Electrical conductivity – *EC*)**
- **Sodium Adsorption Ratio (*SAR*)**
- **Exchangeable Sodium Percentage (*ESP*)**

$$SAR = \frac{(Na^+)}{\sqrt{\frac{(Ca^{2+}+Mg^{2+})}{2}}}$$







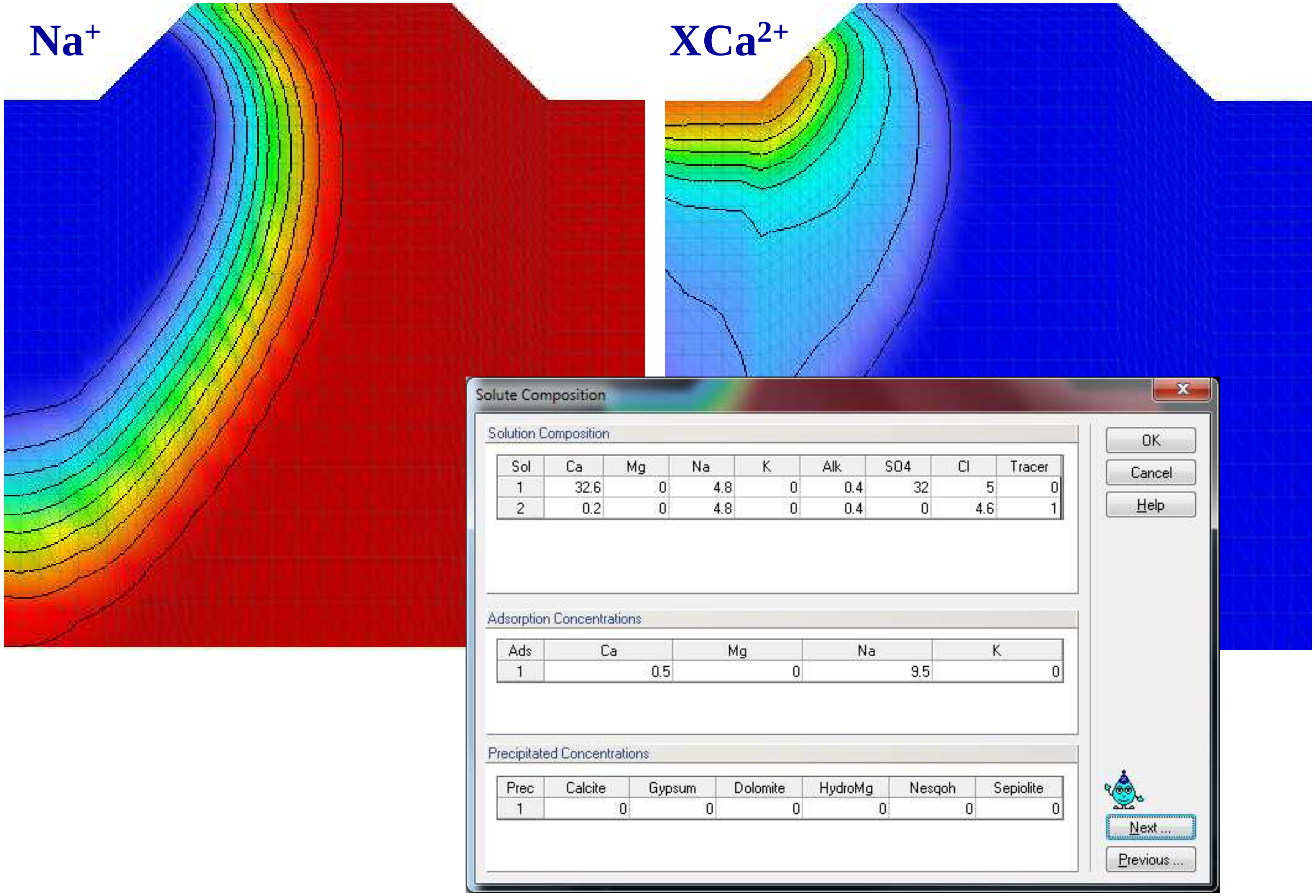


Gonçalves, M. C., J. Šimůnek, T. B. Ramos, J. C. Martins, M. J. Neves, and F. P. Pires, Multicomponent solute transport in soil lysimeters irrigated with waters of different quality, *Water Resources Research*, *42*, 17 pp., 2006.

Ramos, T. B., J. Šimůnek, M. C. Gonçalves, J. C. Martins, A. Prazeres, N. L. Castanheira, and L. S. Pereira, Field evaluation of a multicomponent solute transport model in soils irrigated with saline waters, *J. of Hydrology*, *407*(1-4), 129-144, 2011.

UNSATCHEM-2D Module

Major Ion Chemistry Module



Solution Composition

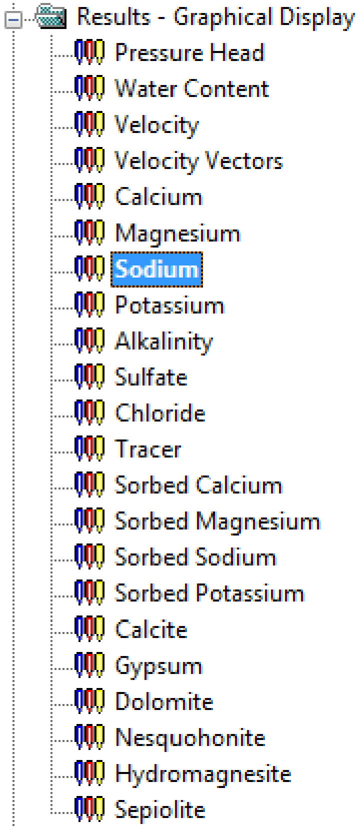
Sol	Ca	Mg	Na	K	Alk	SO4	Cl	Tracer
1	32.6	0	4.8	0	0.4	32	5	0
2	0.2	0	4.8	0	0.4	0	4.6	1

Adsorption Concentrations

Ads	Ca	Mg	Na	K
1	0.5	0	9.5	0

Precipitated Concentrations

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



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.

HYDRUS and its Modules

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  (fate and transport of fumigants)

Wetland Module

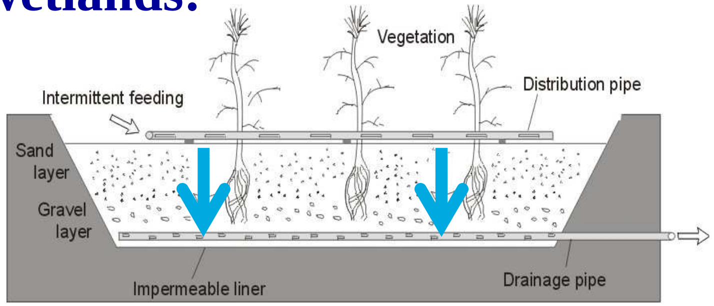
Constructed Wetlands (CWs) or wetland treatment systems

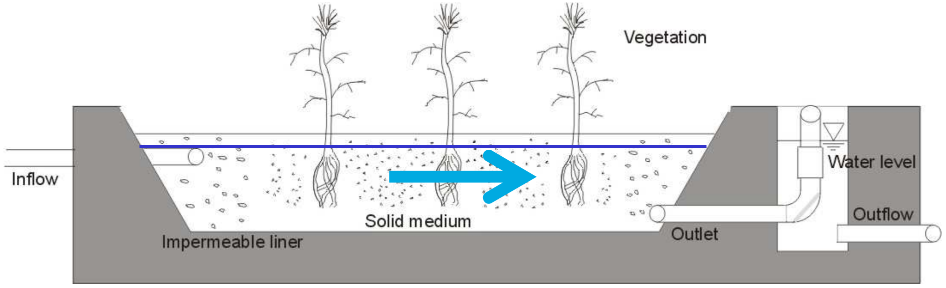
- are systems designed to improve water quality
- use the same processes that occur in natural wetlands but have the flexibility of being constructed
- effective in treating organic matter, nitrogen, phosphorus, and additionally for decreasing the concentrations of heavy metals, organic chemicals, and pathogens

CW2D : aerobic and anoxic processes for organic matter, nitrogen and phosphorus (Langergraber and Šimůnek, 2005)

CWM1: aerobic, anoxic and anaerobic processes for organic matter, nitrogen and sulphur (Langergraber et al., 2005)

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



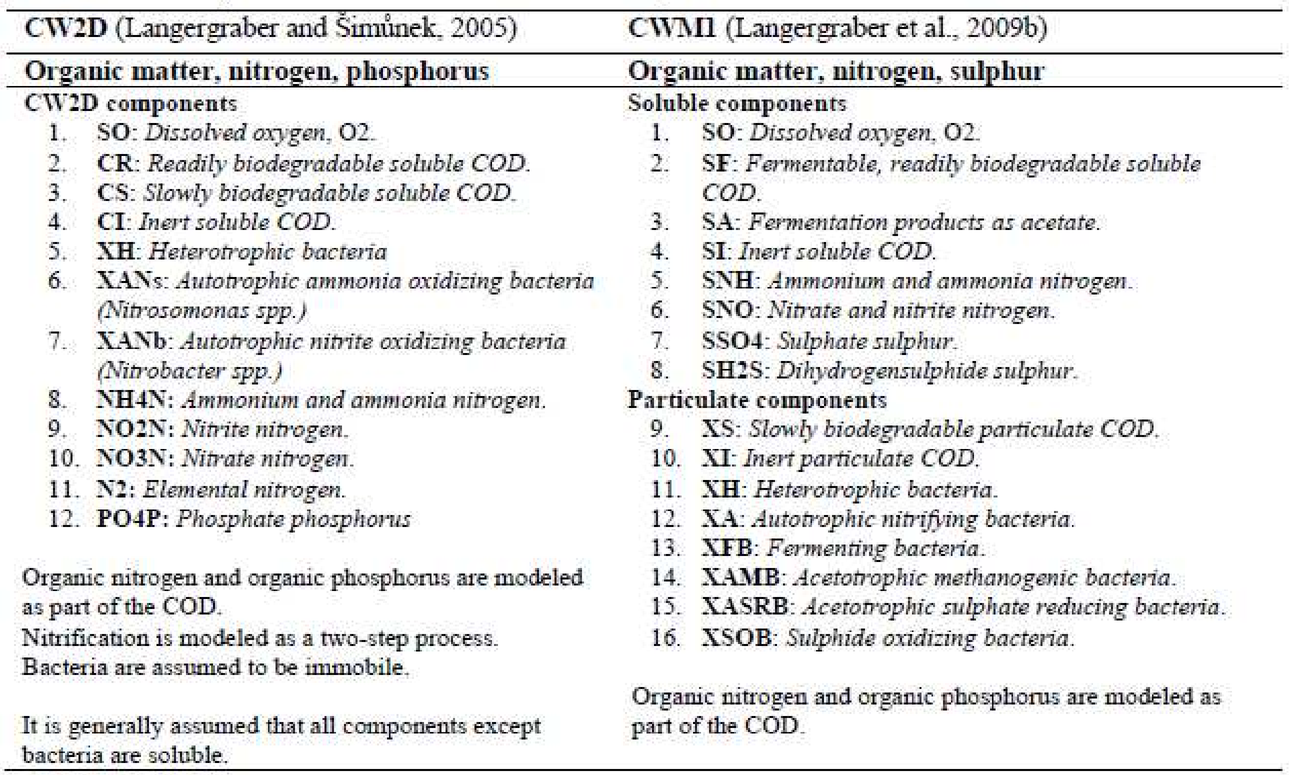


Wetland Modules: Components

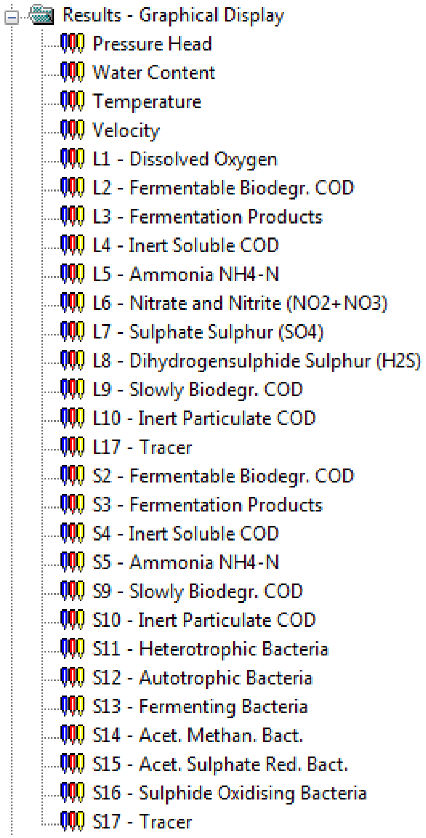
CW2D : aerobic and anoxic processes for organic matter, nitrogen and phosphorus

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

Components:



CW2D (Langergraber and Šimůnek, 2005)	CWM1 (Langergraber et al., 2009b)
Organic matter, nitrogen, phosphorus	**Organic matter, nitrogen, sulphur**
CW2D components 1. **SO**: *Dissolved oxygen, O2.* 2. **CR**: *Readily biodegradable soluble COD.* 3. **CS**: *Slowly biodegradable soluble COD.* 4. **CI**: *Inert soluble COD.* 5. **XH**: *Heterotrophic bacteria* 6. **XANs**: *Autotrophic ammonia oxidizing bacteria (Nitrosomonas spp.)* 7. **XANb**: *Autotrophic nitrite oxidizing bacteria (Nitrobacter spp.)* 8. **NH4N**: *Ammonium and ammonia nitrogen.* 9. **NO2N**: *Nitrite nitrogen.* 10. **NO3N**: *Nitrate nitrogen.* 11. **N2**: *Elemental nitrogen.* 12. **PO4P**: *Phosphate phosphorus*	**Soluble components** 1. **SO**: *Dissolved oxygen, O2.* 2. **SF**: *Fermentable, readily biodegradable soluble COD.* 3. **SA**: *Fermentation products as acetate.* 4. **SI**: *Inert soluble COD.* 5. **SNH**: *Ammonium and ammonia nitrogen.* 6. **SNO**: *Nitrate and nitrite nitrogen.* 7. **SSO4**: *Sulphate sulphur.* 8. **SH2S**: *Dihydrogensulphide sulphur.* **Particulate components** 9. **XS**: *Slowly biodegradable particulate COD.* 10. **XI**: *Inert particulate COD.* 11. **XH**: *Heterotrophic bacteria.* 12. **XA**: *Autotrophic nitrifying bacteria.* 13. **XFB**: *Fermenting bacteria.* 14. **XAMB**: *Acetotrophic methanogenic bacteria.* 15. **XASRB**: *Acetotrophic sulphate reducing bacteria.* 16. **XSOB**: *Sulphide oxidizing bacteria.*
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.	Organic nitrogen and organic phosphorus are modeled as part of the COD.

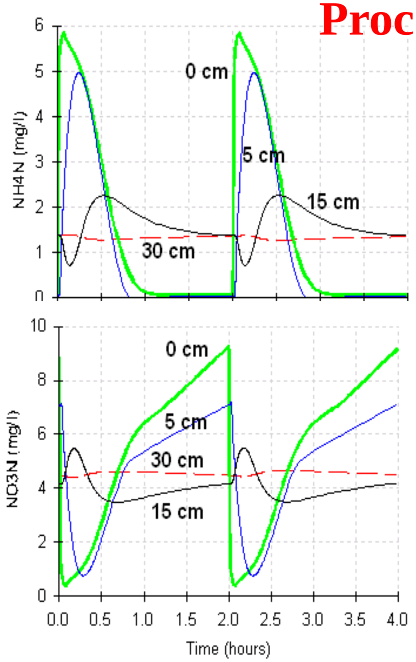


- Results - Graphical Display
  - Pressure Head
  - Water Content
  - Temperature
  - Velocity
  - L1 - Dissolved Oxygen
  - L2 - Fermentable Biodegr. COD
  - L3 - Fermentation Products
  - L4 - Inert Soluble COD
  - L5 - Ammonia NH4-N
  - L6 - Nitrate and Nitrite (NO2+NO3)
  - L7 - Sulphate Sulphur (SO4)
  - L8 - Dihydrogensulphide Sulphur (H2S)
  - L9 - Slowly Biodegr. COD
  - L10 - Inert Particulate COD
  - L17 - Tracer
  - S2 - Fermentable Biodegr. COD
  - S3 - Fermentation Products
  - S4 - Inert Soluble COD
  - S5 - Ammonia NH4-N
  - S9 - Slowly Biodegr. COD
  - S10 - Inert Particulate COD
  - S11 - Heterotrophic Bacteria
  - S12 - Autotrophic Bacteria
  - S13 - Fermenting Bacteria
  - S14 - Acet. Methan. Bact.
  - S15 - Acet. Sulphate Red. Bact.
  - S16 - Sulphide Oxidising Bacteria
  - S17 - Tracer

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.

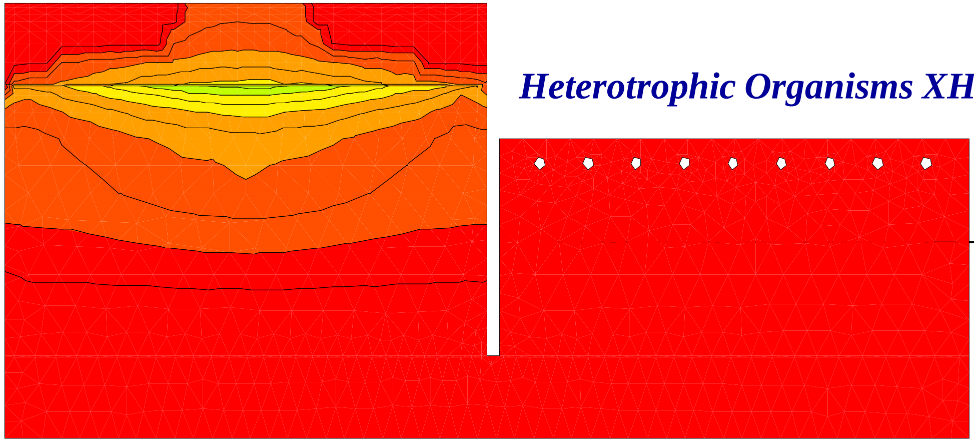
Langergraber, G., D. Rousseau, J. Garcia, and J. Mean, CWM1 - A general model to describe biokinetic processes in subsurface flow constructed wetlands, *Water Science Technology*, 59(9), 1687-1697, 2009.

Wetland Modules: Processes

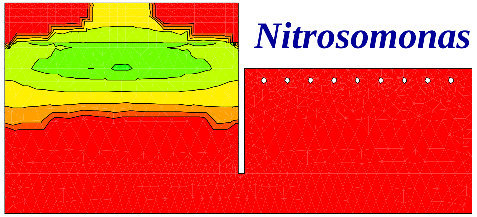


Processes:

CW2D (Langergraber and Šimůnek, 2005)	**CWM1** (Langergraber et al., 2009b)
Heterotrophic bacteria: 1. *Hydrolysis:* conversion of CS into CR. 2. *Aerobic growth of XH on CR* (mineralization of organic matter). 3. *Anoxic growth of XH on CR* (denitrification on NO2N). 4. *Anoxic growth of XH on CR* (denitrification on NO3N). 5. *Lysis of XH.*	*Heterotrophic bacteria:* 1. *Hydrolysis*: conversion of XS into SF. 2. *Aerobic growth of XH on SF* (mineralization of organic matter). 3. *Aerobic growth of XH on SA* (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: 6. *Aerobic growth of XANs on SNH* (ammonium oxidation). 7. *Lysis of XANs.* 8. *Aerobic growth of XANb on SNH* (nitrite oxidation). 9. *Lysis of XANb.*	*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. 17. Lysis of XSOB.



Heterotrophic Organisms XH



Nitrosomonas XANs

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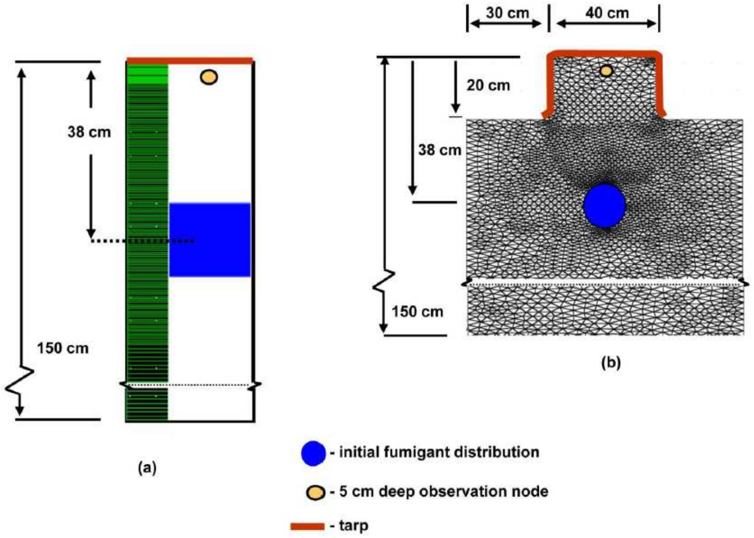
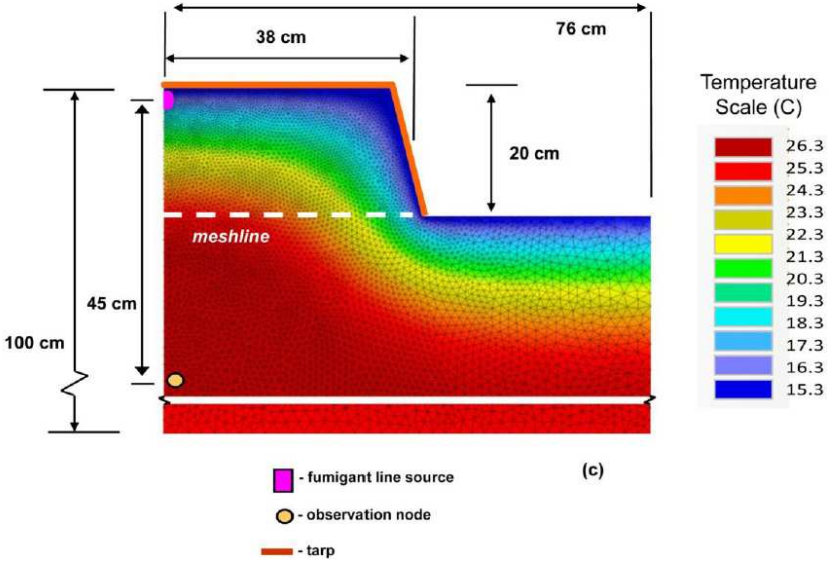
- **HYDRUS + Fumigant**
  (fate and transport of fumigants)

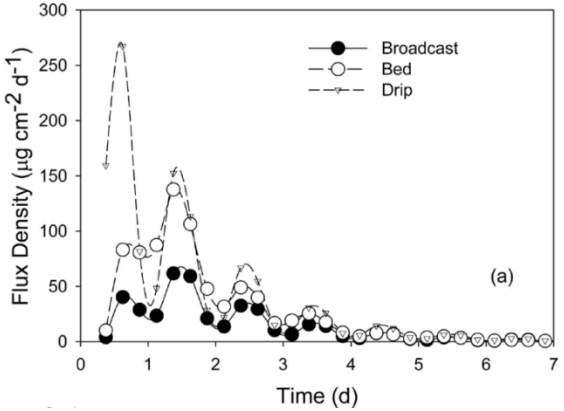
HYDRUS + Fumigant

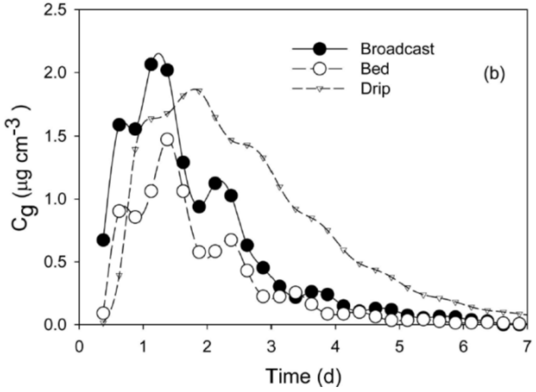
- **HYDRUS-1D and HYDRUS (2D/3D)**
  - Variably-Saturated Water Flow
  - Solute Transport
  - Heat Transport
  - Root Water Uptake
- **Fumigant**
  - Presence or absence of a Surface Tarp
  - Temperature dependence of Tarp properties
  - Removal of Tarp at specified time
  - Additional injection of fumigants into the transport domain at a specified location at specified time

Application of the Fumigant Module









Spurlock, F., J. Šimůnek, B. Johnson, and A. Tuli, Sensitivity analysis of vadose zone fumigant transport and volatilization, *Vadose Zone Journal*, *12*(2), 12 pp., 2013.

HYDRUS and its Future Modules?

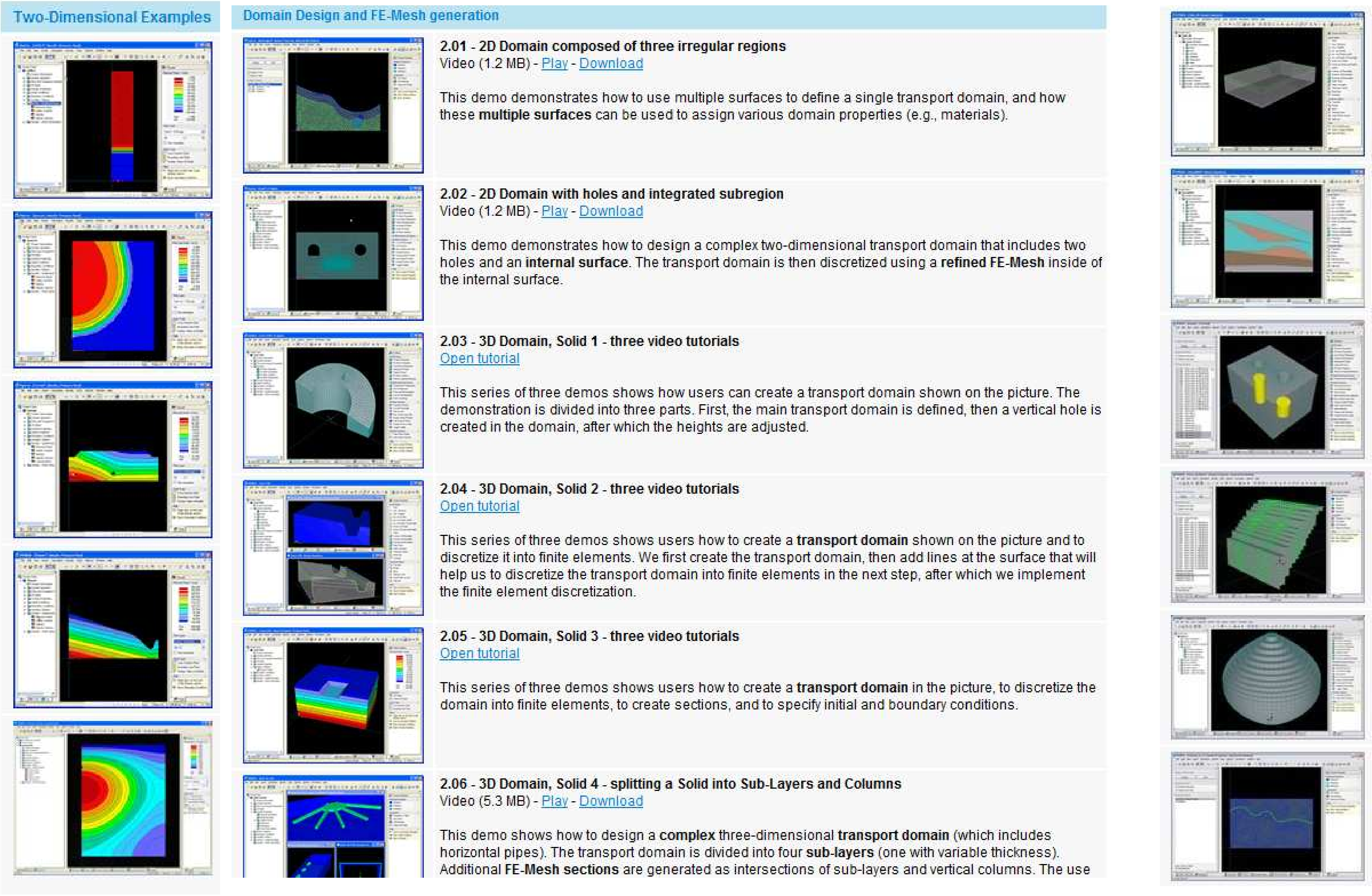
- **HYDRUS + Overland Flow**
  (surface runoff and overland flow)
- **HYDRUS + Freezing/Thawing, Meteo**
  (atmosphere)…
- **HYDRUS + Soil Mechanical Stresses**
  (effects of hydrological processes on slope stability)
- **HYDRUS + Global Optimization**
  (genetic algorithm, AMALGAM, DREAM, …)
- **HYDRUS + MODFLOW**
  (hydrological processes at a large scale)

HYDRUS Web Site

Over 3 thousand downloads in 2008, over 5 thousand in 2009,
and about 10 thousand downloads in 2010 and 2011;
over 10 thousand registered members.

http://www.pc-progress.com/en/Default.aspx

HYDRUS Tutorials



Two-Dimensional Examples

Domain Design and FE-Mesh generation

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).

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.

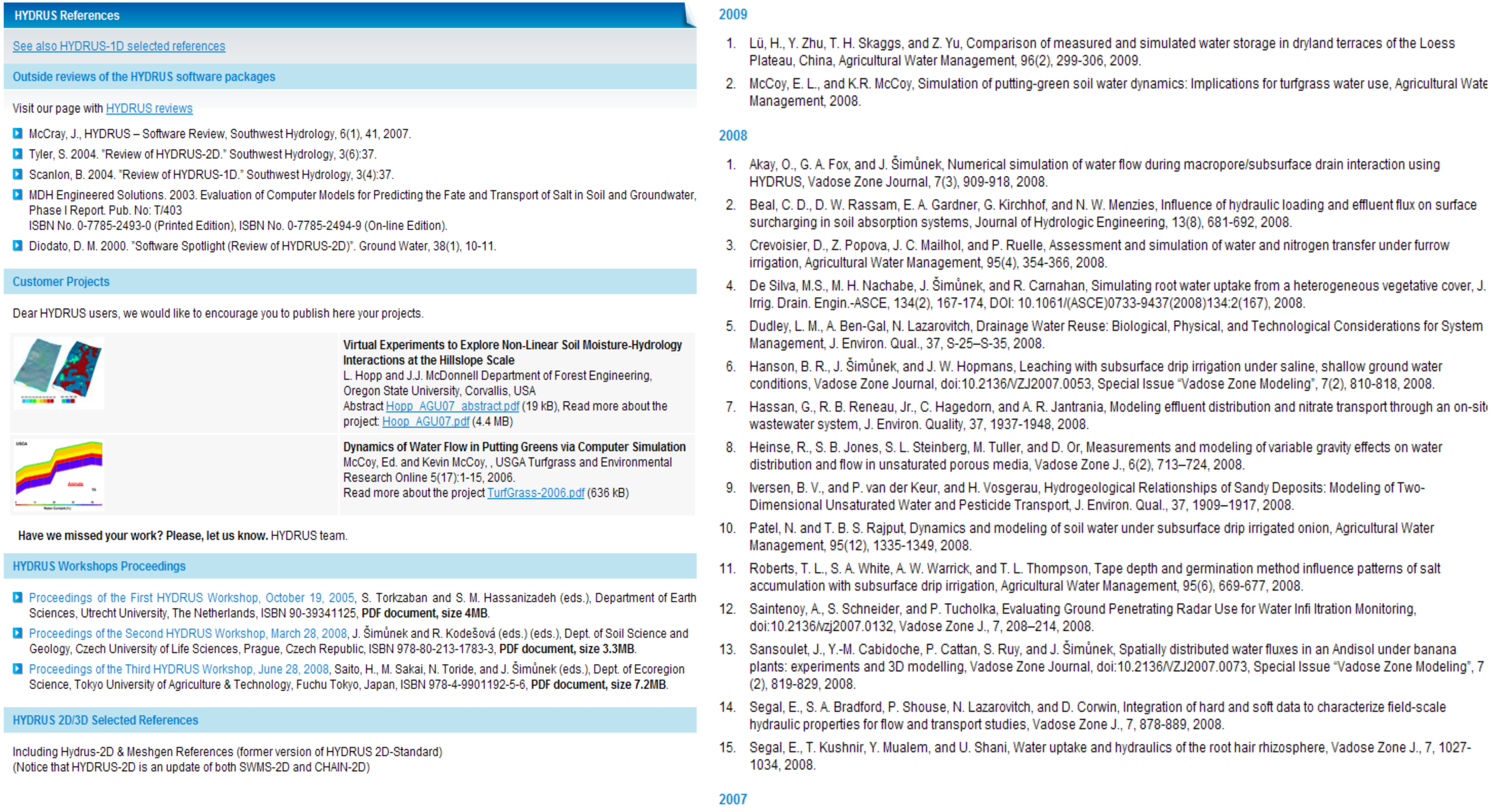
2.05 - 3D Domain, Solid 3 - three video tutorials
Open tutorial

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

HYDRUS Web Site: References



HYDRUS References

See also HYDRUS-1D selected references

Outside reviews of the HYDRUS software packages

Visit our page with HYDRUS reviews

- McCray, J., HYDRUS – Software Review, Southwest Hydrology, 6(1), 41, 2007.
- Tyler, S. 2004. "Review of HYDRUS-2D." Southwest Hydrology, 3(6):37.
- Scanlon, B. 2004. "Review of HYDRUS-1D." Southwest Hydrology, 3(4):37.
- MDH Engineered Solutions. 2003. Evaluation of Computer Models for Predicting the Fate and Transport of Salt in Soil and Groundwater, Phase I Report. Pub. No: T/403
  ISBN No. 0-7785-2493-0 (Printed Edition), ISBN No. 0-7785-2494-9 (On-line Edition).
- 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 Hopp_AGU07_abstract.pdf (19 kB), Read more about the project: Hoop_AGU07.pdf (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 TurfGrass-2006.pdf (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.**
- Proceedings of the Second HYDRUS Workshop, March 28, 2008, J. Šimůnek and R. Kodešová (eds.) (eds.), Dept. of Soil Science and Geology, Czech University of Life Sciences, Prague, Czech Republic, ISBN 978-80-213-1783-3, **PDF document, size 3.3MB.**
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HYDRUS 2D/3D Selected References

Including Hydrus-2D & Meshgen References (former version of HYDRUS 2D-Standard)
(Notice that HYDRUS-2D is an update of both SWMS-2D and CHAIN-2D)

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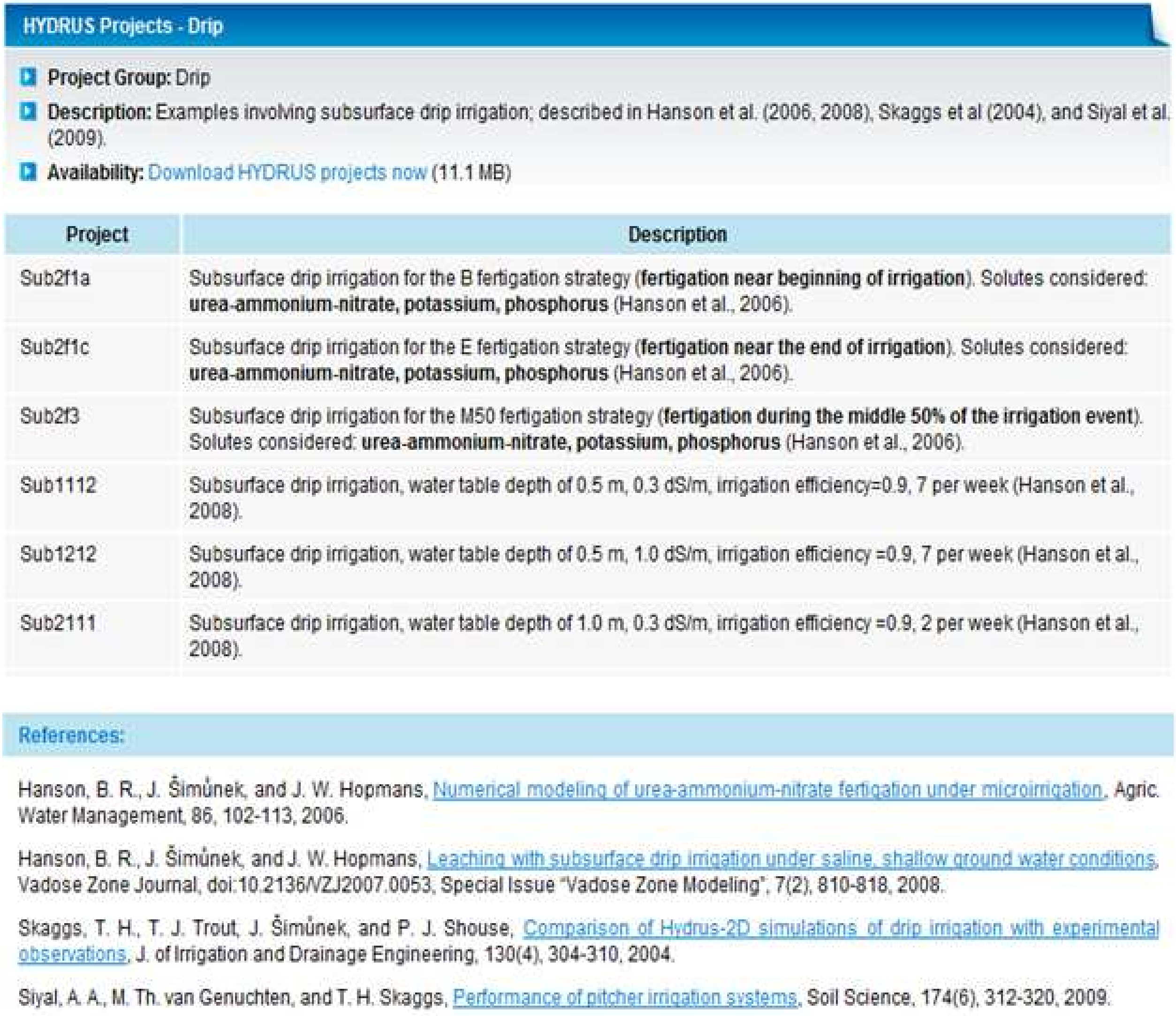
Over one thousand applications of HYDRUS-1D and HYDRUS (2D/3D) published in peer-reviewed journal articles, and many more unpublished.

Public Library of HYDRUS Projects



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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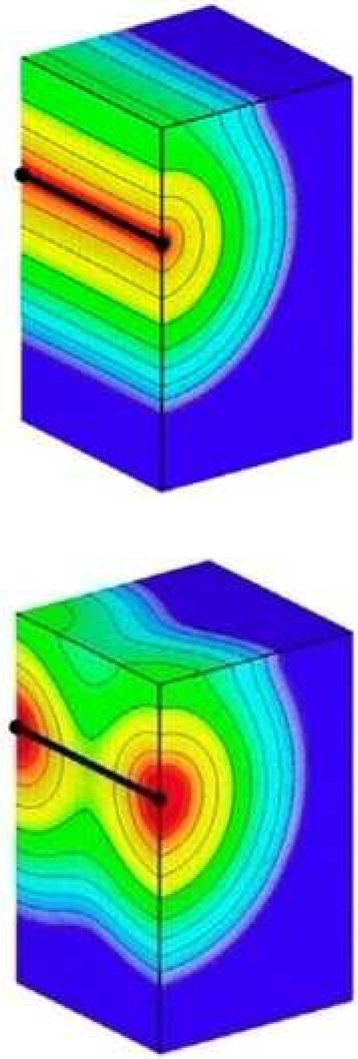


Mathematical/Numerical Models

Mathematical Models have the potential to be powerful tools to help understand and quantify the complexities of various processes in the subsurface.

Mathematical Models are:

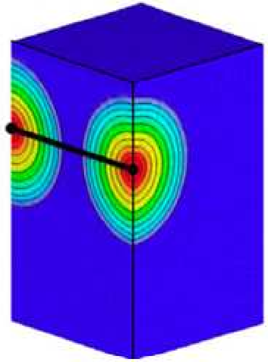
- **a repository for currently available knowledge**
- **represent a practical tool to improve our understanding of and ability to quantify various processes**

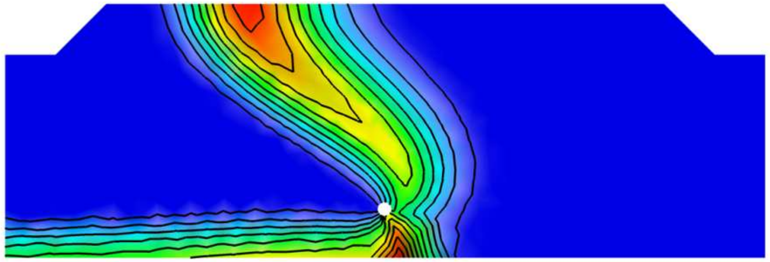
Meaningful applications of Mathematical Models include:

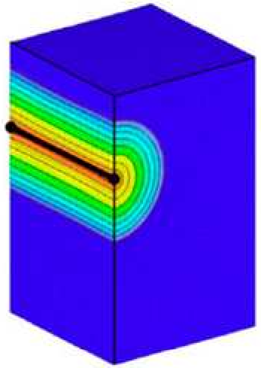
- **predicting outcomes under given assumptions**
- **testing hypotheses**
- **identifying conditions and locations of increased risk**
- **developing treatment strategies, and**
- **informing management decisions**

However, it should be acknowledged that Mathematical Models are not expected to be precise predictors of reality, but are only as good as their input parameters and modeling assumptions.

Questions and Suggestions?







Thank you for your attention